

NUMERICAL SIMULATION OF THE STRUCTURAL BEHAVIOUR OF CONCRETE FOCUSING ON THE INFLUENCE OF NON- UNIFORM MOISTURE DISTRIBUTION

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IN MEMORY OF MANUEL FERREIRA AND CASIMIRO BARREIRA

ABSTRACT

Concrete is the most widely used building material in the world. However, cement production is responsible for a significant proportion of global carbon dioxide emissions. In the context of a more sustainable construction environment, it is essential to rationalise the use of cement-based materials. One set of solutions includes improving design efficiency and extending the service life of existing structures, using numerical tools as decision support.

Numerical tools help engineers predict deterioration mechanisms, assess design options, and plan maintenance interventions. Among these mechanisms, long-term drying and moisture transport processes pose a significant challenge to the serviceability of concrete elements. In thick elements, drying can take decades or even centuries, making experimental characterisation of time-dependent behaviour difficult or impractical. Numerical simulations, if calibrated adequately on short-term tests, offer a viable path toward understanding and investigating the structural influence of long-term moisture-related effects.

Moisture loss in concrete is non-uniform across the cross-section of structural elements. This leads to spatial variation in mechanical properties such as shrinkage, creep, and strength. A reliable numerical tool for long-term behaviour assessment requires numerical models that simulate concrete behaviour locally based on moisture and temperature distributions.

This PhD thesis presents the development of a pointwise thermo-hygro-mechanical (THM) model designed to simulate concrete behaviour from the early ages to the long term. The proposed framework calculates temperature and relative humidity at each finite element node and uses these as input to the mechanical model. Cement hydration is simulated through models incorporating temperature and moisture effects, while shrinkage is captured through rate equations driven by local relative humidity. Creep is modelled using the microprestress solidification theory, and fracture is simulated through smeared crack models employing rotating and fixed crack concepts. The numerical models are discussed in detail, revised, and implemented in the pointwise THM model. The models implemented in the pointwise THM model are validated against benchmarks and experimental data, focusing on the influence of the moisture content on the material behaviour.

The pointwise THM model is used to investigate a series of case studies where drying plays an important role in the structural response. The case studies involve shrinkage in specimens of various sizes, analysis of ring-test configurations, the behaviour of thick reinforced concrete elements over their lifetime, cracking patterns in restrained reinforced concrete members, comparison of the pointwise THM model regarding other numerical approaches in the numerical simulation of the service life of a thick RC tie and the effect of different reinforcement design solutions and degree of restraint in long-term crack widths. Some conclusions about the case studies include the need to consider different shrinkage models for the simulation of shrinkage in modern concrete mixtures; the numerical simulations show that the moisture distribution, influenced by the shape of the structural element and drying conditions, significantly affects the shrinkage and creep response. This effect is not adequately captured by analytical approaches,

requiring the introduction of shape factors to take it into account; the numerical analyses provided a detailed study of the structural behaviour of the ring test and the advantages of different ring test geometries; the numerical simulation of the long-term behaviour of a concrete element shows a reduction in the tensile capacity of thick structural elements to withstand additional loads owing to the transition from stresses developed in the early ages to long-term stresses; the numerical simulation of crack patterns of thick reinforced concrete elements show the interaction between primary and secondary cracks, and the investigations into the effectiveness of different reinforcement design approaches have identified possible reductions in the amount of reinforcement used for the same initial design considerations, resulting in practical material savings.

Due to the complex phenomena associated with moisture distribution and its influence on the behaviour of concrete elements, any findings should be interpreted with caution and considered valid only for the specific concrete mixtures and boundary conditions considered in the simulated case studies. The numerical tool developed must be used for each specific case, providing a robust and versatile platform for future research and design in the construction world. Engineers and scientists can use it to select and interpret experimental tests more effectively, simulate long-term performance in realistic environmental conditions and assess the influence of design variables on the durability of concrete structures.

RESUMO

O betão é o material de construção mais utilizado no mundo. No entanto, a produção de cimento é responsável por uma parte significativa das emissões globais de dióxido de carbono. Por isso, no contexto de um ambiente de construção mais sustentável, é essencial racionalizar a utilização de materiais à base de cimento. Um conjunto de soluções pode incluir a melhoria da eficiência do projeto e o prolongamento da vida útil das estruturas existentes, utilizando ferramentas numéricas como apoio à decisão.

As ferramentas numéricas ajudam os engenheiros a prever os mecanismos de deterioração, a avaliar as opções de conceção e a planear as intervenções de manutenção. Entre estes mecanismos, os processos de secagem a longo prazo e de transporte de humidade representam um desafio significativo para o serviço dos elementos de betão. Em elementos espessos, a secagem pode demorar décadas ou mesmo séculos, tornando difícil ou impraticável a caracterização experimental do comportamento dependente do tempo. As simulações numéricas, se adequadamente calibradas em ensaios de curto prazo, oferecem um caminho viável para a compreensão e investigação da influência estrutural destes efeitos retardados.

A perda de humidade no betão é desuniforme ao longo da secção transversal dos elementos estruturais. Este facto leva à variação espacial das propriedades mecânicas, como a retração, a fluência e a resistência. Uma ferramenta numérica fiável para a avaliação do comportamento a longo prazo requer modelos numéricos que simulem localmente o comportamento do betão com base nas distribuições de humidade e temperatura.

Esta tese de doutoramento apresenta o desenvolvimento de um modelo termo-higro-mecânico (THM) pontual concebido para simular o comportamento do betão desde as primeiras idades até ao longo prazo. A estrutura proposta calcula a temperatura e a humidade relativa em cada nó do elemento finito e utiliza-as como entrada para o modelo mecânico. A hidratação do cimento é simulada através de modelos que incorporam os efeitos da temperatura e da humidade, enquanto a retração é captada através de equações de taxa determinadas pela humidade relativa local. A fluência é modelada utilizando a microprestress solidification theory, e a fratura é simulada através de modelos de fissuras locais considerando conceitos de fissuras rotativas e fixas. Os modelos numéricos são discutidos em pormenor, revistos e implementados no modelo THM pontual. Os modelos implementados no modelo THM pontual são validados com base em dados de referência e dados experimentais, focando a influência do teor de humidade no comportamento do material.

O modelo THM pontual é utilizado para investigar uma série de casos de estudo em que a secagem desempenha um papel importante na resposta estrutural. Os casos de estudo envolvem a retração em provetes de várias dimensões, a análise de configurações de ensaios em anel, o comportamento de elementos espessos de betão armado ao longo da vida útil, os padrões de fissuração em elementos de betão armado com restrições, a comparação do modelo THM pontual com outras abordagens numéricas na simulação numérica da vida útil de um tirante espesso de betão armado e o efeito de diferentes soluções de dimensionamento de armaduras e do grau de restrição na

abertura de fendas a longo prazo. Nestas aplicações, o modelo THM pontual demonstra uma maior precisão e uma melhor capacidade de simular o comportamento dependente do tempo do que as abordagens de modelação tradicionais. Algumas conclusões sobre os estudos de caso incluem a necessidade efectiva de considerar diferentes modelos de retração para a simulação da retração em misturas de betão modernas; as simulações numéricas mostraram que as diferenças na configuração e na geometria da humidade não são tidas em conta nas abordagens analíticas para a retração e fluência, exigindo, por conseguinte, a utilização de factores de forma; as análises numéricas forneceram um estudo pormenorizado sobre o comportamento estrutural do ensaio em anel e as vantagens de diferentes geometrias de ensaio em anel; a simulação numérica do comportamento ao longo da vida útil de um elemento de betão demonstra a redução da capacidade de tração de elementos estruturais espessos para suportar cargas adicionais devido à transição de tensões desenvolvidas nas primeiras idades para tensões a longo prazo; a simulação numérica de padrões de fissuras espessas mostra a interação entre fissuras primárias e secundárias, e as investigações sobre a eficácia de diferentes soluções de conceção de armaduras mostram uma redução das armaduras para as mesmas considerações iniciais de conceção, resultando em poupanças práticas de material.

Devido à complexidade do fenómeno relacionado com a influência da distribuição da humidade no comportamento dos elementos de betão, cada conclusão sobre um caso de estudo presente deve ser abordada cuidadosamente e limitada às misturas de betão consideradas nos casos de estudo simulados, sendo que esta conclusão serve de suporte aos objectivos do presente trabalho de doutoramento. A ferramenta numérica desenvolvida deve ser utilizada para cada caso específico, providenciando uma forma robusta e versátil para projetos de investigação com base em simulações numéricas. Engenheiros e cientistas podem utilizá-la para seleccionar e interpretar ensaios experimentais de forma mais eficaz, simular o desempenho a longo prazo em condições ambientais realistas e avaliar a influência das variáveis de projeto na durabilidade das estruturas de betão.

RÉSUMÉ

Le béton est le matériau de construction le plus utilisé au monde. Cependant, la production de ciment est responsable d'une part importante des émissions mondiales de dioxyde de carbone. Dans le contexte d'un environnement de construction plus durable, il est essentiel de rationaliser l'utilisation des matériaux à base de ciment. L'une des solutions consiste à améliorer l'efficacité de la conception et à prolonger la durée de vie des structures existantes, en utilisant des outils numériques comme aide à la décision.

Les outils numériques aident les ingénieurs à prédire les mécanismes de détérioration, à évaluer les options de conception et à planifier les interventions de maintenance. Parmi ces mécanismes, les processus de séchage à long terme et de transport de l'humidité constituent un défi important pour la fonctionnalité des éléments en béton. Dans les éléments épais, le séchage peut prendre des décennies, voire des siècles, ce qui rend la caractérisation expérimentale du comportement en fonction du temps difficile, voire impossible. Les simulations numériques, si elles sont correctement calibrées à partir d'essais à court terme, offrent une voie viable pour comprendre et étudier l'influence structurelle des effets à long terme liés à l'humidité.

La perte d'humidité dans le béton n'est pas uniforme sur toute la section transversale des éléments structurels. Cela entraîne des variations spatiales des propriétés mécaniques telles que le retrait, le fluage et la résistance. Un outil numérique fiable pour l'évaluation du comportement à long terme nécessite des modèles numériques qui simulent le comportement du béton localement en fonction des distributions d'humidité et de température.

Cette thèse de doctorat présente le développement d'un modèle thermo-hygro-mécanique (THM) ponctuel conçu pour simuler le comportement du béton depuis son jeune âge jusqu'à long terme. Le cadre proposé calcule la température et l'humidité relative à chaque nœud d'élément fini et utilise ces données comme entrées pour le modèle mécanique. L'hydratation du ciment est simulée à l'aide de modèles intégrant les effets de la température et de l'humidité, tandis que le retrait est capturé à l'aide d'équations de vitesse déterminées par l'humidité relative locale. Le fluage est modélisé à l'aide de la théorie de *microprestress solidification theory*, et la fracture est simulée à l'aide de modèles de fissures étalées utilisant les concepts de fissures rotatives et fixes. Les modèles numériques sont discutés en détail, révisés et mis en œuvre dans le modèle THM ponctuel. Les modèles mis en œuvre dans le modèle THM ponctuel sont validés par rapport à des références et des données expérimentales, en mettant l'accent sur l'influence de la teneur en humidité sur le comportement du matériau.

Le modèle THM ponctuel est utilisé pour étudier une série d'études de cas dans lesquels le séchage joue un rôle important dans la réponse structurelle. Ces études de cas portent sur le retrait dans des échantillons de différentes tailles, l'analyse de configurations d'essais en anneau, le comportement d'éléments en béton armé épais au cours de leur durée de vie, les schémas de fissuration dans les éléments en béton armé restraints, la comparaison du modèle THM ponctuel avec d'autres approches numériques dans la simulation numérique de la durée de vie d'un élément de traction en béton armé épais, et l'effet de différentes solutions de conception d'armature et de

différents degrés de restriction sur la largeur des fissures à long terme. Certaines conclusions tirées des études de cas incluent la nécessité de prendre en compte différents modèles de retrait pour la simulation du retrait dans les mélanges de béton modernes; les simulations numériques montrent que la distribution de l'humidité, influencée par la forme de l'élément structurel et les conditions de séchage, affecte de manière significative le retrait et le fluage. Cet effet n'est pas suffisamment pris en compte par les approches analytiques, ce qui nécessite l'introduction de facteurs de forme pour en tenir compte; les analyses numériques ont permis d'étudier en détail le comportement structurel de l'essai sur anneau et les avantages des différentes géométries d'essai sur anneau; la simulation numérique du comportement à long terme d'un élément en béton montre une réduction de la capacité de traction des éléments structurels épais à supporter des charges supplémentaires en raison du passage des contraintes développées au début à des contraintes à long terme; la simulation numérique des schémas de fissuration des éléments épais en béton armé montre l'interaction entre les fissures primaires et secondaires, et les études sur l'efficacité des différentes approches de conception des armatures ont mis en évidence des réductions possibles de la quantité d'armatures utilisées pour les mêmes considérations de conception initiales, ce qui se traduit par des économies de matériaux concrètes.

En raison de la complexité des phénomènes liés à la répartition de l'humidité et à son influence sur le comportement des éléments en béton, toute conclusion doit être interprétée avec prudence et considérée comme valable uniquement pour les mélanges de béton et les conditions limites spécifiques pris en compte dans les études de cas simulées. L'outil numérique développé doit être utilisé pour chaque cas spécifique, offrant une plateforme robuste et polyvalente pour la recherche et la conception futures dans le domaine de la construction. Les ingénieurs et les chercheurs peuvent l'utiliser pour sélectionner et interpréter plus efficacement les essais expérimentaux, simuler les performances à long terme dans des conditions environnementales réalistes et évaluer l'influence des variables de conception sur la durabilité des structures en béton.

KURZFASSUNG

Beton ist der weltweit am häufigsten verwendete Baustoff. Allerdings ist die Zementproduktion für einen erheblichen Teil der globalen Kohlendioxidemissionen verantwortlich. Im Hinblick auf eine nachhaltigere Bauwirtschaft ist es unerlässlich, den Einsatz von zementbasierten Materialien zu rationalisieren. Eine Reihe von Lösungen umfasst die Verbesserung der Konstruktionseffizienz und die Verlängerung der Lebensdauer bestehender Bauwerke unter Verwendung numerischer Werkzeuge als Entscheidungshilfe.

Numerische Werkzeuge helfen Ingenieuren dabei, Verschleißmechanismen vorherzusagen, Konstruktionsoptionen zu bewerten und Wartungsmaßnahmen zu planen. Unter diesen Mechanismen stellen langfristige Trocknungs- und Feuchtigkeitstransportprozesse eine erhebliche Herausforderung für die Gebrauchstauglichkeit von Betonelementen dar. In dicken Elementen kann die Trocknung Jahrzehnte oder sogar Jahrhunderte dauern, was eine experimentelle Charakterisierung des zeitabhängigen Verhaltens schwierig oder unpraktisch macht. Numerische Simulationen bieten, wenn sie anhand von Kurzzeittests angemessen kalibriert werden, einen gangbaren Weg zum Verständnis und zur Untersuchung des strukturellen Einflusses langfristiger feuchtigkeitsbedingter Effekte.

Der Feuchtigkeitsverlust in Beton ist über den Querschnitt von Bauteilen hinweg ungleichmäßig verteilt. Dies führt zu räumlichen Schwankungen der mechanischen Eigenschaften wie Schwinden, Kriechen und Festigkeit. Ein zuverlässiges numerisches Werkzeug zur Bewertung des Langzeitverhaltens erfordert numerische Modelle, die das Verhalten von Beton lokal auf der Grundlage von Feuchtigkeits- und Temperaturverteilungen simulieren.

Diese Doktorarbeit präsentiert die Entwicklung eines punktwisen thermo-hygro-mechanischen (THM) Modells, das das Verhalten von Beton vom frühen Alter bis zur Langzeitentwicklung simulieren soll. Der vorgeschlagene Rahmen berechnet die Temperatur und relative Feuchte an jedem Finite-Elemente-Knoten und verwendet diese als Eingabe für das mechanische Modell. Die Zementhydratation wird durch Modelle simuliert, die Temperatur- und Feuchteeffekte berücksichtigen, während die Schwindung durch Geschwindigkeitsgleichungen erfasst wird, die von der lokalen relativen Feuchte gesteuert werden. Das Kriechen wird anhand der *microprestress solidification theory* modelliert, und Brüche werden durch Smeared-Crack-Modelle unter Verwendung von rotierenden und festen Risskonzepten simuliert. Die numerischen Modelle werden ausführlich diskutiert, überarbeitet und im punktwisen THM-Modell implementiert. Die im punktwisen THM-Modell implementierten Modelle werden anhand von Benchmarks und experimentellen Daten validiert, wobei der Schwerpunkt auf dem Einfluss des Feuchtigkeitsgehalts auf das Materialverhalten liegt.

Das punktwise THM-Modell wird verwendet, um eine Reihe von Fallstudien zu untersuchen, in denen die Trocknung eine wichtige Rolle für das Strukturverhalten spielt. Die Fallstudien umfassen das Schwinden von Probekörpern unterschiedlicher Größe, die Analyse von Ringversuchskonfigurationen, das Verhalten von dicken Stahlbetonelementen über ihre Lebensdauer, Rissmuster in gespannten Stahlbetonbauteilen, den Vergleich des punktwisen

THM-Modells mit anderen numerischen Ansätzen bei der numerischen Simulation der Lebensdauer einer dicken Stahlbetonverbindung sowie den Einfluss verschiedener Bewehrungslösungen und Spannungsgrade auf die langfristige Rissbreite. Zu den Schlussfolgerungen aus den Fallstudien gehört die Notwendigkeit, verschiedene Schwindungsmodelle für die Simulation der Schwindung in modernen Betonmischungen zu berücksichtigen. Die numerischen Simulationen zeigen, dass die Feuchtigkeitsverteilung, die durch die Form des Bauelements und die Trocknungsbedingungen beeinflusst wird, das Schwindungs- und Kriechverhalten erheblich beeinflusst. Dieser Effekt wird durch analytische Ansätze nicht ausreichend erfasst, sodass Formfaktoren eingeführt werden müssen, um ihn zu berücksichtigen. Die numerischen Analysen lieferten eine detaillierte Untersuchung des strukturellen Verhaltens des Ringtests und der Vorteile verschiedener Ringtestgeometrien. Die numerische Simulation des Langzeitverhaltens eines Betonelements zeigt eine Verringerung der Zugfestigkeit dicker Strukturelemente, die zusätzlichen Belastungen standhalten müssen, aufgrund des Übergangs von Spannungen, die in der Anfangsphase entstehen, zu Langzeitspannungen. Die numerische Simulation von Rissmustern dicker Stahlbetonelemente zeigt die Wechselwirkung zwischen Primär- und Sekundärrissen, und die Untersuchungen zur Wirksamkeit verschiedener Bewehrungskonzepte haben mögliche Reduzierungen der Bewehrungsmenge bei gleichen Auslegungsgrundlagen aufgezeigt, was zu praktischen Materialeinsparungen führt.

Aufgrund der komplexen Phänomene im Zusammenhang mit der Feuchtigkeitsverteilung und deren Einfluss auf das Verhalten von Betonelementen sollten alle Ergebnisse mit Vorsicht interpretiert und nur für die spezifischen Betonmischungen und Randbedingungen als gültig angesehen werden, die in den simulierten Fallstudien berücksichtigt wurden. Das entwickelte numerische Tool muss für jeden einzelnen Fall verwendet werden und bietet eine robuste und vielseitige Plattform für zukünftige Forschung und Planung in der Baubranche. Ingenieure und Wissenschaftler können es nutzen, um experimentelle Tests effektiver auszuwählen und zu interpretieren, die Langzeitleistung unter realistischen Umgebungsbedingungen zu simulieren und den Einfluss von Entwurfsvariablen auf die Dauerhaftigkeit von Betonkonstruktionen zu bewerten.

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TABLE OF CONTENTS

ABSTRACT	V
RESUMO	VII
RÉSUMÉ	IX
KURZFASSUNG	XI
ACKNOWLEDGEMENTS	XIII
TABLE OF CONTENTS	XV
LIST OF SYMBOLS AND ABBREVIATIONS	XXI
1 INTRODUCTION	1
1.1 OBJECTIVES.....	3
1.2 ORGANISATION OF THE THESIS.....	4
2 THERMO-HYGRO-CHEMO-MECHANICAL BEHAVIOUR OF CONCRETE	5
2.1 CEMENT HYDRATION	5
2.1.1 <i>Cement Hydration Kinetics Theory</i>	6
2.1.2 <i>Cement Hydration of Alite Compound</i>	9
2.1.3 <i>Degree of Hydration</i>	11
2.1.3.1 Simple autocatalytic model	12
2.1.3.2 Affinity model	13
2.1.3.3 Multiple-particle cement hydration models	14
2.1.4 <i>Mechanical Properties and Maturity of Concrete</i>	14
2.1.4.1 Mechanical properties of concrete based on the degree of hydration	15
2.1.4.2 Mechanical properties of concrete based on time.....	17
2.2 MOISTURE IN CONCRETE	18
2.2.1 <i>General Concepts</i>	18
2.2.2 <i>Sorption Isotherm</i>	21
2.2.3 <i>Transport Mechanisms</i>	23
2.2.3.1 Darcy's law	24
2.2.3.2 Fick's law	25
2.2.4 <i>Differential Equations for Moisture Transport</i>	26
2.2.5 <i>Boundary Conditions</i>	30

2.2.6	<i>Effect of Cracking on Moisture Transport</i>	31
2.2.7	<i>Moisture Effect in the Cement Hydration Evolution</i>	32
2.3	SHRINKAGE	34
2.3.1	<i>Basic Shrinkage and Self-desiccation</i>	35
2.3.2	<i>Drying Shrinkage</i>	37
2.4	CONCRETE CREEP	39
2.4.1	<i>Concepts and Mechanisms</i>	40
2.4.2	<i>Basic Creep</i>	41
2.4.2.1	Solidification theory	41
2.4.2.2	Burger mechanical model for basic creep	46
2.4.3	<i>Drying Creep</i>	48
2.4.3.1	Microprestress-solidification theory	49
2.4.3.2	Microprestress-solidification theory formulation in order to viscosity	54
2.4.3.3	Extended microprestress-solidification theory	55
2.4.3.4	Improved microprestress-solidification theory	58
2.4.3.5	Burger mechanical model for drying creep	58
2.4.4	<i>Simulation of Concrete Creep</i>	59
2.4.4.1	Initial considerations	59
2.4.4.2	Kelvin chain model	60
2.4.4.3	Maxwell chain model	63
2.4.4.4	Second-order exponential approach	64
2.5	TEMPERATURE EFFECTS ON HYDRATION, MOISTURE DIFFUSION AND CREEP	65
2.5.1	<i>Temperature Effects on Hydration</i>	67
2.5.2	<i>Temperature Effects on Moisture Diffusion</i>	67
2.5.3	<i>Temperature Effects on Shrinkage</i>	68
2.5.4	<i>Temperature Effects on Concrete Creep</i>	68
2.6	CONCRETE FRACTURE	69
2.6.1	<i>Cracking in Reinforced Concrete Structures</i>	69
2.6.1.1	Experimental investigation on early-age cracking in concrete elements	72
2.6.1.2	Experimental investigation on cracking patterns in thick concrete elements	73
2.6.1.3	Experimental investigation of the combined effect of bending and axial restraint in slab-like specimens	75

2.6.2	<i>Numerical Simulation of Concrete Cracking</i>	76
3	POINTWISE THERMO-HYGRO-MECHANICAL MODEL FOR THE NUMERICAL SIMULATION OF CONCRETE	79
3.1	JUSTIFICATIONS AND OBJECTIVES.....	79
3.2	GENERAL ASPECTS OF THE NUMERICAL THM FRAMEWORK	81
3.3	HYGROTHERMAL MODEL.....	82
3.3.1	<i>Numerical Simulation of Moisture Transport in Concrete</i>	82
3.3.2	<i>Numerical Simulation of Heat Conduction in Concrete</i>	88
3.4	ARCHITECTURE OF THE POINTWISE MECHANICAL MODEL	89
3.5	CEMENT HYDRATION	90
3.5.1	<i>Contextual Introduction</i>	90
3.5.2	<i>Implementation Details</i>	91
3.5.2.1	Transformed times model	91
3.5.2.2	Cement hydration of a single particle controlled by diffusion through barrier shells of C-S-H..	93
3.6	HYGROTHERMAL STRAINS.....	99
3.6.1	<i>Contextual Introduction</i>	99
3.6.2	<i>Implementation Details</i>	100
3.6.2.1	Shrinkage model.....	100
3.6.2.2	Thermal strains model.....	104
3.6.2.3	Eigenstrains computation	104
3.7	CONCRETE CREEP AND ELASTICITY	104
3.7.1	<i>Contextual Introduction</i>	104
3.7.2	<i>Implementation Details</i>	105
3.7.2.1	Solidified material volume	105
3.7.2.2	Post-Widder approach	107
3.7.2.3	Evaluation of the viscoelastic parameters.....	108
3.7.2.4	Evaluate the flow strain	109
3.7.2.5	Incremental modulus of elasticity and creep strains.....	112
3.8	CONTINUUM OR FRACTURE MODEL	113
3.8.1	<i>Contextual Introduction</i>	113
3.8.2	<i>Implementation Details</i>	114
3.8.2.1	Linear behaviour	114

3.8.2.2	General aspects of the cracking models	115
3.8.2.3	Total strain crack model with rotating cracks	117
3.8.2.4	Total strain model with fixed crack	126
3.8.2.5	Time dependencies on the total strain model	131
3.8.2.6	Single-crack model with strain decomposition	133
3.9	CONSIDERATIONS AND LIMITATIONS IN THE IMPLEMENTATION OF THE USER-SUPPLIED ROUTINE	139
3.9.1	<i>Iterative Method for Nonlinear Analysis</i>	140
3.9.2	<i>Convergence Criteria</i>	142
3.10	EXAMPLE OF DATA INPUT IN THE POINTWISE MECHANICAL MODEL.....	143
3.11	VALIDATION OF THE NUMERICAL IMPLEMENTATION OF THE POINTWISE MECHANICAL MODEL.....	148
3.11.1	<i>Test 1 - Tension Softening Model with Imposed Deformation</i>	150
3.11.1.1	Test 1.1 - Tension softening model	150
3.11.1.2	Test 1.2 and Test 1.3 – Creep effects on the tension softening model	151
3.11.2	<i>Test 2 – Reloading and Unloading Tests</i>	153
3.11.2.1	Test 2.1 – Unloading under tension, followed by reloading.....	153
3.11.2.2	Test 2.2 – Unloading into compression, followed by reloading.	155
3.11.2.3	Test 2.3 – Unloading into compression after full exhaustion of the tension softening model, followed by reloading.....	156
3.11.3	<i>Test 3 – Rotational Tests for the Crack Directions and Principal Directions</i>	156
3.11.3.1	Test 3.1 – Load cases 1 and 2 applied simultaneously	157
3.11.3.2	Test 3.2 – Unloading into compression after full exhaustion of the tension softening model.	160
3.11.4	<i>Test 4 – Eigenstrains and Strain Localisation</i>	163
3.11.5	<i>Final Remarks on the Benchmark Tests for Validating the Pointwise THM Model</i>	165
3.12	REINFORCEMENT AND BOND-SLIP.....	165
4	APPLICATIONS OF THE POINTWISE THERMO-HYGRO-MECHANICAL MODEL	169
4.1	HYGROMECHANICAL BEHAVIOUR OF CONCRETE	169
4.1.1	<i>Numerical Simulation of the Relative Humidity and Shrinkage Tests of the IntegraCrete Experimental Campaign</i>	170
4.1.1.1	Hygrometric simulation of the relative humidity tests.....	170
4.1.1.2	Mechanical simulation of the shrinkage test using different shrinkage models	173
4.1.2	<i>Shrinkage and Creep Tests from Bryant and Vadhanavikkit</i>	176
4.1.2.1	Introduction to the experimental campaign	176

4.1.2.2	Numerical simulation of the shrinkage specimens.....	177
4.1.2.3	Creep simulation using the microprestress-solidification theory.....	185
4.1.2.4	Notional size in slab and prismatic specimens	196
4.1.3	<i>Numerical Simulation of the Shrinkage in an Unrestrained Ring Test.....</i>	<i>199</i>
4.1.3.1	Material characterisation	201
4.1.3.2	Numerical simulation of the shrinkage prisms	202
4.1.3.3	Numerical simulation of the unrestrained ring test	204
4.1.4	<i>Numerical Simulation of the Ring Test</i>	<i>206</i>
4.1.4.1	Materials, experimental data and input parameters	207
4.1.4.2	Thermo-hygral model parameters	210
4.1.4.3	Simulation of free shrinkage	211
4.1.5	<i>Numerical Investigation of Different Ring Test Geometries with Different Drying Conditions</i>	<i>221</i>
4.1.5.1	Different ring test geometries and finite element meshes	221
4.1.5.2	Numerical results and discussion	223
4.2	ADJUSTABLE RESTRAINING FRAMES FROM TU GRAZ	231
4.2.1	<i>Experimental Campaign</i>	<i>232</i>
4.2.2	<i>Numerical Simulation of the ARF Tests</i>	<i>234</i>
4.2.2.1	Numerical model.....	235
4.2.2.2	Material parameters	236
4.2.2.3	Numerical results	237
4.3	MODIFIED FRAME AND CRACK PATTERNS IN THICK MEMBERS	242
4.3.1	<i>Experimental Campaign</i>	<i>243</i>
4.3.2	<i>Numerical Model.....</i>	<i>244</i>
4.3.3	<i>Numerical Results.....</i>	<i>245</i>
4.4	RC TIE RESTRAINED SINCE THE EARLY AGES.....	246
4.4.1	<i>Material Behaviour in the Pointwise THM Model</i>	<i>247</i>
4.4.2	<i>Hygrothermal Analysis of the 0.5 m RC Tie and Dependent Properties of Hygrothermal Results</i>	<i>250</i>
4.4.3	<i>Numerical Simulation of the 0.50 m Thick RC Tie.....</i>	<i>252</i>
4.4.4	<i>Results and Discussion of the Numerical Simulations of the 0.5 m RC Tie</i>	<i>253</i>

4.4.5	<i>Investigation of the Reinforcement Design and Degree of Restraint on Long-term Crack Widths</i>	256
4.4.5.1	Minimum reinforcement design according to Eurocode 2.....	256
4.4.5.2	Results and discussion.....	258
5	CONCLUSIONS	263
5.1	THERMO-HYGRO-MECHANICAL FRAMEWORK	263
5.2	NUMERICAL SIMULATION OF THE RELATIVE HUMIDITY AND SHRINKAGE TESTS.....	266
5.3	NUMERICAL SIMULATION OF THE SHRINKAGE AND CREEP TESTS FROM BRYANT AND VADHANAVIKKIT	267
5.4	NUMERICAL SIMULATION OF THE UNRESTRAINED RING TEST	267
5.5	NUMERICAL SIMULATION OF THE RING TEST	268
5.6	NUMERICAL SIMULATION OF THE DIFFERENT RING TEST GEOMETRIES.....	269
5.7	NUMERICAL SIMULATION OF THE ARF TESTS.....	270
5.8	NUMERICAL SIMULATION OF THE MODIFIED FRAME TEST	270
5.9	NUMERICAL SIMULATION OF THE 0.50 M RC TIE RESTRAINED SINCE EARLY AGES	271
5.10	FINAL REMARKS.....	272
	REFERENCES.....	275

LIST OF SYMBOLS AND ABBREVIATIONS

Symbols and abbreviations are defined upon their first appearance in the text. The following list is presented in alphabetical order and does not include some symbols and notations of a secondary order (whose concern is limited to specific applications).

Roman Letters

A^*	Constant dependent on the chemical reaction
A_c	Cross-sectional area of the concrete
ACI	American Concrete Institute
AFt	Ettringite
ARF	Adjustable restraining frame
ASR	Alkali-silica-reaction
A_s	Cross-sectional area of the reinforcement
$A_{s,min}$	Minimum reinforcement
a	Aggregates content in the concrete mixture
a_0	Average cement particle size (initial cement particle radius)
BET	Brunauer-Emmett-Teller model
BFGS	Broyden-Fletcher-Goldfarb-Shanno
B_v	Surface vapour transfer coefficient
$\mathbf{C}$	Elastic compliance matrix
C	Concentration (amount of substance per unit of volume)
CFD	Computational Fluid Dynamics
C_v	Molar concentration of water vapour
C_2S	Dicalcium silicate (Belite)
C_3A	Tricalcium aluminate
C_3S	Tricalcium silicate (Alite)
C_4AF	Tetracalcium aluminoferrite
$Ca(OH)_2$ or CH	Calcium hydroxide (Portlandite)
CO_2	Carbon dioxide
C-S-H	Calcium silicate hydrate
c	Cement content in the concrete mixture
c	Effective specific heat capacity of concrete per unit mass
c_0	Parameter of the microprestress creep model
$\mathbf{D}$ or $\mathbf{D}^{CO}$ or $\mathbf{D}_{lin}$	Elastic stiffness matrix
D	Diffusion coefficient
$\mathbf{D}_{cr}$	Cracking stiffness matrix

D_g	Diffusion coefficient of the gas (water vapour and air)
D_h	Diffusion coefficient for hygral analysis
DLL	Dynamic Link Library
D_w	Diffusivity due to cracking
D_0	Diffusion coefficient value at the reference temperature and reference gas pressure
d_v	Damage function for the Poisson's ratio calculation in total strain models
E	Modulus of elasticity
$\tilde{E}$	Incremental modulus
EC2	Eurocode 2 – EN1992
E_{sec}	Elastic secant modulus
E_μ	Modulus of elasticity of the Kelvin-Voigt element μ
EDS	Energy dispersive spectroscopy
EMP	Electron microprobe analysis
Env	Environment
e.g.	Abbreviation of “for example”
FDM	Finite differences method
FEA	Finite element analysis
FEM	Finite element method
FVM	Finite volume method
$f(\alpha)$	Function of the kinetic model
f_{bl}	Blaine fineness of cement
f_c	Compressive strength
f_{cm}	Mean compressive strength
f_{ct}	Tensile strength
f_{ctm}	Mean tensile strength
$\mathbf{f}_{ext}$	External force vector
$\mathbf{f}_{int}$	Internal force vector
G	Gibbs free energy
GGBFS	ground granulated blast-furnace slag
G_f	Fracture energy
G_{ij}	Shear modulus at directions ij
g	Gravitational acceleration
$\mathbf{g}_i$	out-of-balance force vector
H	Water molecule
H_t	Total head
h	Relative humidity

h	Crack bandwidth (in the cracking models)
h_{bs}	Relative humidity drops due to basic shrinkage (self-desiccation model)
h_{cr}	Combined convective/radiation heat transfer coefficient
h_{env}	Environment relative humidity
h_m	Constant surface emissivity coefficient
h_s	Relative humidity consumption due to cement hydration (self-desiccation)
I	Identity matrix
IMPS	Improved microprestress solidification theory
i.e.	Abbreviation of “that is”
J	Diffusion flux
$J(t, t')$	Compliance function of concrete creep
$J_f(t, t')$	Compliance function for the flow part of creep
$J_v(t, t')$	Compliance function for the viscoelastic part of creep
$J_0(t, t')$	Non-ageing creep compliance
JSCE	Japan Society of Civil Engineers
j_v	Max flux of water vapour
j_l	Mass flux of liquid water
j_w	Outward flux of water
K_0	Intrinsic permeability
K_h	Hydraulic permeability
K_i	Stiffness matrix
k	Thermal conductivity
k_{dc}	Elastic modulus for the Burger creep model
k_h	Parameter that depends on the element thickness
k_{sh}	Shrinkage coefficient
MC2010	fib Model code 2010
MMPS	Modified microprestress solidification theory
MPS	Microprestress solidification theory
M_r	Molar mass
M_w	Molar mass of water
n_g	Number of cement particles per unit volume of cement
ODE	Ordinary differential equation
PDE	Partial differential equation
p_a	Pressure of air
p_{atm}	Atmospheric pressure
p_c	Capillary pressure
p_g	Pore gas pressure

p_v	Water vapour pressure
p_{sat}	Saturated vapour pressure
Q	Heat released during cement hydration
$Q(t, t')$	Ageing function of concrete creep
Q_e, Q_r, Q_s	Activation energy for hydration Q_e , viscous processes Q_r and microprestress relaxation Q_s
Q_{total}	Total heat accumulated at full hydration
q_1	Instantaneous strain due to a unit stress
q_2	Creep model parameter related to the ageing part of the creep
q_3	Creep model parameter related to the non-ageing part of the creep
q_4	Creep model parameter related to the flow part of the creep
QXRD	X-ray diffraction analysis
R	Universal gas constant
RC	Reinforced concrete
RH	Relative humidity
RMPS	Refined microprestress solidification theory
S	Microprestress
SCM	Supplementary cementitious materials
S_l	Saturation degree
s	Slip value
$\dot{s}$	Rate of instantaneous microprestress induced by changes in the capillary pressure, surface tension and crystal growth
T	Transformation matrix
T	Temperature
T_{env}	Environment temperature
THM	Thermo-hygro-mechanical
TSTM	Temperature-stress-testing-machine
T_0	Reference temperature
t	Concrete age
t_{eq} or t_e	Equivalent concrete age
t_r	Reduced time
t_s	Reduced microprestress time
$\mathbf{u}_i$	Displacement vector
V_a	Volume of aggregates
V_c	Volume of cement
V_{CH}	Volume of portlandite
V_g	Volume of gas
V_{gel}	Volume of cement gel

V_l	Volume of liquid
V_s	Volume of a solid
V_m	Molar volume
V_w	Volume of water
$v(t)$	Solidified material volume
v_l	Flux of liquid water that overpasses a porous medium
v_v	velocity of the water vapour
XMPS	Extended microprestress solidification theory
XRD	X-ray powder diffraction
$X_i(\alpha)$	Property X for the degree of hydration α
$X_i(t_{eq})$	Property X for equivalent age t_{eq}
$X_{28,i}$	Hypothetical value of the property X at 28 days
$X_{\infty,i}$	Hypothetical value of the property X at full hydration
$W_{chem,w}$	Weight of chemically bonded water
$W_{max,chem,w}$	Amount of chemically bonded water at complete hydration
w	Moisture or water content in the concrete mixture
w_{cr}	Crack width
w_d	Design crack widths
w_e	Evaporable water
w_{lim}	Nominal limit value of the crack width
w_n	Non-evaporable water (chemically bonded water)
w_s	Moisture consumption due to cement hydration (self-desiccation)
γ_{gl}	Surface tension
z	Actual shell radius

Greek Letters

α	Degree of hydration
α	Internal damage variables used in the total strain model
α_{bs}	Basic shrinkage parameter
$\alpha_e, \alpha_r, \alpha_s$	Model parameters that affect the relative humidity function β_{ih} , for hydration α_e , viscous processes α_r and microprestress relaxation α_s
α_i	Initial degree of hydration
α_{max}	Maximum degree of hydration
α_{set}	Degree of hydration at setting
α_0	Parameter of the diffusion model
β	Shear retention factor

β_μ	Coefficient for the second-order exponential algorithm
β_{ih}	Coefficients to account for the relative humidity on hydration β_{eh} , viscous processes β_{rh} and microprestress relaxation β_{sh}
β_{eT}	Coefficients to account for the temperature on hydration β_{eT} , viscous processes β_{rT} and microprestress relaxation β_{sT}
Γ	Boundary surface
ε	Strain
ε_{cbs}	Basic shrinkage of concrete
ε_{cbs0}	Asymptotic value of the basic shrinkage
ε_{cr}	Inelastic part of the total strain (crack strain)
$\varepsilon_{cr,switch}$	Crack strain for the switch from the total strain rotating model to the total strain fixed model
ε_{creep}	Creep strains that would occur under constant stress
ε_{dc}	Drying creep strain in the Burger mechanical model
ε_{eigen}	Eigenstrains due to hygrothermal effects
ε_f	Flow strain
$\tilde{\varepsilon}_{nst}$	Equivalent uniaxial strains
ε_{sh}	Free shrinkage
$\varepsilon_{sh,ult}$	Shrinkage upon total (or almost total) drying
ε_v	Viscoelastic strain
$\zeta_{prod,react}$	Volume expansion of the reaction of a cement particle
$\eta(t)$ or $\eta(S)$	Viscosity modulus dependent on time or microprestress
η_{dc}	Non-linear viscosity modulus for the Burger creep model
η_e	Surface emissivity
η_e^*	Adjusted surface emissivity
η_l	Dynamic shear viscosity
$\eta_M(S, \dot{S})$	Macroscale viscosity
$\eta_n(S)$	Nanoscale viscosity
$\eta_{flow}(S)$	Viscosity due to the water flow or the rate of any other phenomenon causing a thermodynamic imbalance in nanopores
λ_μ	Coefficient for the second-order exponential algorithm
μ	Kelvin-Voigt element number
ν or ν_{ij}	Poisson's coefficient (directions ij)
$\mathcal{P}$	Orthotropic matrix for Poisson's ratio
ρ	Mass density
ρ_l	Density of liquid water
σ	Stress
σ_c	Concrete stress

σ^d or σ'	Deviatoric stresses
σ_e	Elastic stress
σ_{nst}	Principal stresses
σ_s	Steel stress
σ^s	Hydrostatic or spherical stresses
σ_v	Viscoelastic stress
σ_α	Auxiliary stress at the internal damage strain values α
τ	Tortuosity
τ_b	Bond stress
τ_{bmax}	Maximum bond stress
τ_μ	Retardation time of the Kelvin-Voigt element μ
Φ_{dif}	Flux of moisture due to the diffusion mechanism
Φ_{per}	Flux of moisture due to the permeability mechanism
Φ_{con}	Flux of moisture due to convection
φ	Porosity
φ_{cap}	Inter-particle porosity (capillary porosity)
φ_{gel}	Gel porosity
φ_{Kp}	Porosity in which the Kelvin equation applies
φ_{np}	Porosity of nanopores
φ_p	Cement paste porosity
$\psi(t - t')$	Relaxation function of the cement gel
ψ_i	Function that accounts for the temperature and relative humidity effects on hydration ψ_e , viscous processes ψ_r and microprestress relaxation ψ_s
Ω	Volume of the solid

1

INTRODUCTION

Concrete is the most used manufactured material, with an annual consumption of more than 2×10^9 ton. Cement production, which is the main constituent of the concrete matrix, is responsible for 5 to 8% of the total CO₂ emissions due to human activities. Consequently, significant efforts have been devoted to optimising the use of material resources, namely:

- i) the development of new efficient structural design procedures, which includes the development and use of new sustainable materials included in the design of future smart cities;
- ii) the cracking/deflection control and increase of the durability of current and future structures through the continuous investigation of the long-term behaviour of the materials used in construction.

Investigating these two topics provides an aesthetic and environmentally friendly perspective, but also, for the particular case of the second topic, contributes to a decrease in the number of interventions in public/private structures, which positively affects the global economy. Excessive deflections or cracking may impair the structure's function, limiting its durability or requiring costly strengthening interventions [1]. Not all structures present the same sensitivity to delayed effects. In the scope of creep effects (but also valid to other delayed effects), Bažant and Baweja [2] proposed to classify the sensitivity of structures into five different levels:

- Level 1 - reinforced concrete beams, frames and slabs with spans under 20 m and heights of up to 30 m, plain concrete footings, and retaining walls;
- Level 2 - prestressed beams or slabs or spans up to 20m, high-rise building frames up to 100m high;
- Level 3 - medium-span box girder, cable-stayed or arch bridges with spans of up to 80m, concrete tanks, silos, pavements and tunnel linings;
- Level 4 - long-span prestressed box girders, cable-stayed or arch bridges; large bridges built sequentially in stages by joining parts; large gravity, arch or buttress dams; cooling towers; large roof shells; very tall buildings;
- Level 5 - record-span bridges, nuclear containments and vessels, large offshore structures, large cooling towers, record-span thin roof shells, record-span slender arch bridges, and super-tall buildings.

The level of sensitivity of the structure grows in this classification. Level 1 presents the least sensitive structures, while level 5 is the most sensitive. This classification should be seen as a quantification of the importance of the design efforts beyond an accurate simulation of the delayed effects on concrete structures. Even structures of level 1 can be evaluated using the most sophisticated models. However, from the constructor's point of view, the outcome of using those in comparison with simpler approaches is negligible and time-wasting. For Levels 1 and 2 of sensitivity, the volumetric changes can be evaluated within the practices of the code-based approaches. Level 3 is a transition level that requires some designer interpretation regarding the structure's sensitivity. Levels 4 and 5 are sensitive structures where the most sophisticated and realistic models must be employed. For those types of structures, numerical approaches that can simulate the physical behaviour of the concrete and efficiently predict long-term deformations are required.

The physical material behaviour of concrete is associated with chemical reactions, thermal conduction and moisture transport, which can vary depending on the morphology of the structural element. In massive concrete elements, the structure exhibits internal restraints because of the non-linear drying and temperature profiles, which generate stresses in the element cross-section. External restraint to the volumetric deformations generally increases the cracking risk. As soon as the tensile strains exceed the tensile strain capacity of concrete, cracking occurs. Due to durability, aesthetics, watertightness or safety reasons, cracking should be limited, controlled or (in some types of structural elements) avoided. Therefore, investigating the mechanisms associated with the delayed strains, like creep and shrinkage, which are directly connected to the hygrothermal effects, is crucial.

Shrinkage is a delayed strain associated with moisture variations in the concrete pores. In a restrained element, shrinkage may lead to cracking. Additionally, moisture content may affect other mechanical properties of concrete. The cement hydration reactions govern the evolution of concrete's strength properties depending on the available moisture content. The moisture content drop slows down the cement hydration, and if it decreases below a particular threshold value, the main chemical reactions associated with the development of the concrete microstructure cease. If the element dries fast, the cement hydration will stop early, leading to poor-quality concrete.

Under constant stress, the concrete element undergoes an increase in strain over time. This phenomenon is called creep and is associated with the sliding of the cement hydration products under a stressed state. The sliding rate is influenced by the amount of water in the nanopores and other thermo-hydrodynamic phenomena, like moisture transport or temperature variations, resulting in increased or decreased creep strains at the macroscale. Consequently, creep depends on moisture content and transport. This influence is also generally grossly simplified in design codes, engineering practices, and even many academic approaches.

The nonlinear internal moisture distribution over the element cross-section increases with the size of the structural element. For instance, in thick concrete elements with ordinary concrete mixtures, the core remains almost near saturation for decades while the exposed concrete at the element's surface dries faster. The concrete at the core is expected to develop a more advanced microstructure than at the element's surface. Therefore, for a correct assessment of the behaviour of sensitive concrete elements,

the numerical analysis must consider the abovementioned factors by including mathematical models that simulate the eigenstrains and the mechanical properties of the concrete element, with dependence on the local temperature and moisture history.

1.1 OBJECTIVES

The present PhD thesis work involved developing numerical tools to investigate the behaviour of concrete structures based on local temperature and moisture content. The ultimate goal is to improve the numerical analysis tools for concrete structures sensitive to drying effects, such as bridges, nuclear power plants, or structures with thick concrete members not in permanent contact with water. Some of the intended applications of the numerical model developed in this PhD include analysing the possibility of extending the service life of this type of structural element, improving the experimental tests used for material characterization, predicting long-term structural behaviour, accessing the effectiveness of reinforcement design solutions for cracking control, investigate and improve new solutions intended to solve problems related to the serviceability and maintenance of concrete structures.

A numerical tool must be developed and validated to reach the ultimate goal, including numerical models that account for concrete's most realistic physical behaviour. The model developed during this PhD work is called the “pointwise thermo-hygro-mechanical (THM) model”. In this context, the term “pointwise” means that the material behaviour is a function of the time history of temperature and moisture content in each integration point.

The first objective is to select state-of-the-art material models that will be implemented in the pointwise THM model. Even though microscopic level simulation is important in porous materials, like cement hydration, the adopted modelling approach concentrates on numerical simulations at the macroscale by discretising the concrete members using solid finite elements for concrete. The implementation of new material models is limited to concrete. The pointwise THM material model includes formulations for simulating cement hydration reactions and maturity effects, concrete creep, and fracture, focusing on the influence of the local relative humidity and temperature. Each justified selected model is implemented, validated and modified (if needed) in the pointwise THM model. Despite the simulated temperature effects in the presented model, the focus is on the influence of moisture on the concrete behaviour. The model is intended to be applied to the numerical simulation of the concrete structure's service life, starting from the setting time until decades after casting.

The pointwise THM model is employed in numerical simulations of case studies to investigate the influence of hygrothermal coupling on concrete elements and the long-term cracking patterns observed in realistic structural scenarios. Simulating elements of varying dimensions will be used to conduct a parametric study of the size effect in shrinkage and creep under different drying conditions. Thick element simulations are validated by numerically replicating an experimental campaign on restrained reinforced concrete members, examining early-age behaviour and crack-pattern development in thick members. Finally, the pointwise THM model is benchmarked against alternative numerical approaches

and used to investigate the analytical solutions for minimum reinforcement design in a thick reinforced concrete tie.

1.2 ORGANISATION OF THE THESIS

The thesis is organised into five chapters. Chapter 1 provides an introduction to the research objectives and methodology. This chapter identifies the civil engineering branch to which this PhD thesis is applied and the main objectives of the PhD research work. Chapter 2 reviews the state of the art in thermo-hygro-chemo-mechanical behaviour of concrete. Different models and research work performed by other authors on the topics addressed during this PhD are presented. This chapter provides an understanding of the physical behaviour of the mechanisms involved and the numerical approaches used to simulate concrete behaviour, forming the background for the numerical models selected and implemented in Chapter 3. Chapter 3 details the implementation of each submodel in the pointwise THM model. This chapter focuses on the details of the numerical implementation of the selected numerical models and their validation through comparison with well-established numerical models available in commercial software. Chapter 4 applies the pointwise THM model to simulate field applications. In this chapter, the pointwise THM model described in Chapter 3 is applied to the numerical simulation of experimental tests and selected field applications, demonstrating the functionalities, capabilities and limitations of the developed pointwise THM model in civil engineering applications. Finally, Chapter 5 summarises the key findings and offers concluding remarks regarding the work presented in Chapters 3 and 4.

2

THERMO-HYGRO-CHEMO-MECHANICAL BEHAVIOUR OF CONCRETE

2.1 CEMENT HYDRATION

Concrete is a solidifying material constituted of cement, water, aggregates and, possibly, admixtures and additions. After the initial mixing and casting, the blend may be seen as a solution or suspension of rigid particles in water or a granular water-filled porous medium [3]. The cement paste is represented by the water and cement, which undergo complex physical and chemical processes. Those processes are denominated as cement hydration reactions or just hydration, and start once the water and cement come into contact. Usually, the cement hydration may be divided into three stages [4, 5]:

1. Stage I – Early stage – once the water and the anhydrous cement particles come into contact, there is an instantaneous reaction between the surface ions of the clinker and water. These highly exothermic reactions occur for a few minutes and designate the pre-induction phase. Subsequently, a dormant period occurs within the next few hours. During this period, the material is workable;
2. Stage II – Intermediate stage – Stage II initiates after the disruption of the mechanism which prevents hydration progression during the dormant period. During this phase, the cement particles, alite C_3S and belite C_2S , hydrate resulting in the production of calcium silicate hydrate C-S-H and crystalline calcium hydroxide CH (Portlandite - $Ca(OH)_2$). Other minor clinker components, like aluminates, react during this phase, forming ettringite, which is converted into monosulphate. The cement hydration reaction is exothermic and has an initial accelerated phase until it reaches the heat generation rate peak (for this stage). A deceleration period is observed due to the newly formed layer of hydration products assembled at the anhydrous cement particle shell. At this time, the hydration rate becomes controlled by water diffusion through the layers of hydrated products. The porosity of the material decreases due to the expansive chemical reactions. Additionally, there is an increase in the stiffness and strength of the concrete element;
3. Stage III – Late stage – this period is controlled by the diffusion hydration that characterises the end of Stage II, but with lower hydration rates due to the increase in the thickness of the hydrated products in the shell of the anhydrous cement particles. As the hydration rate decreases, the generation of heat and the evolution rate of the material's mechanical properties will also decrease.

Fig. 1 shows the formation of several hydration products during the different cement hydration stages.

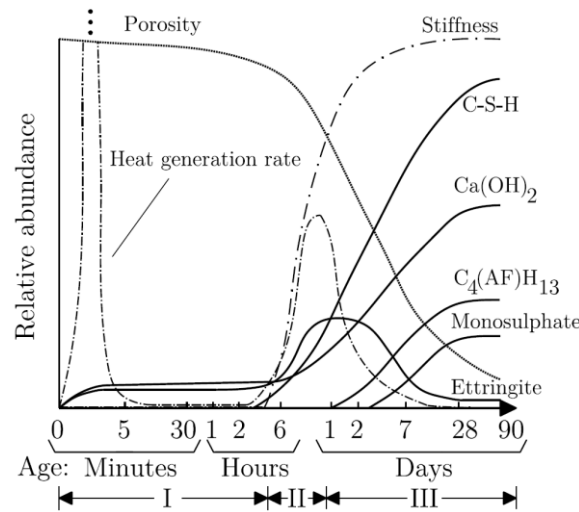


Fig. 1 – Formation of several hydration products with time, together with porosity and heat generation rate evolution (adapted from [5, 6]).

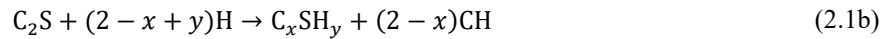
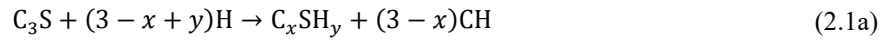
2.1.1 CEMENT HYDRATION KINETICS THEORY

The constituents and proportions of cement clinker are influenced by the specific chemical compositions of the raw materials. Nevertheless, the principal oxides present in ordinary Portland cement are calcium oxide (lime, $\text{CaO} = \text{C}$), silicon dioxide (silica, $\text{SiO}_2 = \text{S}$), aluminium oxide (alumina, $\text{Al}_2\text{O}_3 = \text{A}$) and iron oxide ($\text{Fe}_2\text{O}_3 = \text{F}$). The resulting compounds in hydrated cement are calcium silicate hydrates (C-S-H) and calcium hydroxide (portlandite CH). The presence of calcium sulfate in cement clinker also contributes to forming hexacalcium aluminate trisulfate hydrate (ettringite, Aft), which, under particular conditions, may be associated with long-term cracking problems [7]. Other components of cement clinker include sulphur trioxide ($\text{SO}_3 = \bar{\text{S}}$), which combined with calcium oxide and water ($\text{H}_2\text{O} = \text{H}$), forms gypsum, resulting in a highly expansive reaction associated with swelling in submerged concrete. Table 1 shows the principal compounds of the Portland cement clinker and the hydrated products.

Table 1 – Principal components of Portland cement clinker and hydrated Portland cement

Type	Name	Chemical Composition	Cement notation
Cement Clinker	Tricalcium silicate (Alite)	3Ca O. Si O_2	C_3S
	Dicalcium silicate (Belite)	2Ca O. Si O_2	C_2S
	Tricalcium aluminate	$3\text{Ca O. Al}_2\text{ O}_3$	C_3A
	Tetracalcium aluminoferrite	$4\text{Ca O. Al}_2\text{ O}_3. \text{Fe}_2\text{O}_3$	C_4AF
Hydrated Cement	Calcium silicate hydrate	$3(\text{CaO}). 2(\text{SiO}_2). 4(\text{H}_2\text{O})$	C-S-H
	Calcium hydroxide (Portlandite)	Ca (OH)_2	CH
	Hexacalcium aluminate trisulfate hydrate (Ettringite)	$6(\text{CaO}). (\text{Al}_2\text{O}_3). 3(\text{SO}_3). 32(\text{H}_2\text{O})$	AFt

The chemical reactions occurring in cement paste are exothermic and chemically activated at ambient temperature by the contact of water with the anhydrous cement. The stoichiometric equations of the chemical reactions occurring with the principal compounds of cement clinker are [8-12]:



The proportions in the stoichiometry equation may vary from case to case. Therefore, the stoichiometry balances for the alite (Equation (2.1a)) and the belite (Equation (2.1b)) are written for the variables ‘ x ’ and ‘ y ’. Common literature values for these variables are $1.5 \leq x \leq 2$ and $1.5 \leq y \leq 7$ [8-12]. The products of alite (C_3S) and belite (C_2S) reaction with water are the calcium silicate hydrated (CSH), and the calcium hydroxide (CH); Equation (2.1c) gives the reaction occurring between tricalcium aluminate (C_3A) and water, which generates calcium aluminate hydrate (C_3AH_6); Equation (2.1d) gives the reaction occurring between tetracalcium aluminoferrite (C_4AF) and water, which produces calcium aluminate hydrate (C_3AH_6) and calcium ferrite hydrate (CFH); Equation (2.1e) presents the solidification process of calcium ferrite hydrate ($\text{C}_3\text{FH}_{x+2}$); and Equation (2.1f) gives the reaction

between tricalcium aluminate (C_3A), calcium sulfate ($C\bar{S}$) and water, resulting in the formation of ettringite (AFt).

Alite (C_3S) has a higher amount of calcium, which makes it more reactive than belite (C_2S). Therefore, the intermediate stage (Stage II) reactions are mainly dominated by the hydration of alite, Equation (2.1a). The belite (C_2S) reaction presented in Equation (2.1b) has lower reactivity and contributes to the late strength development identified in Stage III [13]. Table 2 summarises the chemical characteristics of the different compounds of Portland cement.

Table 2 - Characteristics of the Portland cement (values from [4])

Clinker Compound		C_3S	C_2S	C_3A	C_4AF
Hydration velocity		High	Moderate	Very high	High
Heat of hydration	Quantity	High (502 J/g)	Low (260 J/g)	Very high (867 J/g)	Moderate (419 J/g)
	Development	Fast	Slow	Fast	Slow
	Contribution to the mechanical resistance	Fast and long-term	Slow and long-term	Very fast and slow duration	Slow and insignificant
Chemical Attack		Small	Moderate	Very small	Big

Different experimental techniques have been used to quantify cement oxides and compounds. Kristmann [14] used electron microprobe analysis (EMP) to study the clinker minerals. Le Saoût et al. [15] determined the amount of oxides through energy dispersive spectroscopy (EDS). Scrivener et al. [16] derived the amount of compound from X-ray diffractometry experiments. Durdziński et al. [17] used X-ray fluorescence spectroscopy and X-ray powder diffraction (XRD) with Rietveld refinement to quantify the number of oxides in the cement clinker.

Based on identifying the oxide quantities, the composition of the clinker can be estimated with high precision using analytical techniques. The most commonly used method for estimating the four main compounds, alite (C_3S), belite (C_2S), tricalcium aluminate (C_3A) and tetracalcium aluminoferrite (C_4AF) in Portland cement clinker is the Bogue calculation [18, 19] or the Modified Bogue calculation (also known as the Taylor model) [20]. An alternative method has been proposed by Shim et al. [21]. Fig. 2 shows the mean compound composition of Portland cement (Type I).

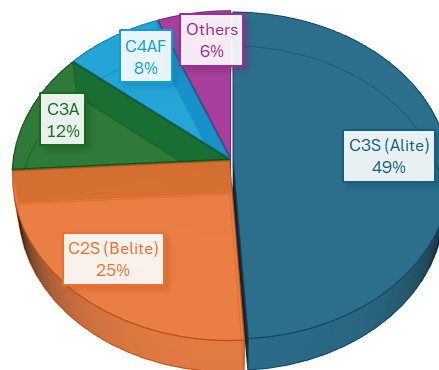


Fig. 2 – Mean compound composition of Portland cement (Type I) [4].

2.1.2 CEMENT HYDRATION OF ALITE COMPOUND

Alite (C_3S), which typically constitutes 50% of cement clinker, is the principal compound, with belite (C_2S) being the second most abundant. Consequently, alite is the main one responsible for the properties of cement-based materials. Fig. 3 compares an anhydrous and hydrated alite particle obtained from scanning electron microscopy [22].

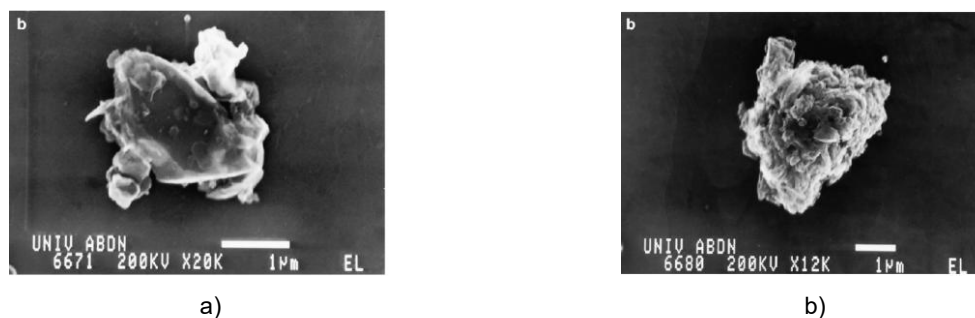


Fig. 3 – Scanning electron microscopy of anhydrous and hydrated alite particles (adapted from [22]): a) unhydrated alite particle; b) hydrated alite particle.

The unhydrated alite particle has a smoother surface than the hydrated alite particle. This is justified by the morphology of the C-S-H, which can be identified as small thin foils that adhere to the surrounding surface of the hydrated alite particle. The cement reaction is expansive, as it results in an increase in the volume of the solid product constituents despite a decrease in the total volume of the reactants [23]. Fig. 4 shows the principal five stages of an idealised model of cement hydration for a single cement particle proposed by Rahimi-Aghdam et al. [24].

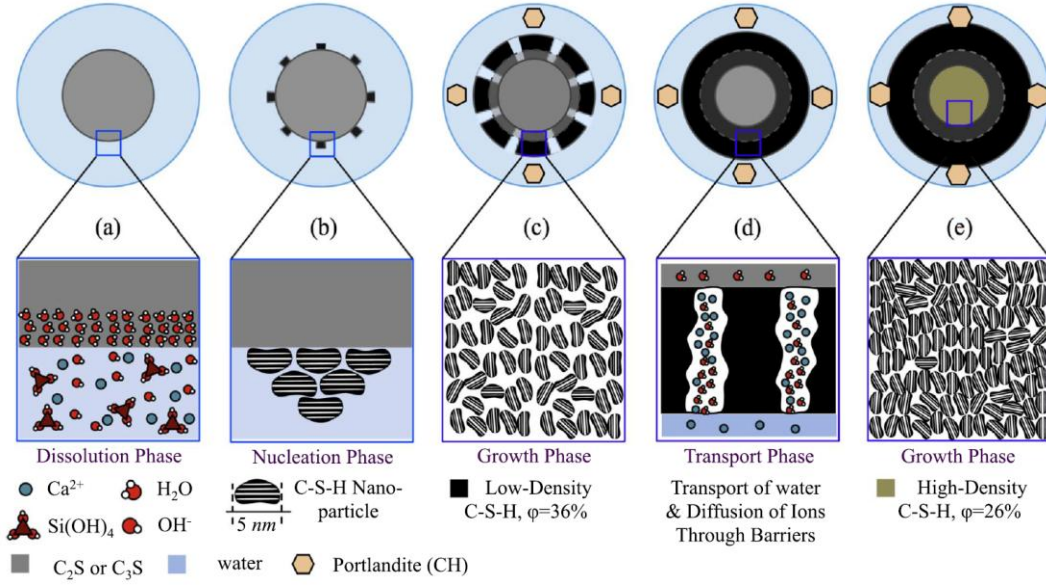


Fig. 4 – Schematics of a five-phase idealised cement hydration model (adapted from [24]).

In Fig. 4, phase a) is the dissolution phase corresponding to the generation of a semi-impermeable layer around cement particles during the dormant period. Phase b) is the nucleation phase and corresponds to the allocation of a constant number of C-S-H particles on the surface of the cement particles. Phase c) is the first growth phase, where an isotropic and self-similar growth of the C-S-H adheres to the cement particle in a spatially constant but time-varying growth rate. In this phase, low-density C-S-H with high porosity (ϕ) is generated. Phase d) is the transport phase, represented by an overlapping of the growing C-S-H nuclei and the coverage of the entire surface with hydration products, which ends the nucleation growth process. Phase e) is the second growth phase, where a uniform growth of C-S-H particles is controlled by the diffusion of water and the ions to the anhydrous cement. In this phase, high-density C-S-H is generated with lower porosity (ϕ) [24]. Phase a) belongs to Stage I or Early-stage (dormant period), while phases b) and c) are relative to Stage II or Intermediate-stage and phases d) and e) are representative of the transition between Stage II and Stage III or Late-stage.

Equation (2.1a) can be used to set up the growing phase for the hydration of an alite particle, hereby described by the following values assumed from [24]:



The volume expansion of the reaction of a cement particle, $\zeta_{prod,react}$ can be formulated according to the following equation [24]:

$$\zeta_{prod,react} = \frac{dV_{prod}}{dV_{react}} = \sum \left(\frac{V_{m,prod} n_{prod}}{V_{m,react} n_{react}} \right), \text{ with } V_m = M_r / \rho \quad (2.3)$$

where dV_{prod} is the volume of the produced compound, dV_{react} is the volume of the consumed compound, V_m is the molar volume, M_r is the molar mass, ρ is the mass density, and n is the number of moles produced or consumed in the stoichiometry Equation (2.2).

Table 3 presents the molar mass and the density of the different components of cement hydration involved in Equation (2.2).

Table 3 – The molar mass and density of cement components [24]

Phase	Molar mass (g/mol)	Density (g/cm ³)
C ₃ S	228.3	3.15
C-S-H (C _{1.7} SH _{1.8})	187.9	1.71
CH	74.1	2.24

Employing Equation (2.3), the volume expansion for alite in the reaction presented in Equation (2.2) becomes:

$$\begin{aligned}
 \zeta_{prod,C3S} &= \zeta_{CSH,C3S} + \zeta_{CH,C3S} = \frac{dV_{CSH}}{dV_{C3S}} + \frac{dV_{CH}}{dV_{C3S}} = \frac{M_{r,CSH}n_{CSH}\rho_{C3S}}{M_{r,C3S}n_{C3S}\rho_{CSH}} + \frac{M_{r,CH}n_{CH}\rho_{C3S}}{M_{r,C3S}n_{C3S}\rho_{CH}} \\
 &= \frac{187.9 \times 1 \times 3.15}{228.3 \times 1 \times 1.71} + \frac{74.1 \times 1.3 \times 3.15}{228.3 \times 1 \times 2.24} \\
 \zeta_{prod,C3S} &= 1.52 + 0.59 \approx 2.11
 \end{aligned} \tag{2.4}$$

Equation (2.4) quantifies the potential solid volume increase resulting from the hydration of an alite cement grain. Each unit of solid volume of alite during hydration produces an additional 2.11 units of solid volume, comprising 1.52 units of C-S-H and 0.59 units of calcium hydroxide. This volume growth analytically confirms the expansive nature of cement hydration.

2.1.3 DEGREE OF HYDRATION

The degree of hydration, α , is a concept introduced to quantify cement hydration. The degree of hydration allows researchers to relate the chemical reactions occurring in cement to the development of the concrete's microstructure and the evolution of its material strength. Overall, the degree of hydration is defined as the ratio between the amount of cement that has reacted and the total amount of cement [23] as follows:

$$\alpha(t) = \frac{\text{amount of cement that has reacted at time } t}{\text{total amount of cement at time } t = 0} \tag{2.5}$$

Since the amount of reacted cement cannot be quantified straightforwardly, some authors propose alternative relationships for the degree of hydration. Methods like quantitative calorimeter tests, X-ray diffraction analysis (QXRD), measurement of non-evaporable water as a loss on ignition with thermogravimetry, and basic shrinkage measurement can be used to monitor cement hydration [25].

Ulm and Coussy [26] suggested that the degree of hydration can be easily obtained based on the actual water mass combined in the solid phase (hydration mass) and the asymptotic value of the water mass

combined in the solid phase. Such an approach is commonly used to determine the degree of hydration based on the chemically bonded water [22].

$$\alpha = \frac{W_{chem,w}}{W_{max,chem,w}} \quad (2.6)$$

where $W_{chem,w}$ is the weight of chemically bonded water and $W_{max,chem,w}$ is the amount of chemically bonded water at complete hydration.

Reinhardt et al. [27] suggest determining the degree of hydration as the ratio between the amount of heat released and the total heat accumulated at full hydration, $\alpha \approx Q/Q_{total}$. This approximation benefits from the exothermic characteristic of the cement hydration and allows the evaluation of the degree of hydration experimentally through calorimeter tests.

Czernin [28] and Geiker and Knudsen [29] measured the degree of hydration based on the basic shrinkage. Other analytical relationships, like the amount of produced portlandite, specific surface of the cement paste, strength evolution or dielectric properties of the cement, have been proposed to quantify the degree of hydration [30].

The degree of hydration should vary between 0 (before mixing) and 1 (representing full hydration). During Stage I (Fig. 1), the contact of water and cement leads to instant reactions that increase the degree of hydration while the mixture still has a viscous fluid consistency. The degree of hydration for which concrete starts to have a solidified structure is usually called the degree of hydration at setting (α_{set}). Most of the degree of hydration evolution is expected to occur during Stage II (Fig. 1). Full hydration means that all the cement compounds should have reacted. Due to the characteristics of Stage III and the multiple physical processes related to moisture content, full hydration would be difficult to achieve in ordinary concretes [31]. Several models have been proposed to evaluate the degree of hydration.

2.1.3.1 Simple autocatalytic model

The simple autocatalytic model is generally given by a differential equation that relates the evolution of the degree of hydration with a temperature function based on the Arrhenius law [30]. The simple case of autocatalytic kinetics can be formulated as:

$$\dot{\alpha} = A^* \cdot f(\alpha) \cdot \beta_{eT}(T) = A^* \cdot f(\alpha) \cdot \exp \left[\frac{Q_e}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \quad (2.7)$$

where A^* is a constant dependent on the chemical reaction, $f(\alpha)$ is the function of the kinetic model (for a simple autocatalytic kinetic model $f(\alpha) = \alpha(1 - \alpha)$), $\beta_{eT}(T)$ is a function that accounts for the temperature effect in the evolution of the chemical reactions, Q_e is the activation energy, R is the universal gas constant, T_0 is the temperature at calibration (typically, $T_0 = 293 \text{ K}$) and T is the temperature.

The parameters used in Equation (2.7) can be determined based on experimental data. Assuming the Reinhardt et al. [27] definition of the degree of hydration, the isothermal calorimetry tests can be used to obtain the normalised function $f(\alpha)$ by dividing the heat ratio by the heat ratio peak:

$$f(\alpha) = \frac{\dot{Q}(t)}{\dot{Q}_{peak}} \quad (2.8)$$

This formulation assumes that the calibration of the function $f(\alpha)$ is independent of the temperature at which the cement hydrates. Similar assumptions are made for the calibration of the parameter A^* and the energy of activation, Q_e . The only parameter dependent on temperature is the function $\beta_{eT}(T)$. Two methods are recurrently used to estimate those parameters based on isothermal calorimetry tests:

- i) the speed method;
- ii) the derivative of the speed method.

These methods are explained in detail by D'Aloia and Chanvillard [32] and D'Aloia [33]. Azenha [5] calibrated the parameters in Equation (2.7) for various cement types using an isothermal calorimetry test for temperatures between 20 °C and 60 °C. He found that considering $f(\alpha)$, Q_e and A^* as temperature-independent variables, it is a practicable approach.

2.1.3.2 Affinity model

The affinity is the force that governs the chemical reactions. For hydration at constant pressure P and temperature T , the affinity is given by the relation between the Gibbs free energy, G and the degree of hydration α .

$$A = -[G/\alpha]_{P,T} \quad (2.9)$$

The affinity is negative in spontaneous reactions. Ulm and Coussy [34] established the relationship between the degree of hydration and the affinity determined at a specific temperature as:

$$\dot{\alpha} = \tilde{A}_{Tref}(\alpha) \cdot \beta_{eT}(T) \cdot \beta_{eh}(h) \quad (2.10)$$

where $\beta_{eT}(T)$ and $\beta_{eh}(h)$ are coefficients to account for the temperature and relative humidity effects on affinity. Considering $\tilde{A}_{Tref}(\alpha) = A^* \cdot f(\alpha)$, Equation (2.7) and Equation (2.10) are identical.

Cervera et al. [35] and Gawin et al. [36] developed an equation for the affinity as:

$$\tilde{A}_{Tref}(\alpha) = B_1(B_2/\alpha_{max} + \alpha)(\alpha_{max} - \alpha) \exp(-\eta_A \cdot \alpha/\alpha_{max}) \quad (2.11)$$

where B_1 , B_2 and η_A are coefficients to be adjusted and represent the micro-diffusion of free water through formed hydrates, α_{max} is the maximum degree of hydration and can be defined using an empirical formula. Powers and Brownyard [23] propose the following expression to determine α_{max} :

$$\alpha_{max} = \min\left(1; \frac{w/c}{0.42}\right) \quad (2.12)$$

Alternatively, Mills [37] proposed an equation for the maximum degree of hydration, which was later updated by Schindler and Folliard [38] to account for the effect of slag and fly ash:

$$\alpha_{max} = \frac{1.031 w/c}{0.194 + w/c} + 0.3 \cdot P_{slag} + 0.5 \cdot P_{FA} \quad (2.13)$$

where P_{slag} and P_{FA} are the weights of slag and fly ash in the mixture, respectively, as a percentage of the total cementitious material.

Lea da Silva and Šmilauer [39] calibrated the Affinity Model and proposed empirical equations for the estimation of the parameters of Equation (2.11):

$$B_1 = 0.738 \cdot C_3S^{-0.206} \cdot C_2S^{-0.128} \cdot C_3A^{0.161} \quad (2.14a)$$

$$B_2 = (-0.0767 \cdot C_4AF + 0.0184) \frac{B_f}{350 \cdot B_f} \quad (2.14b)$$

$$\eta_A = 10.95 \cdot C_3S + 11.25 \cdot C_2S - 4.10 \cdot C_3A - 0.892 \quad (2.14c)$$

where B_f is the cement fineness (m^2/kg) and C_3S , C_2S , C_3A and C_4AF are the mass percentage of each mineral.

2.1.3.3 Multiple-particle cement hydration models

More sophisticated models for cement hydration simulation are the multi-particle cement hydration models. Several teams have investigated and developed numerical tools that allow the complex simulation of cement hydration based on multiple-particle models. This includes the works of Jennings and Johnson [40], Bentz [41] (CEMHYD3D), Van Breugel [42] (HYMOSTRUCT), Navi and Pignat [43], Maekawa [44] (DuCOM) and Lin and Meyer [45]. In these models, the cement hydration is simulated in a closed envelope, usually in a cubic shape.

2.1.4 MECHANICAL PROPERTIES AND MATURITY OF CONCRETE

The evolution of concrete's microstructure is correlated with cement hydration [46]. Additionally, cement hydration kinetics and the proportions of cement, water, aggregates, admixtures and additions, and aggregate type influence concrete's mechanical properties. Fig. 5 shows the typical compressive strength evolution due to each of the four principal compounds of Portland cement.

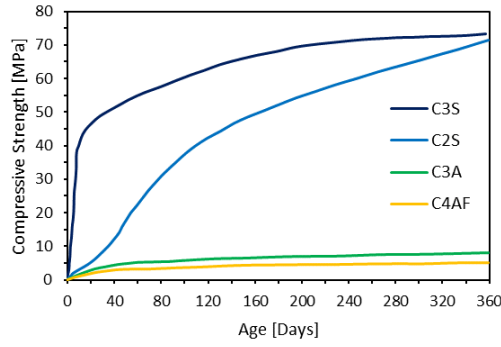


Fig. 5 – Compressive strength evolution due to the different compounds of cement (adapted from [12])

Alite is the clinker compound primarily responsible for early compressive strength development, with a rapid strength gain in the first 20 days and a slower rate after 40 days. In contrast, belite develops strength more slowly at early ages compared to alite. However, after 40 days, belite's compressive strength gain rate surpasses alite's, and after one year, belite reaches similar compressive strength levels. The effects of tricalcium aluminate and tetracalcium aluminoferrite on concrete's compressive strength are negligible compared to the alite and belite compounds. Since alite is the main compound of the cement clinker Type I (Fig. 2), most of the strength evolution in concrete specimens is expected to occur in the early ages (first 20 days), while long-term strength evolution can be primarily associated with the hydration of belite.

2.1.4.1 Mechanical properties of concrete based on the degree of hydration

De Schutter and Taerwe [47] proposed that the mechanical properties of concrete, compressive strength, tensile strength and elastic modulus can be formulated based on the degree of hydration and the asymptotic value of the evaluated properties:

$$X_i(\alpha) = X_{\infty,i} \left(\frac{\alpha - \alpha_i}{1 - \alpha_i} \right)^{\eta_i} \quad (2.15)$$

where α is the degree of hydration, α_i is the initial degree of hydration and parameter η_i is a coefficient that depends on the mechanical property being evaluated. ($\eta_i = 1.5$ for compressive strength; $\eta_i = 1.0$ for tensile strength; $\eta_i = 0.5$ for elastic modulus), and $X_{\infty,i}$ is the general property value, X_i , upon full hydration.

Ulm and Coussy [26] proposed an equation that evaluates the increase of compressive strength proportionally with the increase of the degree of hydration as:

$$\frac{df_c}{dt} = c \frac{d\alpha}{dt} \quad (2.16)$$

where c is a constant.

Maekawa [44] proposed an equation that evaluates the compressive strength of concrete based on the volume ratio of hydration products.

$$f_c = f_\infty \left(1 - \exp \left(-k_1 (D_{hyd,out})^{k_2} \right) \right) \quad (2.17)$$

where f_c is the compressive strength, f_∞ is the ultimate strength, k_1 and k_2 are material constants that may take into account additional effects on the mechanical properties, $D_{hyd,out}$ is the volume ratio of the outer hydration products that form outside the original cement particle volume ($V_{hyd,out}$) and the initial capillary space volume ($V_{cap,ini}$):

$$D_{hyd,out} = \frac{V_{hyd,out}}{V_{cap,ini}} = \frac{V_{hyd,total} - V_{hyd,in}}{V_{cap,ini}} \quad (2.18)$$

where $V_{hyd,total}$ is the total volume of hydration products, and $V_{hyd,in}$ is the volume of hydration products that form inside the original cement particle. Fig. 6 shows the relationship between the degree of hydration and the volume fractions.

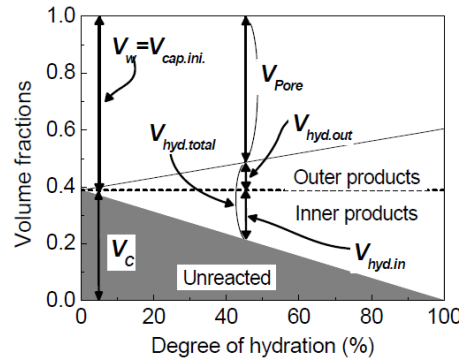


Fig. 6 – Change in component volume and its indicator for strength development (adapted from [44]).

Powers and Brownyard [23] proposed a formulation for the strength of cement paste based on the gel space, which is the ratio of gel volume to the volume of available space. Wang and Park [48] developed a model for evaluating the compressive strength of concrete based on the gel-space ratio as follows:

$$f_c(t) = F_1 (x_{pc})^{F_2} \quad (2.19)$$

where F_1 is the intrinsic strength of the material, F_2 is the strength exponent, x_{pc} is the gel-space ratio of cement calculated as:

$$x_{pc} = \frac{V_v(T) \cdot (1/\rho_c) \cdot \alpha}{(1/\rho_c) \cdot \alpha + w/c} \quad (2.20)$$

where α is the degree of hydration and $V_v(T)$ is the volume of hydration products in a unit volume of cement determined as [42]:

$$V_v(T) = \frac{\text{Volume of hydration products at } T}{\text{Volume of reacted cement at } T} = v_{293} \cdot \exp(-28 \times 10^{-6} (T - 293)^2) \quad (2.21)$$

where T is the temperature in K and v_{293} is the volume of hydration products in a unit volume of cement at 293 K (i.e., 20 °C) and can be taken as $v_{293} = 2.2$.

2.1.4.2 Mechanical properties of concrete based on time

Kanstad et al. [49] proposed adjusting the equation suggested by De Schutter and Taerwe [47], based on the time evolution or equivalent time, resulting in:

$$X_i(t_{eq}) = X_{28,i} \left(\exp \left[s \left(1 - \sqrt{28/(t_{eq} - t_0)} \right) \right] \right)^{\eta_i} \quad (2.22)$$

The coefficient η_i depends on the mechanical property being evaluated: for the compressive strength, the parameter $\eta_i = 1$, for tensile strength, it can vary between 0.5 and 0.7, and for the elastic modulus, it can vary between 0.3 and 0.45. Fig. 7 compares the evolution of the different mechanical properties, normalised with respect to the property value at 28 days, for representative η_i values.

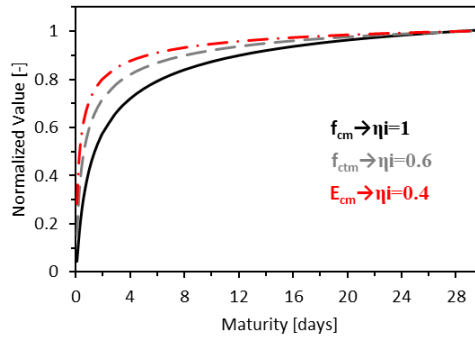


Fig. 7 – Comparison between the evolution of the different mechanical properties of concrete.

The MC2010 [50] and Eurocode 2 [51] adopt the equations proposed by Kanstad et al. [49] for describing the time evolution of concrete's mechanical properties, specifying values for $X_{\infty,i}$ based on the compressive strength and for s based on the cement type.

Azenha et al. [52] and Granja and Azenha [53] developed the *Elastic Modulus Measurement from the Ambient Response Method* (EMM-ARM) to evaluate the evolution of the modulus of elasticity since the casting of concrete. The setup is based on an implicit calculation based on the eigen frequency of the first vibration mode of a supported beam (or a cantilever) periodically excited at the middle span in a long-range frequency spectrum.

An investigation of the early age evolution of the modulus of elasticity concluded that the evolution of the properties of concrete at the setting time might not be correctly simulated using Equation (2.22). Carette and Staquet [54] proposed an alternative equation based on the sum of two exponential functions:

$$E(t) = \alpha_1 \exp \left(- \left(\frac{\tau_1}{t} \right)^{\beta_1} \right) + \alpha_2 \exp \left(- \left(\frac{\tau_2}{t} \right)^{\beta_2} \right) \quad (2.23)$$

where $\alpha_1, \alpha_2, \tau_1, \tau_2, \beta_1$ and β_2 are constants obtained from experimental calibration.

Fig. 8 compares the modulus of elasticity results obtained through cyclic compression in cylinders (CC) with those measured by the EMM-ARM for the COST ACTION 1404 concrete [55]. The best curve fitting from equations (2.22) and (2.23) is also presented.

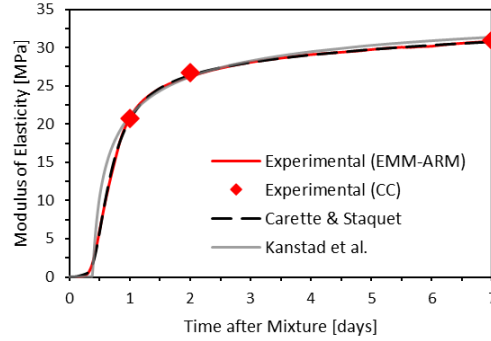


Fig. 8 – Comparison between different modulus of elasticity experimental tests and analytical models [55].

The Carette and Staquet [54] equation better fits the modulus of elasticity evolution for times below one day. This occurs because the time t_0 in Kanstad et al. [49] equation is approximately equal to the setting time and does not capture in detail the initial hardening processes of concrete.

2.2 MOISTURE IN CONCRETE

Concrete is a porous material containing water in different states in the pores. The pore water is essential for cement hydration and affects other hygral-dependent phenomena, like shrinkage and creep. Moisture content within the pores may change due to transport mechanisms or chemical reactions. Accurately describing moisture transport in porous materials is essential to reproduce the multiphysics behaviour of concrete. The moisture transport is generally described by the theory of partially saturated porous media [56-60], with the theoretical support of thermodynamics of multiphase systems [61-63]. Ideally, moisture transport should be considered simultaneously with heat transport and chemical processes due to their influence on the evolution of the porous structure. Sophisticated thermo-hygro-chemo-mechanical models have been proposed in the literature to simulate the multiphysics behaviour of porous materials [36, 64]. The numerical simulation of moisture transport remains challenging since the limits between the solid and fluid phases are blurred and variable in time. Furthermore, some model parameters are difficult to quantify or hard to determine. Therefore, some simplifications are usually made. This chapter presents the principal theories behind moisture transport and the simplifications made toward the numerical simulation of moisture content.

2.2.1 GENERAL CONCEPTS

In concrete pores, water may exist in different states. Some water is located in the capillary pores; others are hindered in the nanopores or chemically bonded in the calcium silicate hydrates (C-S-H). In a

thermodynamic equilibrium of a stabilised microstructure of an ordinary concrete mixture, three different phases of water can be distinguished [65]:

- i) capillary water, which consists of liquid water in the capillary pores bounded by the capillary menisci;
- ii) water vapour, which consists of most of the evaporable water in the capillary pores at a partial pressure p_v below the saturated vapour pressure p_{sat} ;
- iii) adsorbed water, which consists of thin layers of water molecules adsorbed to the wall of the pores in contact with water vapour and hindered adsorbed water in the cement gel nanopores.

Moisture, w , is defined as the amount of water in concrete in these three phases. Fig. 9 shows the moisture in a concrete capillary pore.

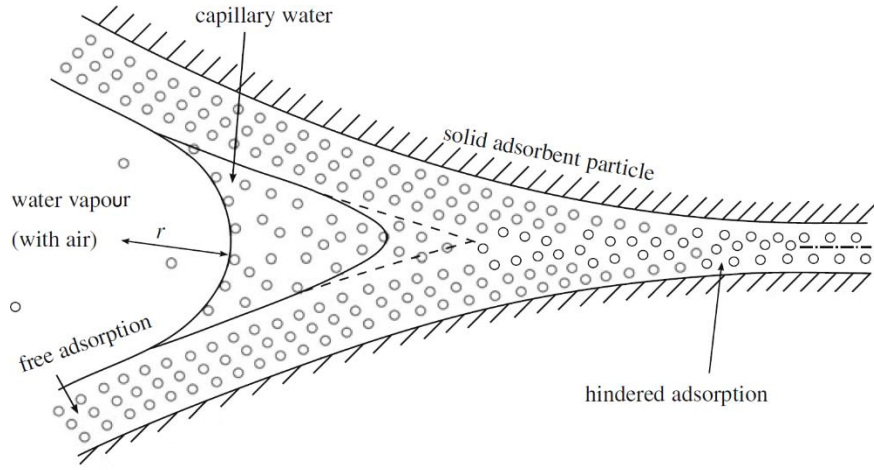


Fig. 9 –Capillary pore with identification of the different water phases (adapted from [65]).

The water chemically bonded in the C-S-H is part of the concrete's solid skeleton and will not evaporate or diffuse through the concrete specimen. The moisture in the concrete pores can be separated into evaporable water, w_e , and non-evaporable water (chemically bonded water), w_n . At the mixing time, all the moisture can be considered evaporable. Owing to cement hydration progression, the quantity of evaporable water decreases while the non-evaporable water increases. Only the evaporable water is subjected to moisture transport. For that reason, in some models, the evaporable water is just called moisture ($w_e = w$) [65].

Since concrete permeability is very low, moisture transport can be considered slow. Therefore, the moisture in the concrete capillary pores is in constant thermodynamic equilibrium, and the moisture variation can be closely related to the pore's relative humidity changes [65]. The following equation expresses the relative humidity, h .

$$h = \frac{p_v}{p_{sat}} \quad (2.24)$$

where p_v is the partial pressure of the water vapour and p_{sat} is the saturated vapour pressure, which represents the limit pressure for condensation. The saturated vapour pressure depends on the temperature [66].

Other recurrent terms used in poromechanics are the saturation degree, $S_l = V_l/(V_l + V_g)$, corresponding to a term used to quantify the extent to which something is saturated with water (or other liquid) and the porosity, $\varphi = (V_l + V_g)/(V_l + V_g + V_s)$, corresponding to a term used to measure a material's void or empty spaces. The parameters V_l , V_g and V_s are the volumes of liquid, gas and solid matter, respectively.

Fig. 9 shows the water in the capillary pores in liquid and vapour states delimited by the meniscus (concave interface between air and liquid water). The pore gas pressure in the capillary pore, p_g , which consists of the sum of the air pressure p_a and water vapour pressure p_v , must differ from the liquid water pressure p_l . The difference between the water vapour pressure, p_g , and liquid water pressure, p_l , is defined as the capillary pressure, p_c . The Young-Laplace equation describes the capillary pressure based on the interface between air and liquid water as follows:

$$p_c = p_g - p_l = \frac{2\gamma_{gl}}{r} \quad (2.25)$$

where γ_{gl} is the surface tension, which depends on the temperature (for the water-air interface at 20 °C is equal to 0.07329 N/m), r is the meniscus radius, which is constant for a sphere or can be determined through the average of the principal curvatures.

The air pressure, p_a , and the water vapour pressure, p_v , can be obtained through the Boyle-Mariotte state equation of ideal gases. Considering that the air pressure, p_a , is negligible compared with the capillary pressure, p_c , and assuming the incompressibility of liquid water and the behaviour of water vapour as an ideal gas, one can formulate the capillary pressure, p_c , regarding the pore relative humidity h as follows [65]:

$$p_c = -\frac{\rho_l RT}{M_w} \ln h \quad (2.26)$$

where M_w is the molar mass of water, ρ_l is the density of the liquid water (it varies with the temperature), and R is the ideal gas constant. Equation (2.26) is also known as the Kelvin equation.

Baroghel-Bouny et al. [67] compared the capillary pressure between ordinary and high-strength cement pastes and between ordinary and high-strength hardened concretes. Fig. 10 shows the experimental results for the evolution of capillary pressure for normal and high-strength cement pastes and concretes [68, 69].

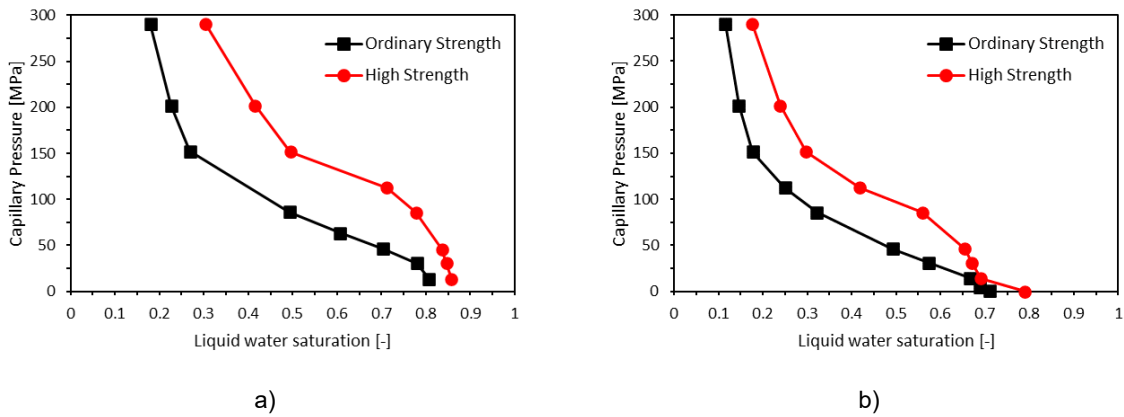


Fig. 10 – Relationship between the capillary pressure and the liquid water saturation, a) for hardened cement pastes; b) for hardened concretes (adapted from [67]).

The capillary pressure increases with the decrease in the liquid water saturation. For any liquid water saturation value, the capillary pressure in high-strength cement pastes or concretes is higher than that in ordinary cement pastes or concretes.

2.2.2 SORPTION ISOTHERM

The sorption isotherm is the relationship between the evaporable water content and the pore relative humidity at a constant temperature. The sorption isotherm may be divided into two subcategories:

- the desorption isotherm, which relates the evaporable water content with the decrease of the relative humidity (drying conditions);
- the adsorption isotherm, which relates the changes in the evaporable water content with the increase of the relative humidity (wetting conditions).

Baroghel-Bouny [70] performed experimental measurements of the desorption and adsorption of ordinary cement mixtures. Fig. 11 presents the sorption isotherm for ordinary cement mixtures.

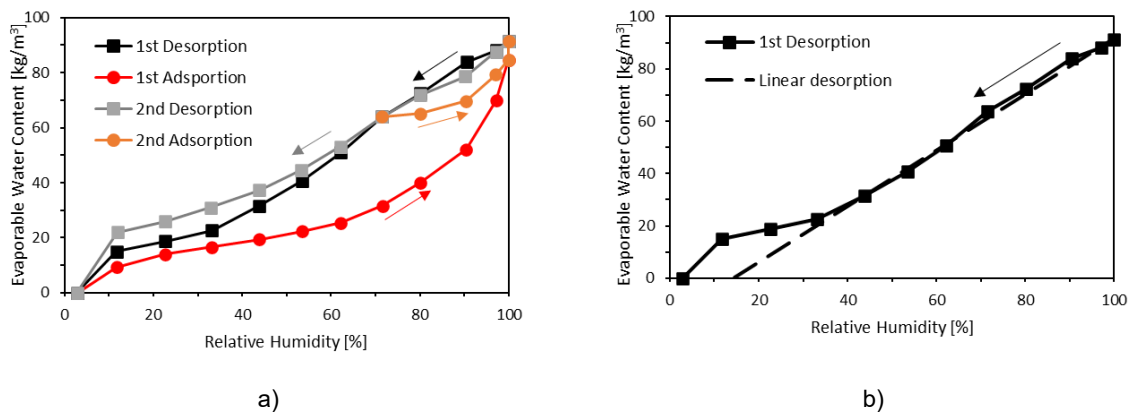


Fig. 11 – Sorption isotherms: a) differences between desorption isotherm and adsorption isotherm; b) linearity of the desorption isotherm (adapted from [70]).

Fig. 11 a) shows the sorption isotherm results for drying and wetting cycles in ordinary concrete mixtures. The experiment starts with a fully saturated specimen that dries from 100% relative humidity

to 3% relative humidity. The first drying stage, labelled as “1st desorption”, is presented in an isolated manner in Fig. 11 b). One can observe that linear desorption behaviour provides an accurate simulation of the desorption isotherm for relative humidity values above 30%. Subsequently, the concrete specimen is wetted from 3% to 100% relative humidity, labelled in Fig. 11 a) as “1st adsorption”. A non-linear curve and hysteretic behaviour are observed, where, for the same relative humidity, the amount of evaporable water content is smaller in the adsorption curve. Such behaviour can be explained by the *ink-bottle effect* [71] (non-uniqueness of the surfaces of capillary menisci of liquid adsorbate in larger pores) or by other mechanisms associated with the theory of sorption hysteresis in nanopores, i.e., the snap-through instabilities [72] and the molecular condensation [73]. Therefore, the hysteresis of the sorption curves is highly dependent on porous sizes and concrete microstructure. A new drying stage provides the “2nd desorption” similar to the “1st desorption”. Generally, Baroghel-Bouny [70] observed that drying and rewetting cycles of the same concrete specimens would lead to similar sorption curves. Additionally, Fig. 11 a) presents a wetting cycle starting at a relative humidity of 72%, labelled as “2nd adsorption”. The new wetting cycle confirms the strong hysteresis in the new adsorption curve. Several authors have proposed numerical models for representing sorption isotherms [74-78].

The relationship between the evaporable water content and the relative humidity can be represented as $w_e = \phi(h)$, where $\phi(h)$ is a function characterizing the sorption isotherm. The variation in the moisture content over time may be related to the relative humidity ratio by the following equation:

$$\dot{w}_e = [\partial\phi(h)/\partial h] \cdot \dot{h} \quad (2.27)$$

where the derivative $[\partial\phi(h)/\partial h]$ is the slope of the sorption isotherm (desorption), and it is named *moisture capacity*. The inverse of the moisture capacity $[\partial\phi(h)/\partial h]^{-1}$ is called the *reciprocal moisture capacity*.

Different models are available to characterise the sorption in ordinary concretes. The most popular ones are the Brunauer-Emmett-Teller (BET) model [76] derived from statistical thermodynamics of adsorption, and modifications of the BET model such as the BDDT model [77], the Hillerborg's formula [78], the FHH model [79] and the BSB model [75]. Other approaches have been adopted based on semi-empirical equations, which account for the evolution of the hydration reactions and the silica fume content [80, 81]. For the simple case of linear desorption, a simplified equation has been proposed by Rahimi-Aghdam et al. [24]:

$$\frac{\partial\phi(h)}{\partial h} = \frac{1}{1 - w/c} \Leftrightarrow \left[\frac{\partial\phi(h)}{\partial h} \right]^{-1} = 1 - w/c \quad (2.28)$$

Xi et al. [74] proposed an update to the BET model [76], which is based on a composed series of Langmuir isotherm single molecular layers [82]. The equation of the model is:

$$w = \frac{C \cdot k \cdot V_m \cdot h}{(1 - k \cdot h) \cdot [1 + (C - 1) \cdot k \cdot h]} \quad (2.29)$$

where w is the moisture content, and h is the relative humidity. The parameter V_m may be calculated as:

$$V_m = \left(0.068 - \frac{0.22}{t}\right) \left(0.85 + 0.45 \frac{w}{c}\right) V_{ct} \quad (2.30)$$

where t is the concrete age.

The parameter C is given by:

$$C = \exp\left(\frac{C_0}{T}\right) \quad (2.31)$$

where $C_0 = 855$ and T is the absolute temperature (Kelvin). The parameter k is given by:

$$k = \frac{\left(1 - \frac{1}{n}\right) C - 1}{C - 1} \quad (2.32)$$

where,

$$n = \left(2.5 + \frac{15}{t}\right) \cdot \left(0.33 + 2.2 \frac{w}{c}\right) N_{ct} \quad (2.33)$$

Equation (2.29) is valid for $t > 5$ days and $0.3 < w/c < 0.7$. The parameter V_{ct} and N_{ct} depend on the type of cement and may be considered as $V_{ct} = 0.9$ and $N_{ct} = 1.1$ for CEM type I, $V_{ct} = 0.9$ and $N_{ct} = 1$ for CEM type II, $V_{ct} = 0.85$ and $N_{ct} = 1.15$ for CEM type III and $V_{ct} = 0.6$ and $N_{ct} = 1.5$ for CEM type IV.

2.2.3 TRANSPORT MECHANISMS

Moisture transferences will occur in the presence of nonuniform ion concentrations or water pressure. According to Bažant and Jirásek [65], the different transport mechanisms occurring in concrete pores are:

- I. molecular diffusion;
- II. effusion (Knudsen diffusion);
- III. surface diffusion;
- IV. advective water flow;
- V. advective flow of pore gas (wet air).

Molecular diffusion is driven by the gradient of the molar concentration of vapour in the pore gas at the capillary pores. Overall, the molecular diffusion diminishes with the decrease in the pore size. The effusion relates to the molecular diffusion in the nanopores. It differs from ordinary molecular diffusion due to increased resistance generated by the molecules' collision with the pore walls. The surface diffusion is a transport process of water molecules adsorbed at the pore walls, which can be considered a special phase or a part of the liquid phase. The advective water flow and the advective flow of pore gas correspond to the moisture movement (liquid and vapour, respectively) due to a gradient of pressures

or convection mechanisms. Both of these mechanisms are associated with the permeability of the pore medium. Generally, the first two mechanisms and mechanism V are associated with water vapour transport. Mechanisms III and IV are associated with the transport of liquid water.

2.2.3.1 Darcy's law

In fully saturated elements, the mechanism that governs water transport is the gradient of pressure. The flux of liquid water that overpasses a porous medium, v_l , is proportional to the gradient of pressure multiplied by the hydraulic permeability K_h [m/s].

$$v_l = -K_h \nabla H_t \quad (2.34)$$

where H_t is the *total head*, which represents the level at which the water would rise in a pipe connected to the vertical coordinate z , and may be related to the liquid pressure $p_l(z)$ as:

$$H_t(z) = z + \frac{p_l(z) - p_{atm}}{\rho_l \cdot g} \quad (2.35)$$

where z is the height of the point above the reference plane, ρ_l is the mass density of the liquid, g is the gravitational acceleration and p_{atm} is the atmospheric pressure.

Combining Equation (2.34) with Equation (2.35) and considering that the density of water is constant, the mass flux of liquid water j_l [kg m⁻²s⁻¹] can be formulated as:

$$j_l = \rho_l \cdot v_l = -\frac{K_h}{g} \nabla p_l - \rho_l K_h e_z \quad (2.36)$$

Equation (2.36) presents Darcy's law for liquid water transport. Hydraulic permeability is a property specific to liquid water. For other fluid types, it can be expressed in terms of the intrinsic permeability, K_0 [m²]. Considering an incompressible Newtonian fluid is characterised by the mass density ρ_l [kg/m³] and the dynamic shear viscosity η_l [Pa.s], the hydraulic permeability K_h is related to the intrinsic permeability, K_0 [m²] by the following equation:

$$K_h = \frac{K_0 \rho_l g}{\eta_l} \quad (2.37)$$

Combining Equations (2.37) and (2.36), Darcy's law can be formulated for any fluid, provided the mass density and the dynamic shear viscosity of the fluid are known:

$$j_l = \rho_l \cdot v_l = -\frac{K_0 \cdot \rho_l}{\eta_l} \nabla p_l - \frac{\rho_l^2 K_0 g}{\eta_l} e_z \quad (2.38)$$

The second term on the right-hand side of Equations (2.36) and (2.38) is essential when the hydrostatic pressure caused by the self-weight of the fluid is non-negligible compared to the pore pressure. For usual

concrete members, it can be omitted, yet it must be kept for large structures like dams or geotechnical problems.

Equation (2.38) has been developed considering fully saturated conditions. For a partially saturated porous medium, the flow can also be considered driven by the total head gradient (∇H_t), but the hydraulic permeability needs to be reduced. This was taken into account by Buckingham [83], who extended Darcy's law to the partially saturated case. Buckingham [83] considered the hydraulic permeability a function of the water content by introducing a reduction factor k_r , called the relative permeability, which depends on water content and varies from 1 at full saturation to 0 at a certain minimum degree of saturation. The general form of Darcy's law for the partially saturated medium becomes:

$$j_l = \rho_l \cdot v_l = -\frac{k_{rl} \cdot K_0 \cdot \rho_l}{\eta_l} \nabla p_l - \frac{\rho_l^2 \cdot k_{rl} \cdot K_0 \cdot g}{\eta_l} e_z \quad (2.39)$$

2.2.3.2 Fick's law

Fick's law characterises the transport mechanism associated with diffusion processes. The law states that a diffusive flux is created from regions with higher concentrations to regions with lower concentrations, and results from the mathematical and physical investigations of Adolf Fick [84] on the experimental work regarding gas effusion conducted by Thomas Graham. Fick's first law is given by:

$$J = D \nabla C \quad (2.40)$$

where J is the diffusion flux, D is the diffusion coefficient, and C is the concentration (amount of substance per unit of volume).

Rewriting the diffusion processes concerning the change in concentration in time leads to Fick's second law:

$$\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) \quad (2.41)$$

The mathematical formulation of diffusion mechanisms is similar to that of permeability mechanisms. The main difference lies in the type of gradient driving each process. In permeability, the flux is governed by pressure gradients, whereas in diffusion, it is controlled by concentration gradients.

In concrete elements, the diffusion processes are mostly associated with water vapour flux. Fick's first law is formulated based on the diffusion flux, $J = C_v v_v$. For convenience, the diffusion processes should be rewritten in terms of the mass flux, $j_v = \rho_v v_v$. Considering the water vapour and air to behave as an ideal gas, the molar concentration of water vapour C_v is given by:

$$C_v = \frac{\rho_v / M_w}{\rho_v / M_w + \rho_a / M_a} = \frac{p_v}{p_v + p_a} = \frac{p_v}{p_g} \quad (2.42)$$

Thus, Fick's first law (Equation (2.40)) can be rewritten as:

$$p_v v_v = -D_g p_g \nabla \left(\frac{p_v}{p_g} \right) \quad (2.43)$$

where v_v is the velocity of the water vapour and D_g is the diffusion coefficient of the gas (water vapour and air).

Finally, Fick's first law applied to the mass flux of water vapour j_v is given by:

$$j_v = \rho_v v_v = \frac{M_w p_v}{RT} v_v = -\frac{M_w}{RT} D_g p_g \nabla \left(\frac{p_v}{p_g} \right) \quad (2.44)$$

The diffusion coefficient D_g depends on the temperature and gas pressure and is given by [84]:

$$D_g = \frac{p_{atm}}{p_g} \left(\frac{T}{T_0} \right)^{1.88} D_0 \quad (2.45)$$

where $D_0 = 2.48 \times 10^5 \text{ m}^2/\text{s}$ is the diffusion coefficient value at the reference temperature and gas pressure.

For concrete elements, the mass flux of water vapour must be reduced by two factors: the porosity φ , which implies the reduction of area across which the diffusing molecules can travel; and the tortuosity τ , which accounts for the constraint effect of pore walls in the diffusing flux. The mass flux of vapour in the concrete element is given by:

$$j_v = -\varphi \tau \frac{M_w}{RT} p_{atm} \left(\frac{T}{T_0} \right)^{1.88} D_0 \nabla \left(\frac{p_v}{p_g} \right) \quad (2.46)$$

The equation can be simplified if $p_g = p_{atm}$ and the temperature is constant in time. Bažant and Najjar [85] formulate the mass flux of water vapour as:

$$j_v = -\varphi \tau [1 - S_l] \frac{M_w D_0 p_{sat}}{R T_0} \nabla h \quad (2.47)$$

where S_l is the saturation degree.

2.2.4 DIFFERENTIAL EQUATIONS FOR MOISTURE TRANSPORT

In fully saturated concrete elements, the moisture in the concrete pores is mostly in the liquid state. Therefore, the moisture transport is associated with the flux of liquid water, mechanisms III and IV, while the diffusion processes can be considered residual. In this stage, moisture transport is generally described exclusively by permeability processes, according to Darcy's law. Following the decrease of moisture content associated with water consumption due to hydration and/or drying, the gaseous moisture phase becomes more and more predominant. Considering that the air pressure in concrete pores

(dry air and water vapour) at ambient temperature is similar to the external atmospheric pressure, the part of the transport mechanisms associated with the permeability of the air, mechanism V, can be discarded. This hypothesis is based on the assumption that the dynamic viscosity of the dry air is very low. Therefore, the pressure variations are fastest dissipated regarding the time scale of drying processes, and the water vapour transport mechanism is of the diffusive type only. In this stage, the moisture transport can be restricted to the diffusion mechanisms I and II, which are described by Fick's law. Simplifications on the numerical models for moisture transport are obtained if the evolution of concrete microstructure is dismissed. The numerical model for moisture transport should account for the transition between the permeability and diffusion mechanisms [86]. The general form of moisture transport is given by [87]:

$$\frac{\partial w}{\partial t} = -\nabla(\Phi_{dif} + \Phi_{per} + \Phi_{con}) - \frac{\partial w_s}{\partial t} - q \quad (2.48)$$

where $\Phi_{dif} = J_v$ is the flux of moisture due to the diffusion mechanism, $\Phi_{per} = J_l$ is the flux of water due to permeability mechanisms, Φ_{con} is the flux of water due to convection, $\partial w_s/\partial t$ is the moisture consumption due to cement hydration called self-desiccation, and q is a term that accounts for other phenomena influencing the moisture transport, like gravity or cracking.

The flux of water due to convection, Φ_{con} , associated with mechanism V, and the term that accounts for other phenomena in the moisture transport, q , can be dismissed [87, 88]. Thus, Equation (2.48) can be rewritten as:

$$\frac{\partial w}{\partial t} = -\nabla(\Phi_{dif} + \Phi_{per}) - \frac{\partial w_s}{\partial t} \quad (2.49)$$

The flux of water due to the diffusion mechanism Φ_{dif} is given by Fick's law, and the flux of water due to the permeability mechanism Φ_{per} is given by Darcy's law for a non-saturated medium. More straightforwardly, the moisture transport may be rewritten in a combined manner where the diffusion and permeability mechanisms are accounted for together by the diffusion coefficient $D(w)$ (moisture coefficient would be a better description of the variable since it includes both permeability and diffusion mechanisms, which are hard to separate in concrete drying; however, the nomenclature presented in the literature is kept unchanged to compare the formulation with previous works):

$$\frac{\partial w}{\partial t} = -\nabla \cdot (D(w)\nabla w) - \frac{\partial w_s}{\partial t} \quad (2.50)$$

Equation (2.50) can be formulated in order to the relative humidity as follows:

$$\frac{\partial w}{\partial h} \frac{\partial h}{\partial t} = \nabla \cdot (D(h)\nabla h) + \frac{\partial h_s}{\partial t} \quad (2.51)$$

where $D(h)$ is the diffusion coefficient $D(w)$ in order to relative humidity and $\partial h_s/\partial t$ is the relative humidity drop due to cement hydration (self-desiccation).

Considering the permeability (Darcy's law) and the diffusion (Fick's law) processes, the diffusion coefficient equation is therefore given by:

$$D(h) = (D_{per} + D_{dif}) = \left(\frac{k_{r,l} K_0 \rho_l^2 R T_0}{n_l M_w h} + -\varphi \tau [1 - S_l] \frac{M_w D_0 p_{sat}}{R T_0} \right) \quad (2.52)$$

where D_{dif} is the coefficient relative to the diffusion of water vapour, D_{per} is the coefficient relative to the permeability, $S_l = V_l/(V_a + V_l)$ is the saturation degree.

Equation (2.52) establishes the diffusion coefficient based on the perception of the microstructure of concrete, which implies the quantification of the porosity n_p and tortuosity τ . These variables are not easily quantified. Therefore, straightforward models based on experimental calibration of the diffusion processes have been proposed in the literature.

Bazant and Najjar [89] proposed a non-linear equation to simulate the diffusion processes in concrete pores:

$$D(h) = D_1 \left(\alpha_0 + \frac{1 - \alpha_0}{1 + \left(\frac{1 - h}{1 - h_c} \right)^{n_h}} \right) \quad (2.53)$$

where $\alpha_0 = D_0/D_1$, D_1 is the maximum diffusion, D_0 is the lower bound for the diffusion parameter, h_c is the relative humidity corresponding to $D = 0.5(D_1 + D_0)$, n_h is a material parameter which may vary between 2 and 15.

The fib [50] suggests the use of $\alpha_0 = 0.05$, $h_c = 0.80$, $n_h = 15$ and the maximum diffusion coefficient D_1 to be estimated as:

$$D_1 = \frac{D_{1,o}}{f_{cm} - 8} \quad (2.54)$$

where $D_{1,o} = 1 \times 10^{-8} \text{ [m}^2/\text{s]}$ and f_{cm} is the mean compressive strength in MPa.

Wang [90] proposed a relationship between the maximum diffusion and the porosity as:

$$D_1 = \frac{D_{1,o}}{A_1 \cdot \exp(A_2 \cdot \varphi^{cap})} \quad (2.55)$$

where $D_{1,o} = 3.9 \times 10^{-6} \text{ m}^2/\text{h}$, $A_1 = 14.5$ and $A_2 = 4.66$ are model parameters and φ^{cap} is the capillary porosity of binder paste in concrete, which can be determined as:

$$\varphi^{cap} = \frac{W_0 - 0.4 \cdot C_0 \cdot \alpha + 0.0625 \cdot C_0 \cdot \alpha}{W_0/\rho_w + C_0/\rho_c} \quad (2.56)$$

where W_0 and C_0 are model parameters and α is the degree of hydration.

Azenha et al. [91] calibrated numerically a hygral model considering the reciprocal moisture capacity, $[\partial w / \partial h]^{-1}$, in the diffusion coefficient $D_h^*(h) = [\partial w / \partial h]^{-1} D_h(h)$.

Another model for the description of the experimental diffusion of moisture in concrete has been proposed by Xi et al. [92]:

$$D(h) = \alpha_h + \beta_h \left(1 - 2^{-10^{\gamma_h(h-1)}}\right) = \alpha_h + \beta_h \left(1 - \exp(-\ln(2) \cdot 10^{\gamma_h(h-1)})\right) \quad (2.57)$$

where α_h , β_h and γ_h are coefficients to be calibrated from test data.

In addition, Xi et al. [92] proposed formulations to estimate the diffusion coefficient based on the water-to-cement ratio:

$$\alpha_h = 1.05 - 3.8 w/c + 3.56 (w/c)^2 \quad (2.58a)$$

$$\beta_h = -14.4 + 50.4 w/c - 41.8 (w/c)^2 \quad (2.58b)$$

$$\gamma_h = 31.3 - 136 w/c + 162 (w/c)^2 \quad (2.58c)$$

The maximum diffusion coefficient in this model is given by $D_1 = \alpha_h + 0.5 \beta_h$.

Fig. 12 shows a comparison between the Bažant and Najjar [89] and Xi et al. [92] diffusion coefficients normalised to the maximum diffusion coefficient D_1 .

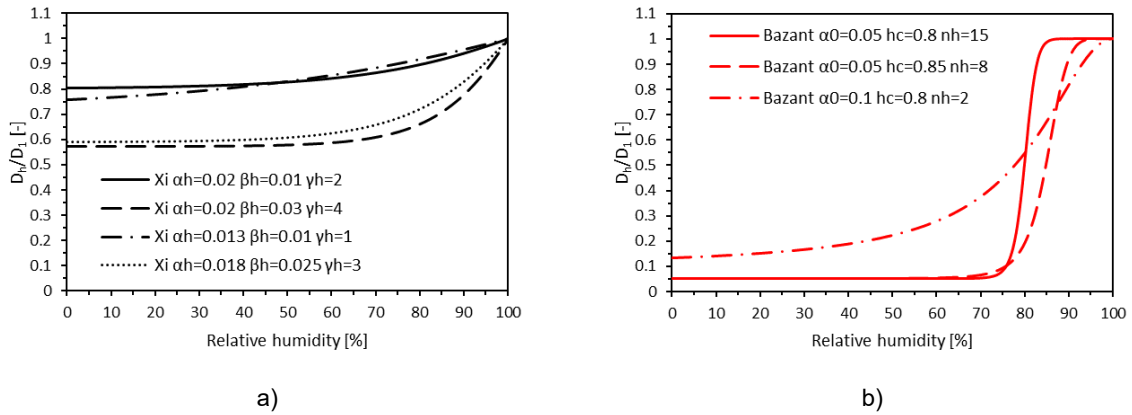


Fig. 12 – Comparison between the different approaches for the diffusion coefficient: a) for the equation of Xi et al. [92]; b) for the equation of Bažant and Najjar [89].

Fig. 12a) presents the diffusion coefficient for commonly used parameters in the equations of Xi et al. [92]. It is observed that the equation provides a soft drop in the diffusion coefficient and, for low relative humidity, the diffusion coefficient is kept above 50% of the maximum diffusion coefficient. Fig. 12 b) presents the diffusion coefficient for commonly used parameters in the equation of Bažant and Najjar [89]. This approach has a considerable drop in the diffusion coefficient after a specific relative humidity. The n_h parameter governs the change in the diffusion gradient, where the lower the n_h value the smoother is the decrease of the diffusion coefficient. For lower relative humidities values, this model presents a residual value of the diffusion coefficient which is delimited by the parameter α_0 .

Alternative models for moisture transport based on different gradients can be found in the literature. Hagentoft et al. [93] proposed a model based on the gradient of the water vapour pressure p_v and on the capillary pressure p_c . Moonen [94] proposed a model based on the gradients of the state variables, the liquid pressure p_l , the gas pressure p_g and the water vapour pressure p_v . Coussy [58] proposed a model based on the gradient of the liquid pressure p_l , gas pressure p_g and the relation between the water vapour pressure and gas pressure (p_v/p_g). Meftah et al. [95] proposed a model for mass transfer processes in the porous medium based on the state variables of capillary pressure p_c and gas pressure p_g . Other models can be found in the literature [65].

2.2.5 BOUNDARY CONDITIONS

The boundary conditions must be formulated to govern the moisture transfer between the exposed surfaces of the concrete element and the surrounding environment. The boundary conditions can be defined by a normal outward flux of water $\mathbf{j}_w \cdot \mathbf{n}$ dependent on the difference between the pressure of water vapour in concrete and the pressure of the environment [65]:

$$\mathbf{j}_w \cdot \mathbf{n} = B_v(p_v - p_{v,env}) \quad (2.59)$$

where $\mathbf{n}$ is the outward unit vector normal to the boundary surface, B_v is the surface vapour transfer coefficient which depends on the movement of air, illumination or partial insulation. Künzle [96] proposed typical values for the B_v in the range between 75×10^{-9} s/m for outdoor conditions and 25×10^{-9} s/m for indoor conditions.

Equation (2.59) can be rewritten depending on the relative humidity as [65]:

$$\mathbf{j}_w \cdot \mathbf{n} = \eta_e(\ln h - \ln h_{env}) \quad (2.60)$$

where η_e is the surface emissivity [kg/m²s], which is equal to the surface vapour transfer coefficient B_v multiplied by the saturated vapour pressure p_v .

Equation (2.60) can be rewritten as a proportional jump in the relative humidity:

$$\mathbf{j}_w \cdot \mathbf{n} = \eta_e^*(h - h_{env}) \quad (2.61)$$

where η_e^* is the adjusted surface emissivity coefficient that should be dependent on the relative humidity of the environment and the relative humidity of the concrete surface:

$$\eta_e^* = \frac{\eta_e \cdot (\ln h - \ln h_{env})}{(h - h_{env})} \quad (2.62)$$

Fig. 13 shows the relation between the adjusted surface emissivity and the surface emissivity coefficient.

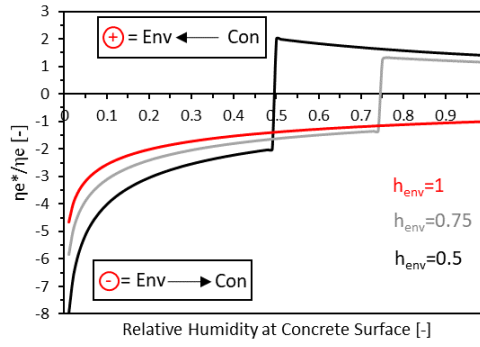


Fig. 13 – Adjusted surface emissivity coefficient for the boundary conditions. Positive: flux between concrete and the environment (drying), Negative: flux between the environment and concrete (wetting)

The positive flux means drying, corresponding to moisture transference from concrete (Con) to the environment (Env). In contrast, the negative flux means wetting, corresponding to moisture transference from the environment (Env) to concrete (Con). It is possible to observe that the adjusted surface emissivity coefficient decreases with the increase in the environment's relative humidity. Additionally, the variation depending on the relative humidity of concrete is non-linear and slowly increases with the decrease of the environment's relative humidity. For the environment's relative humidity of 0.5, the adjusted emissivity coefficient varies between $1.39\eta_e$ at full saturation to $2\eta_e$ at the concrete surface relative humidity of 0.5.

2.2.6 EFFECT OF CRACKING ON MOISTURE TRANSPORT

Cracks are often observed in reinforced concrete structures. Concrete cracks can provide additional surface exposure to ambient air, enhancing the moisture transfer in the directions parallel to the cracks. Bazant and Raftshol [97] proposed an equation to estimate the increment of diffusivity due to cracking, assuming a viscous laminar flow of air with water vapour:

$$\Delta D_w = \alpha_w \frac{\rho_v \cdot p_{sat} \cdot [\partial \phi(h) / \partial h]^{-1}}{12\eta_v} \times \frac{w_{cr}^3}{s} \quad (2.63)$$

where α_w is a coefficient that considers the orientation of the cracks and can be taken as $\alpha_w = 1$ if the cracks are perfectly planar, η_v is the viscosity of the water vapour, w_{cr} is the crack width and s is the spacing of cracks.

Equation (2.63) should be seen as an increment of diffusivity based on the average moisture transport in a control region within the crack depth and not as a local property at the crack location. The obtained value should be added as a contribution to the maximum diffusivity $D_1^* = D_1 + \Delta D_w$. Bazant et al. [98] experimentally validated Equation (2.63) through drying tests in C-shaped beams.

Fig. 14 shows a comparison between the increase of diffusivity given by Equation (2.63) and the diffusivity $D_{1,0}$ presented in Equation (2.54) for different crack width and crack spacing values. In this analysis, it was considered $\alpha_w = 1$ (perfectly planar smooth cracks, which represents the worst

scenario), $\rho_v(RH = 75\%) = 0.013 \text{ kg/m}^3$, $\eta_v = 1.8 \times 10^{-5} \text{ Pa/s}$, $p_{sat} = 2338 \text{ Pa}$ and $[\partial\phi(h)/\partial h]^{-1} = 9 \times 10^{-3} \text{ m}^3/\text{kg}$.

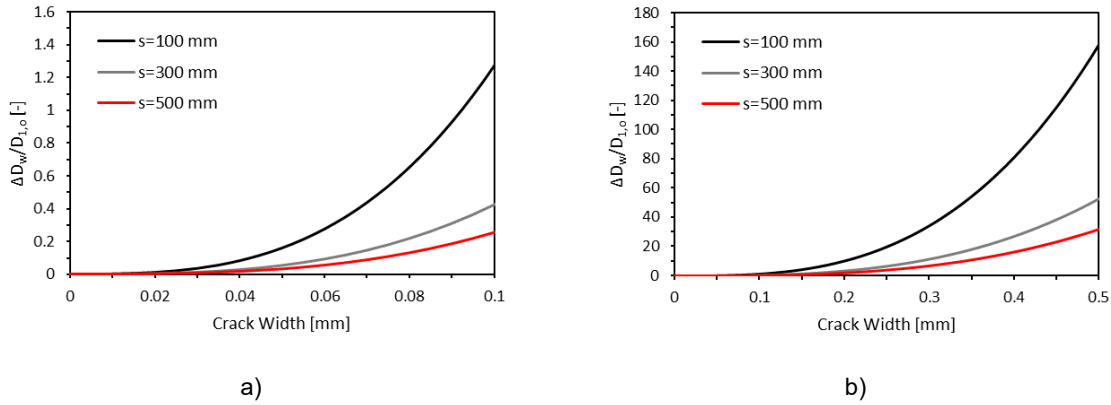


Fig. 14 – Comparison of diffusivity increment and initial diffusivity for different crack widths and spacing values: a) for crack width values below 0.1 mm; b) for crack width values below 0.5 mm.

Increased cracking density and crack widths lead to a substantial rise in moisture diffusivity. For example, for a crack width of 0.1 mm and a spacing between cracks of 300 mm, in the worst scenario, the diffusivity coefficient boosts up by an additional $\approx 0.4(f_{cm} - 8)$ times the initial maximum diffusivity. The effect increases for larger cracks, as shown in Fig. 14 b).

2.2.7 MOISTURE EFFECT IN THE CEMENT HYDRATION EVOLUTION

The cement hydration is dependent on the available water content. Hence, it is predictable that moisture transport will affect the hydration rate. Powers [99] was the first to notice that the cement hydration will practically stop at a relative humidity below 80%. Jensen et al. [22] investigated the hydration of cement clinker minerals at reduced relative humidity and performed a thermodynamic analysis of the effect of self-desiccation [100]. They estimated the hydration of anhydrous cement minerals exposed to water vapour at 20 °C to halt for relative humidity values of 85%, 90% and 60% for C_3S , C_2S and C_3A respectively. Mullin [101] investigated the crystallisation processes' velocity and identified the nucleation-controlled induction period's duration for different temperatures and relative humidity values. They concluded that the induction period of nucleation would exponentially increase with the decrease of saturation and decrease with the temperature increase. Flatt et al. [31] showed that the cement hydration of the alite mineral would stop for relative humidity below 80% due to the change in water activity. Wyrzykowski and Lura [102] confirmed this statement by investigating the effect of relative humidity decrease due to self-desiccation in hydration. They proposed a multiplication factor to the rate of hydration given by:

$$\beta_{RH}(RH) = \min\left(1; 3.7 \times \left(\frac{RH}{100}\right)^{25}\right) \quad (2.64)$$

Bažant [103] proposed replacing the concrete age in the hydration or any dependent models, like strength evolution, basic creep or self-desiccation, with the equivalent age, which considers the effect of temperature and relative humidity in concrete.

$$\frac{dt_e}{dt} = \beta_{eT}(T) \cdot \beta_{eh}(h) \quad (2.65)$$

where $\beta_{eT}(T)$ is a parameter that takes into account the temperature evolution and $\beta_{eh}(h)$ is a parameter that takes into account the effect of relative humidity and is given by:

$$\beta_{eh}(h) = \frac{1}{1 + [\alpha_e(1 - h)]^4} \quad (2.66)$$

where h is the relative humidity and α_e is a model parameter that, in the absence of experimental data, can be considered equal to 10. Lacarrière et al. [104] proposed to consider the term $\alpha_e = 5$ in β_{eh} instead of $\alpha_e = 10$. Such an approach leads to an extension of the cement hydration beyond relative humidity values below 80% at a slower pace (instead of stopping), which may be more accurate for modern concretes with special admixtures, such as silica fume, where the cement hydration may continue until relative humidity values of 60% [67].

Rahimi-Aghdam et al. [24] proposed a model where hydration is governed by the diffusion of water from capillary pores through the barrier shell toward the interface with anhydrous cement. To evaluate the effect of relative humidity drop on hydration, they considered a multiplication factor to the rate of hydration, f_0 , based on the diffusion model of Bažant and Najjar [85]:

$$f_0 = c_f + \frac{1 - c_f}{1 + \left(\frac{1 - h}{1 - h^*}\right)^{n_h}} \quad (2.67)$$

where c_f , h^* and n_h are model parameters that can be taken as 0, 0.88 and 8, respectively.

Fig. 17 shows a comparison between Equation (2.64) – Wyrzykowski and Lura, Equation (2.66) - Bažant and Equation (2.67) – Rahimi-Aghdam, et al.

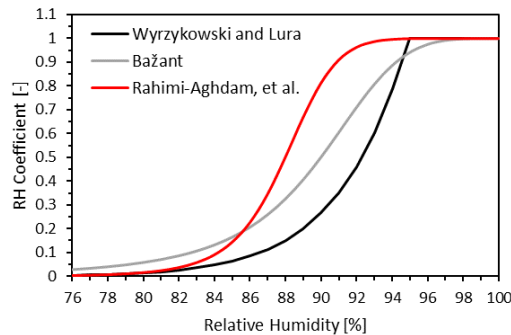


Fig. 15 – Effect of relative humidity coefficient on the cement hydration rate.

The effect of the relative humidity in the range of 80% to 94% varies in these different models. However, all the equations show that the cement hydration can be considered to practically cease after the relative

humidity drops below 80%. The best curing conditions are also verified for relative humidity values in the concrete pores above 94%.

2.3 SHRINKAGE

In the absence of load, concrete elements sustain volume variations due to physical phenomena related to cement hydration and drying. This volume decrease is called *shrinkage* (note that the hydration of a concrete element in water immersion leads to a swelling effect, but this does not occur under foggy conditions). Generally, the code-based approaches [50, 51, 105, 106] consider shrinkage as the average cross-section deformation, while morphological aspects and moisture transport are simplified through empirical parameters. The shrinkage that occurs without internal restraint is defined as free shrinkage. The free shrinkage can be directly related to the moisture content. Therefore, the free shrinkage varies in the depth of the concrete element and differs from the average shrinkage. Fig. 16 shows the comparison between shrinkage and free shrinkage.

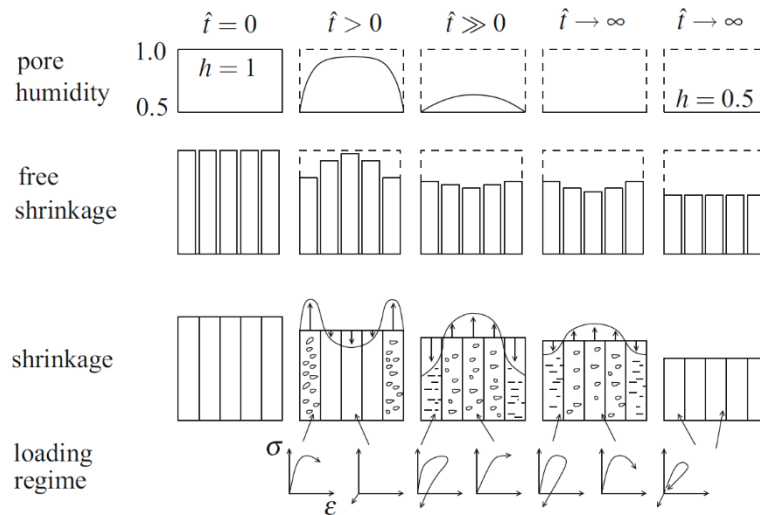


Fig. 16 – Evolution of the pore relative humidity, free shrinkage and shrinkage (adapted from [107]).

Theoretically, the free shrinkage will be hard to quantify once drying profiles generally occur in most concrete elements, and only shrinkage is accessible through experimental measurements. Nevertheless, reasonable estimations are obtained when considering small-sized specimens.

Different sources of shrinkage in cement-based materials have been identified in the literature:

- chemical shrinkage quantifies the shrinkage due to the chemical reactions during cement hydration. Due to the microstructure stresses generated in the porous medium during hydration, chemical shrinkage can only be measured in a fully saturated cement paste without the generation of a solid microstructure;
- autogenous shrinkage is the part of shrinkage that occurs in concrete elements due to the chemical reactions owing to cement hydration in the absence of moisture transfer. The autogenous shrinkage is smaller than the chemical shrinkage as a result of the internal restraint in the solid skeleton of concrete;

- plastic shrinkage is the superficial shrinkage generated by water loss in freshly poured concrete due to rapid moisture evaporation before hardening;
- drying shrinkage is the shrinkage that occurs due to moisture transport in the capillary pores.

The main shrinkage mechanisms responsible for mechanical stresses and deformations in hardened concrete are autogenous and drying shrinkage. Autogenous shrinkage occurs during cement hydration and is commonly pronounced in concretes with lower water-to-cement ratios. In contrast, drying shrinkage is pronounced in concretes with higher water-to-cement ratios and depends on moisture transport, which can last for decades.

2.3.1 BASIC SHRINKAGE AND SELF-DESICCATION

The volume of cement hydration products is smaller than the original volume of cement and reacted water [23, 108]. In concrete elements, this phenomenon results in the so-called autogenous shrinkage. Generally, autogenous shrinkage is characterised by the volume decrease in a concrete element under sealed conditions. Even in the absence of drying, the chemical reactions consume water. The moisture content drop due to hydration is called self-desiccation. Therefore, some authors considered that autogenous shrinkage depends not only on the chemical reactions but also on the moisture drop in the capillary pores, like the drying shrinkage, and should be considered in a unified manner and not in an additive way [65]. Despite the global decrease in volume, the solid volume of the concrete skeleton increases, which explains the swelling effect of elements immersed in water. Fig. 17 shows the volume change due to the hydration of a single cement grain.

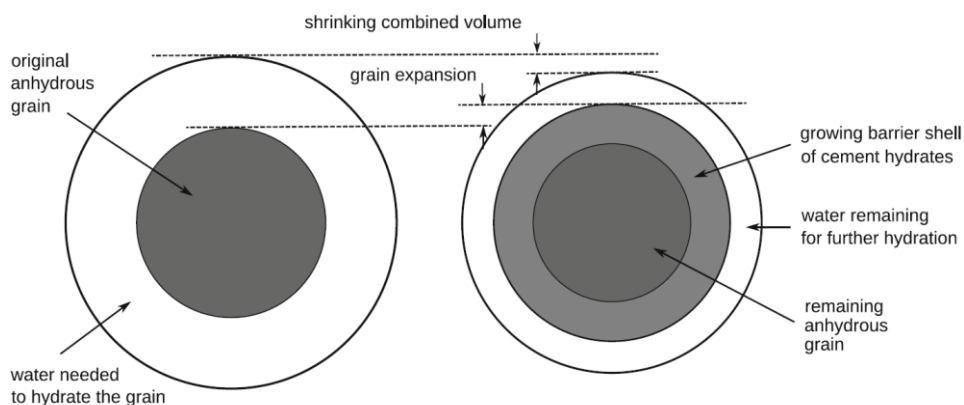


Fig. 17 - On the left, the anhydrous cement grain is surrounded by the exact amount of water required for full hydration; on the right, the hydration process of the cement grain (adapted from [65]).

Acker and Ulm [109] reported that the stresses generated by the full restraint of the autogenous shrinkage rapidly reach values equal to the material's tensile strength. Several models for autogenous shrinkage have been proposed in the literature [50, 51, 105, 106, 110]. The MC2010 [50] introduced the basic shrinkage, which represents the shrinkage occurring without moisture loss (it should be “moisture transfer” or “moisture loss to the environment” since hydration leads to moisture loss, but the source definition is kept) and can be considered equal to the autogenous shrinkage in sealed specimens. The basic shrinkage is given by:

$$\varepsilon_{cbs}(t) = \varepsilon_{cbs0} \cdot [1 - \exp(-0.2 \cdot \sqrt{t})] \quad (2.68)$$

where ε_{cbs} is the basic shrinkage and

$$\varepsilon_{cbs0} = -\alpha_{bs} \cdot \left(\frac{0.1 \cdot f_{cm}}{6 + 0.1 \cdot f_{cm}} \right)^{2.5} \cdot 10^{-6} \quad (2.69)$$

where α_{bs} is a coefficient dependent on the type of cement and f_{cm} is the mean compressive strength at 28 days in [MPa].

The self-desiccation $h_s(h)$ presented in Equation (2.51) can be calculated based on the amount of water consumed during hydration [65]:

$$h_s(h) = - \left[\frac{\partial \phi(h)}{\partial h} \right]^{-1} \left(\frac{\partial \phi(h)}{\partial t} + \frac{dw_n(t)}{dt} \right) \quad (2.70)$$

where w_n is the chemically bonded water, and $\partial \phi(h, t)/\partial t$ is water supplied. If the water supplied is null or smaller than the rate of chemically bonded water during hydration $dw_n(t)/dt$, self-desiccation will take place.

Rahimi-Aghdam et al. [111] proposed a model to calculate self-desiccation based on the total volume of water consumed as the sum of the water consumed by the hydration of the different minerals. Such a model requires integration with a sophisticated cement hydration model. Additionally, based on the experimental results obtained by Bentz [112], they proposed a simplified equation for self-desiccation where the main variable is the degree of hydration:

$$h_s = h_s^f \left(\frac{\alpha - \alpha_{set}}{\alpha_u - \alpha_{set}} \right)^{n_{wc}} \quad (2.71)$$

with:

$$n_{wc} = 25(w/c - 0.1) \quad (2.72a)$$

$$h_s^f = 0.5(w/c)^{-0.26} - 0.53 \quad (2.72b)$$

$$\alpha_u = 0.46 + 0.95(w/c - 0.17)^{0.6} < 1 \quad (2.72c)$$

Zhao et al. [113] proposed a model for water loss rate during hydration $\dot{w}_n$ based on the rate of variation of density of liquid water ρ_l , saturation S_l , and porosity φ :

$$\frac{\partial w_n}{\partial t} = \varphi S_{l,0} \frac{\partial \rho_l}{\partial t} + \rho_l \left(\varphi \frac{\partial S_l}{\partial t} + S_0 \frac{\partial n_p}{\partial t} \right) \quad (2.73)$$

The hydration mechanism is driven only by liquid water. Since the variation of the density of liquid water due to temperature changes is almost negligible, the first term of the right-hand side of Equation (2.73) can be neglected, and only the second term needs to be developed. This equation shows an

alternative approach where the previous term of chemically bonded water is substituted by porosity evolution in concrete. The previous approaches share the same theoretical background since the chemically bonded water and concrete porosity depend on cement hydration.

2.3.2 DRYING SHRINKAGE

The drying shrinkage is related to the loss of water in the capillary pores of concrete due to moisture transport. Granger [114] proposed the following relationship between free shrinkage and moisture loss:

$$\varepsilon_{sh} = k_{sh} \dot{w} \quad (2.74)$$

where k_{sh} is the shrinkage coefficient that relates the shrinkage to moisture loss.

Bissonnette et al. [115] investigated key parameters influencing drying shrinkage, i.e., the environment's relative humidity, specimen size, water/cement ratio and paste volume. Fig. 18 shows the relationship between shrinkage and weight loss for cement paste (P), mortar (M) and concrete (C). The first number indicates the water-to-cement ratio, while the second refers to the mixture number for mortar specimens and the paste volume fraction for concrete specimens.

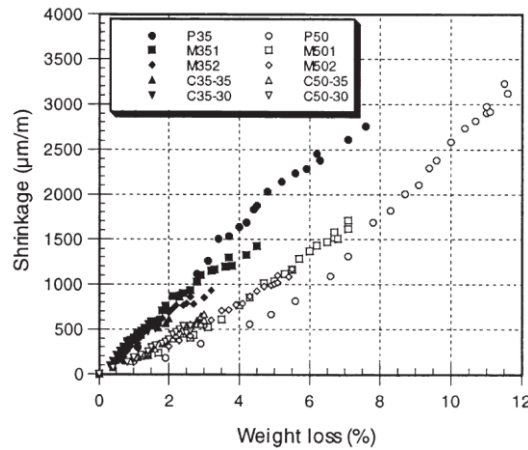


Fig. 18 – Relation between shrinkage and weight loss (adapted from [115])

The shrinkage and weight loss relationship may differ for cement paste, mortar and concrete. However, this relationship seems almost linear and independent of the environment's relative humidity [115, 116]. Therefore, for the considered ordinary concrete mixtures, the coefficient k_{sh} in Equation (2.74) can be assumed constant.

Rewriting Equation (2.74) in order to the relative humidity, one obtains:

$$\varepsilon_{sh} = k_{sh}^* \dot{h} \quad (2.75)$$

where $k_{sh}^* = [\partial w / \partial h] \cdot k_{sh}$. In the particular case that a linear desorption behaviour is assumed ($\partial w / \partial h = \text{const}$) and $k_{sh} = \text{const}$, then k_{sh}^* can be considered constant.

Van Zijl [117] proposed a constant, linear or parabolic equation for the coefficient that relates shrinkage with relative humidity based on the experimental results of Alvaredo [118]. In this formulation, the parameter k_{sh}^* in Equation (2.75) can be determined assuming one of the three approaches:

$$k_{sh}^{*(van\ Zijl)}(h) = \begin{cases} \frac{\varepsilon_s^\infty}{H_{env} - H_0} & \text{for constant behaviour} \\ \left(\frac{2 \cdot \varepsilon_s^\infty}{H_{env}^2 - H_0^2} \right) \cdot h & \text{for linear behaviour} \\ \left(\frac{3 \cdot \varepsilon_s^\infty}{H_{env}^3 - H_0^3} \right) \cdot h^2 & \text{for parabolic behaviour} \end{cases} \quad (2.76)$$

where ε_s^∞ is the final volumetric shrinkage strain, H_{env} is the environment's relative humidity and H_0 is the initial internal relative humidity of the sample. Van Zijl [117] found that the parabolic behaviour in Equation (2.76) is more suitable for the numerical representation of the experimental data of Alvaredo [118]. Idiart [119] reformulated Equation (2.76) for moisture loss.

Yuan and Wan [120] proposed a model for drying shrinkage based on the mechanisms associated with the evolution of the capillary pressure. The approach is based on the stress state of the solid skeleton $\sigma_{sk} = p_c \cdot A_{sk}$ and assumes a linear relation between strain and stresses based in the Hooke's law:

$$\varepsilon_{sh} = \frac{\sigma_{sk}}{E_{s,c}} = \frac{p_c \cdot A_{sk}}{E_{s,c}} \quad (2.77)$$

where A_{sk} is the representative area, which is expressed as the volume of liquid water per volume of concrete and $E_{s,c}$ is the elastic modulus for the capillary pressure. The capillary pressure is linked to the relative humidity by Equation (2.26).

Han and Lytton [121] proposed a similar expression to the shrinkage evolution based on the integration of the law proposed by Powers [122].

$$\varepsilon_{sh} = b \ln \left(1 + \frac{p_c}{a} \right) \quad (2.78)$$

where b and a are two empirical constants.

Kwak et al. [123] proposed a new model that relates the drying shrinkage to the local relative humidity through a cubic power relation:

$$\varepsilon_{sh} = \varepsilon_{sh,ult} \cdot [0.97 - 1.895 \cdot (h - 0.2)^3] \quad (2.79)$$

where $\varepsilon_{sh,ult}$ is the shrinkage upon total (or almost total) drying.

Rahimi-Aghdam et al. [124] proposed a model for the relationship between relative humidity and drying shrinkage considering the evolution of the microstructure of concrete through the degree of hydration concept:

$$\dot{\epsilon}_{sh} = \frac{\alpha_{max} - \alpha_i}{\alpha - \alpha_i} k_{sh}^* \dot{h} \quad (2.80)$$

where α_{max} is the ultimate degree of hydration in sealed conditions and $\alpha_i = 0.9\alpha_{set}$, is a model parameter referring to the initial degree of hydration and α_{set} is the degree of hydration at setting time.

In this model, the autogenous shrinkage is combined with the drying shrinkage since the authors assume both shrinkage components are driven by the capillary moisture drop. The degree of hydration function, $f_\alpha = \frac{\alpha_u - \alpha_i}{\alpha - \alpha_i}$, allows accounting for the effect of microstructure evolution in the shrinkage coefficient.

2.4 CONCRETE CREEP

Under constant load, a concrete element sustains increasing deformation over time. This phenomenon is called creep and is associated with the viscoelastic behaviour of cement gel [65]. Creep may be affected by the loading age and intensity, concrete composition, environmental conditions and geometry of the concrete element. Accurately predicting concrete creep is fundamental for assessing a concrete structure's long-term serviceability, including deflections, prestress loss, or stress relaxation. Several models are available in the literature. The design codes like Eurocode 2 [51] (EC2), fib Model Code 2010 [50] (MC2010), the ACI 209 [105] and the JSCE [125] allow calculating the creep coefficient based on the composition, strength class and environmental conditions. These models are based on a macroscopic interpretation of the creep phenomena and assume an average deformation of the cross-section of the concrete element. The models suggest empirical formulations to determine the creep coefficient. The models were developed under the guidance of scientific committees. This process involved synthesising information from technical bulletins, pre-existing models, and comprehensive databases of creep data. Specific research on creep that influenced these models includes the works of Rüsche et al. [126] and Müller et al. [127] for EC2 and MC2010, ACI SP-27 [128] and ACI 209R-92 [129] and Pauw [130] for ACI 209, and Nagataki and Yonekura [131] and Sakata et al. [132] for the JSCE.

Academic models like model B3 [2], model B4 [133], GL2000[134] and SAK [135] provide the creep curves considering the different mechanisms of creep. These models are calibrated from a large amount of creep data (similar to the design code models) but are usually more sophisticated than design code models. Other models have been employed to simulate creep based on experimental data calibration. It is the case of the Double power law [136], which is used to simulate creep for assessing the early-age behaviour of mass structures.

Benboudjema [87] proposed a model for biaxial solicitations based on the decomposition of the stress tensor into hydrostatic and deviatoric stresses. Aili et al. [137] proposed a model to consider the viscoelastic and eigenstrains (mechanical deformations not caused by external mechanical stress) in a unified manner based on the poromechanical behaviour of concrete.

Several THM material models have been used to simulate thermal and hygral strains [65, 117, 123, 138] and creep strains associated with ageing, drying creep and transitional thermal creep [34, 65, 109, 139-

144]. Some creep models employed in pointwise modelling approaches are the microprestress solidification theory (MPS), initially published by Bažant et al. [145], [146] and improved by Rahimi-Aghdam et al. [124], Jirásek and Havlásek [147], Yu et al. [148], and the Burger concrete model [87, 149-152].

2.4.1 CONCEPTS AND MECHANISMS

In the absence of moisture transport, the lower the evaporable water content of the sample, the lower the creep. Creep strains can even become negligible in pre-dried specimens [109]. However, creep tests performed in a drying environment result in higher creep strains, which can scale up to five times more than in sealed specimens [153]. Overall, the concrete creep is divided into the sum of two parcels:

- basic creep, which consists of the creep strains under sealed conditions;
- drying creep, which consists of the additional creep strains (compared to basic creep strains) observed under drying conditions. These additional creep strains are also referred to as the Pickett effect.

The basic and drying creep strains are commonly considered cumulative. Fig. 19 shows the total deformation of a drying specimen with the identification of the source of creep.

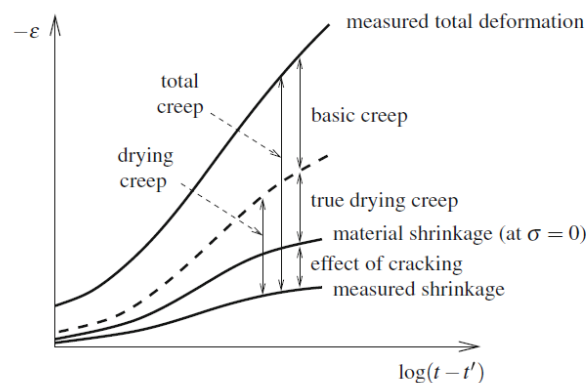


Fig. 19 – Different sources of creep (adapted from [65]).

Different mechanisms for explaining creep have been presented and discussed in the literature [34, 109, 139-144]. Three phenomena are linked with concrete creep [65]:

- 1) the ageing of concrete, which is associated with the decrease of the creep compliance observed for different loading ages. Two mechanisms can explain this:
 - a) *short-term chemical ageing*, which is interpreted as a growth of the volume fraction of solidifying constituents;
 - b) *long-term nonchemical ageing*, which is evidenced by the decrease of creep compliance with the loading age even for many years and probably many decades after the hydration ceased.

- 2) the drying creep effect, which is a transient effect resulting from the fact that the apparent creep during drying is much larger than the basic creep. The source of this phenomenon may be associated with two different mechanisms:
 - a) *apparent macroscopic mechanism* arising from the impossibility of measuring the free shrinkage. This mechanism is associated with the effect of microcracking (see Fig. 16) owing to non-linear moisture distribution, which vanishes or decreases in compressive creep tests (Fig. 19);
 - b) *true nanoscale mechanism*, which is explained by the hypothesis that the rate of shear (slip) due to breakages and restoration of bonds in the C-S-H is influenced by the magnitude of the microprestress acting in the slip planes and controlled by changes in the chemical potential of pore water due to drying.
- 3) The transitional thermal creep, which represents a transient increase of creep due to temperature variations. This phenomenon is also explained by two mechanisms similar to the drying creep effect:
 - a) *apparent macroscopic mechanism*, due to thermally induced microcracking owing to non-linear temperature profiles;
 - b) *true nanoscale mechanism*, due to a change in the level of microprestress caused by a thermally induced change in the nanopores' moisture content.

Mechanisms 2 - a) and 3 - a) operate on the macroscopic scale of the whole specimen or structure (on the scale of centimetres to meters) and are simulated by adopting an adequate fracture model. Mechanism 1 - a) operates on the micrometre scale and is explained by the solidification theory. Mechanisms 1 - b), 2 - b) and 3 - b) operate on the nanometer scale and are explained by the microprestress-solidification theory [65].

2.4.2 BASIC CREEP

The ageing nature of basic creep is justified mainly by the chemical reactions occurring during hydration. The hydration products form the cement gel, which consists mainly of C-S-H and hindered water and is responsible for the viscoelastic behaviour associated with creep. In general, the volume of the hydration products and the volume of the solid load-bearing skeleton in the cement paste are increasing at the cost of diminishing the volume of evaporable water and anhydrous cement. Therefore, the ageing properties of basic creep must be associated with the volume growth of the cement gel, which serves as the basis for the solidification theory proposed by Bazant and Prasannan [154] presented below.

2.4.2.1 Solidification theory

2.4.2.1.1 Micromechanics-based creep model for solidifying material

In the solidification theory, the total strain of a concrete specimen under constant stress is expressed as:

$$\varepsilon = \frac{\sigma}{E_0} + \varepsilon_{creep} + \varepsilon_0, \quad \text{where } \varepsilon_{creep} = \varepsilon_v + \varepsilon_f \quad (2.81)$$

where σ is the stress, E_0 is the elastic modulus, ε_{creep} is the creep strain, ε_v is the viscoelastic strain, ε_f is the flow strain and ε_0 is the sum of the cracking strains and the hygrothermal strains, such as drying shrinkage, thermal dilatation and basic shrinkage. Fig. 20 shows an illustration of the present model.

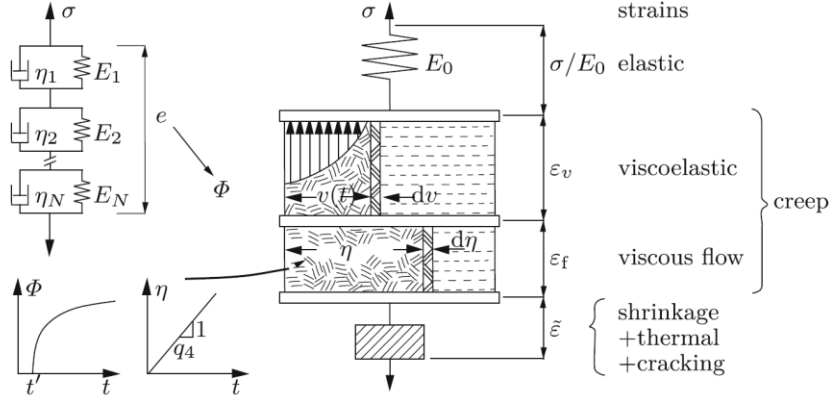


Fig. 20 – Model for solidification in creep (adapted from [154])

The elastic strain (σ/E_0) is a result of the deformation of the aggregates and the microscopic elastic particles in the hardened cement paste, including the anhydrous cement grains, the calcium hydroxide crystals and the crystalline particles (sheets and needles) in cement gel. Owing to their nature, the elastic properties of all those components are constant in time, and therefore, these components can be considered non-ageing. However, the elastic strain of concrete is generally dependent on the loading age ($\sigma/E(t)$), where the ageing elastic modulus $E(t)$ is a property dependent on the concrete age, t . In the solidification theory, the ageing elastic modulus $E(t)$ is divided into a constant elastic modulus E_0 , which is a material constant and should be defined as the *asymptotic elastic modulus* for an infinitesimal time after loading and a short-term creep that characterises the ageing dependency of the ageing elastic modulus.

The *viscoelastic strain* ε_v represents the microstrain to which the cement gel is subjected, and it is associated with the *solidified material volume*, $v(t)$. The ongoing cement hydration leads to the increase of the *relative volume of solidified material*, $dv(t)$, which gets attached to the previous volume $v(t)$. All the solidified material volume is subjected to the same strain increments. The macroscopic stress σ is the result of all the microstress endured by the solidified material volume. An increment of the viscoelastic strain $d\varepsilon_v(t')$ at the loading age t' , generates a microstress $\psi(t - t')d\varepsilon_v(t')$ at the time t , where $\psi(t - t')$ is the relaxation function of cement gel. The macroscopic stress is given by the combination of all the microstress:

$$\sigma(t) = \int_0^t v(t') \cdot \psi(t - t') d\varepsilon_v(t') \quad (2.82)$$

Owing to the ongoing increase of the solidified material volume, the viscoelastic strain ε_v , is only partially recoverable. Therefore, Bazant and Prasannan [154] proposed to consider the *effective*

viscoelastic strain, $e(t)$, which is the fully recovered strain after unloading. The effective viscoelastic strain ratio can be related to the viscoelastic rate through the solidified volume at a certain time, $\dot{e}(t) = v(t) \cdot \dot{\varepsilon}_v$. Replacing the viscoelastic strain with the effective viscoelastic strain and inverting the stress-strain relaxation of Equation (2.82), Bazant and Prasannan [154] obtained:

$$e(t) = \int_0^t \phi(t - t') d\sigma(t') \quad (2.83)$$

where $\phi(t - t')$ represents the non-ageing compliance function of the cement gel (inverse kernel of the relaxation function $\psi(t, t')$ [65]).

The strain-stress relationship within the linear regime is commonly described by the compliance function $J(t, t')$, which represents the creep strain caused by a unit of stress. The macroscopic compliance function associated with the viscoelastic behaviour of the cement gel $J_v(t, t')$ is given by the sum of the instantaneous compliance $J_v(t', t') = \phi(0)/v(t')$ and the viscoelastic compliance rate $\dot{J}_v(t, t') = \dot{\phi}(t - t')/v(t)$:

$$J_v(t, t') = J_v(t', t') + \int_{t'}^t \dot{J}_v(s, t') ds = \frac{\phi(0)}{v(t')} + \int_{t'}^t \frac{\dot{\phi}(s - t')}{v(s)} ds \quad (2.84)$$

Equation (2.84) links the microscopic with the macroscopic behaviour of the solidifying material. From the macroscopic point of view, viscoelastic compliance depends on the loading age t' and the concrete age t .

As shown in Equation (2.81), the viscoelastic strain $\varepsilon_v(t)$ is not enough to fully describe concrete basic creep and the flow strain $\varepsilon_f(t)$ must be included. The flow strain is considered the irreversible part of the creep strain, and it is modelled by a viscous dashpot. Therefore, the rate of flow $\dot{\varepsilon}_f(t)$ is given by:

$$\dot{\varepsilon}_f(t) = \frac{\sigma(t)}{\eta(t)} \quad (2.85)$$

where $\eta(t)$ is the viscosity modulus and should be considered an age-dependent parameter.

The flow compliance function $J_f(t, t')$ is given by integrating Equation (2.85) under the assumption of unit stress:

$$J_f(t, t') = \int_{t'}^t \frac{1}{\eta(s)} ds \quad (2.86)$$

Recalling Equation (2.81) and ignoring the term ε_0 , it is possible to establish the complete creep compliance $J(t, t')$ as:

$$J(t, t') = \frac{1}{E_0} + J_v(t, t') + J_f(t, t') \quad (2.87)$$

The first term of Equation (2.87) represents the instantaneous elastic strain, which is fully recoverable, while the viscoelastic strain $J_v(t, t')$ is partially recoverable and the flow strain $J_f(t, t')$ is unrecoverable.

2.4.2.1.2 Constitutive relationship

The creep model becomes complete with the characterisation of a constitutive relation for the non-ageing compliance function $\phi(t - t')$, the volume growth function $v(t)$ and the time-dependent flow viscosity $\eta(t)$. In this previous investigation, Bazănt [107] reproduced the basic creep curves using power curves $(t - t')^n$ for short load duration $(t - t')$ and logarithmic curves for long time durations, with a smooth transition between both curves. Since the $\ln(1 + x^n)$ is close to x^n for small values of x and close to $n \cdot \ln(x)$ for large values of x , Bazănt and Prasannan [154] proposed to consider the non-ageing compliance function as:

$$\phi(t - t') = q_3 \ln \left[1 + \left(\frac{t - t'}{\lambda_0} \right)^n \right] \quad (2.88)$$

where n , λ_0 , q_3 and q_4 are empirical material parameters.

Since the asymptotic elastic modulus E_0 is a non-ageing parameter, Equation (2.88) for no lag time should be equal to zero, $\phi(0) = 0$.

The inverse of the solidified material volume $v(t)$ can be described by a power-law function [155, 156]:

$$\frac{1}{v(t)} = 1 + \frac{1}{\alpha_v} \left(\frac{\lambda_0}{t} \right)^m \quad (2.89)$$

where m and α_v are empirical constants and $\lambda_0 = 1$ day.

Combining Equation (2.88) and Equation (2.89), the compliance function for the solidifying constituent is given by:

$$J_v(t, t') = q_3 \ln \left[1 + \left(\frac{t - t'}{\lambda_0} \right)^n \right] + q_2 Q(t, t'), \quad \text{where } q_2 = \frac{q_3}{\alpha_v} \quad (2.90)$$

where:

$$Q(t, t') = n \lambda_0^m \int_{t'}^t \frac{s^{-m}}{s - t' + \lambda_0^n (s - t')^{1-n}} ds \quad (2.91)$$

Equation (2.91) cannot be integrated in a closed form. An approximation solution is given by:

$$Q(t, t') \approx Q_f(t') \left[1 + \left(\frac{Q_f(t')}{Z(t, t')} \right)^{r(t')} \right]^{-1/r(t')} \quad (2.92)$$

where:

$$r(t') = 1.7 \cdot (t')^{0.12} + 8 \quad (2.93a)$$

$$Z(t, t') = (t')^{-m} \cdot \ln[1 + (t - t')^n] \quad (2.93b)$$

$$Q_f(t') = \left[0.086(t')^{\frac{2}{9}} + 1.21(t')^{\frac{4}{9}} \right]^{-1} \quad (2.93c)$$

Bazant and Baweja [2] proposed considering $m = 0.5$ and $n = 0.1$. Within the loading time range between $1 \leq t' \leq 10\,000$ days and the load duration time between $0.01 \leq t - t' \leq 10\,000$ days, the errors obtained from the use of the explicit approximation form for the calculation of $Q(t, t')$ are generally less than $\pm 0.5\%$ with a coefficient of variation of 0.2% . The final values Q_f (for $t \rightarrow \infty$) have errors less than $\pm 0.09\%$ with a coefficient of variation of 0.01% . Such accuracy usually is sufficient for good practice [154].

Considering the flow compliance function $J_f(t, t')$ and since $\int 1/\eta(t) dt \propto \ln(t)$ if $\eta(t) \propto t$, Bazant and Prasannan [154] proposed to determine the flow viscosity modulus $\eta(t)$ as:

$$\frac{1}{\eta(t)} = \frac{q_4}{t} \quad (2.94)$$

where q_4 is an empirical material parameter.

Combining Equation (2.94) and Equation (2.86), Bazant and Prasannan [154] obtained:

$$J_f(t, t') = \int_{t'}^t \frac{1}{\eta(s)} ds = q_4 \ln\left(\frac{t}{t'}\right) \quad (2.95)$$

Considering Equation (2.90), Equation (2.95) and a new empirical parameter $q_1 = 1/E_0$, the generalized form of the creep compliance $J(t, t')$ in equation (2.87) is given by:

$$J(t, t') = q_1 + q_2 Q(t, t') + q_3 \ln\left[1 + \frac{(t - t')^n}{\lambda_0}\right] + q_4 \ln\left(\frac{t}{t'}\right) \quad (2.96)$$

The empirical parameters q_2 , q_3 and q_4 presented in Equation (2.96) correspond to the nondimensionalized forms of ageing viscoelastic compliance, non-ageing viscoelastic compliance, and flow compliance, respectively. The dimensions of these empirical constants are $(\text{stress})^{-1}$. The dimension of the constant λ_0 is time, and it is generally assumed as $\lambda_0 = 1$ day.

2.4.2.1.3 Model B3 and Model B4 parameters

Model B3 and Model B4 propose equations based on concrete strength and composition to estimate the empirical parameters used in Equation (2.96) [2, 133, 157, 158]. Table 4 presents the mathematical formulation for calculating these empirical parameters.

Table 4 – Model B3 and Model B4 empirical parameter equations.

Model B3		Model B4	
$q_1 = \frac{0.6 \times 10^6}{E_{28}}$	(2.97a)	$q_1 = \frac{p_1}{E_{28}},$	(2.98a)
$q_2 = 185.4 \sqrt{c} f_{cm}^{-0.9}$	(2.97b)	$q_2 = \frac{p_2}{1 \text{ GPa}} \cdot \left(\frac{w/c}{0.38}\right)^{p_{2w}}$	(2.98b)
$q_3 = 0.29(w/c)^4 q_2$	(2.97c)	$q_3 = p_3 \cdot q_2 \cdot \left(\frac{a/c}{6}\right)^{p_{3a}} \left(\frac{w/c}{0.38}\right)^{p_{3w}}$	(2.98c)
$q_4 = 20.3(a/c)^{-0.7}$	(2.97d)	$q_4 = \frac{p_4}{1 \text{ GPa}} \left(\frac{a/c}{6}\right)^{p_{4a}} \left(\frac{w/c}{0.38}\right)^{p_{4w}}$	(2.98d)

Table 5 gives the parameters p_i , p_{ia} and p_{iw} used in model B4.

Table 5 – Creep parameters dependent on the cement type (model B4 [133]).

Parameter	R(Normal)	RS (Rapid Hardening)	SL (Slow Hardening)
p_1	0.70	0.60	0.80
p_2	58.6×10^{-3}	17.4×10^{-3}	40.5×10^{-3}
p_3	39.3×10^{-3}	39.3×10^{-3}	39.3×10^{-3}
p_4	3.4×10^{-3}	3.4×10^{-3}	3.4×10^{-3}
p_{2w}	3.00	3.00	3.00
p_{3a}	-1.10	-1.10	-1.10
p_{3w}	0.40	0.40	0.40
p_{4a}	-0.90	-0.90	-0.90
p_{4w}	2.45	2.45	2.45

Bažant and Baweja [2] proposed to calculate the ageing elastic modulus at 28 days as:

$$E_{28} = 4734 \sqrt{f_{cm}/\text{MPa}} \quad (2.99)$$

2.4.2.2 Burger mechanical model for basic creep

The Burger mechanical model was developed by the “*Électricité de France – Research and Development*” (EDF R&D) [87, 149, 150] and improved by Sellier and Buffo-Lacarrière [151]. The strain vector is decomposed into the sum of four components:

$$\boldsymbol{\varepsilon}^{to} = \boldsymbol{\varepsilon}^{el} + \boldsymbol{\varepsilon}^{sh} + \boldsymbol{\varepsilon}^{bc} + \boldsymbol{\varepsilon}^{dc} \quad (2.100)$$

where $\boldsymbol{\varepsilon}^{to}$ is the total strain, $\boldsymbol{\varepsilon}^{el}$ is the elastic strain, $\boldsymbol{\varepsilon}^{sh}$ is the shrinkage strain, $\boldsymbol{\varepsilon}^{bc}$ is the basic creep strain and $\boldsymbol{\varepsilon}^{dc}$ is the drying creep strain.

The stress-dependent strains are modelled in an element (called the Burger model) which divides the stress tensor into the sum of the deviatoric and hydrostatic stresses $\sigma = \sigma^d + \sigma^s I$, where σ^d are the deviatoric stresses and $\sigma^s = I_1/3 = \sigma_{kk}/3$ is the hydrostatic stress (or spheric stress), I_1 represents the first invariant of the stress tensor and σ_{kk} is the first invariant of stress tensors represented in the Einstein summation convention (implied summation over repeated indices i, j, k, l, m, n) $I_1 = \sigma_{kk} = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}$. Fig. 21 shows the rheological Burger model.

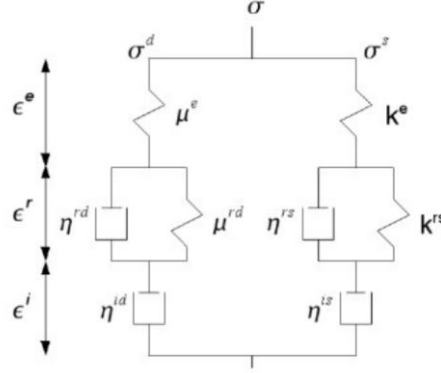


Fig. 21 - Rheological Burger model (adapted from [150])

Each chain part is divided into an elastic part, the reversible creep part (denoted by r) and the irreversible part (denoted by i). The elastic strain is given by the sum of the strain provided by the two spring elements, one for the deviatoric stresses σ^d and the other for the hydrostatic stress σ^s :

$$\varepsilon_{ij}^{el} = \varepsilon_s^{el} + \varepsilon_{d,ij}^{el} = \frac{1}{k^{el}} \delta_{ij} \frac{\sigma_{kk}}{3} + \frac{1}{2 \cdot u^{el}} \sigma'_{ij} = \frac{1}{k^{el}} \cdot \sigma^s + \frac{1}{2 \cdot u^{el}} \sigma^d \quad (2.101)$$

where ε_s^{el} is the elastic strain due to hydrostatic stress, $\varepsilon_{d,ij}^{el}$ is the elastic strain due to deviatoric stresses, $k^{el} = -E/(4\nu + 1)$ is the elastic bulk constant, $u^{el} = G = E/(2(\nu + 1))$ is the shear modulus, and $\sigma'_{ij} = \sigma_{ij} - 1/3 \cdot \delta_{ij} \cdot \sigma_{kk}$ are the deviatoric stresses [87]. Delamonte et al. [152] described the elastic strain due to hydrostatic stresses as $\varepsilon_s^{el} = p \cdot 1/(3k^{el})$, where p is “pressure”. This formulation leads to $k^{el} = E/(6\nu - 3)$ (note that authors consider p as pressure, which, strictly speaking, is an external force divided by a surface area. In constitutive models, the mechanical responses are governed by stresses, an internal material property. Therefore, p would be better described as the stress or internal material response to the pressure. Nevertheless, the authors’ original nomenclature is preserved for the present formulation).

The basic creep due to the hydrostatic stresses depends on the material's relative humidity. The reversible part is given by a Kelvin-Voigt element:

$$k^{rs} \cdot \varepsilon^{bc,rs} + \eta^{rs} \cdot \dot{\varepsilon}^{bc,rs} = h \cdot \sigma^s \quad (2.102)$$

where k^{rs} is the stiffness of the spring and η^{rs} is the viscosity modulus of the Kelvin-Voigt element and h is the relative humidity.

Equation (2.102) shows that the model depends on the local relative humidity, which affects the hydrostatic stress's contribution to creep.

A non-linear dashpot gives the irreversible part of creep:

$$\eta^{is} \cdot \varepsilon^{bc,is} = h \cdot \sigma^s \quad (2.103)$$

with:

$$\eta^{is} = \eta_0^{is} \cdot \exp\left(\frac{\|\varepsilon_m^{ibc}\|}{k}\right) \quad (2.104)$$

where $\|\varepsilon_m^{ibc}\| = \max_{\tau \in [0, t]} \sqrt{\varepsilon^{ibc}(\tau) : \varepsilon^{ibc}(\tau)}$, ε_m^{ibc} is the current state of the irreversible strains, k is an empirical parameter, η_0^{is} is the initial viscosity modulus and η^{is} is the viscosity modulus that varies according to the maximum mechanical strain.

The deviatoric chain model is similar to the spheric chain model, where the hydrostatic stresses and model parameters are replaced by the deviatoric stresses and a new set of model parameters to replace the ones used in the spheric chain model. The reversible part of the deviatoric chain is given by:

$$k^{rd} \cdot \varepsilon^{bc,rd} + \eta^{rd} \cdot \dot{\varepsilon}^{bc,rd} = h \cdot \sigma^d \quad (2.105)$$

where k^{rs} is the stiffness of the spring and η^{rs} is the viscosity modulus of the Kelvin-Voigt element.

The irreversible creep of the deviatoric chain model is given by:

$$\eta^{id} \cdot \varepsilon^{bc,id} = h \cdot \sigma^d \quad (2.106)$$

with:

$$\eta^{id} = \eta_0^{id} \cdot \exp\left(\frac{\|\varepsilon_m^{ibc}\|}{k}\right) \quad (2.107)$$

2.4.3 DRYING CREEP

Pickett [159] observed that an additional creep deformation occurs under drying conditions. The excess of creep at drying over the sum of shrinkage and basic creep is called drying creep. Initially, Pickett assumed that drying creep might be caused by a nonlinearity between creep strain and stress. Other authors [160, 161] explained drying creep through the seepage theory, which states that the excess of creep may be caused by consolidation, like in clays, where the pore water is squeezed out of the specimen under stress. The theory was disapproved since compressive stresses do not increase the water loss of concrete [162, 163]. Another suggestion is the viscous shear theory [164], according to which creep results from the sliding movements occurring in the cement gel particles, where the water flux increases the sliding rate. This theory was also disproved once there was no increased creep in saturated load specimens under constant water permeation rates [139]. The microprestress-solidification theory [145, 146] justifies and quantifies the drying creep through the concept of microprestress.

2.4.3.1 Microprestress-solidification theory

The microprestress-solidification theory states that the drying creep is associated with the magnitude and relaxation of the microprestress that accelerates or decelerates the mechanism of slip breakages and restorations of the atomic bonds in the slip planes of C-S-H [145, 165]. The microprestress is a prestress acting at the micropores generated as an equilibrium response to the disjoining pressure generated due to hindered adsorption layers on the micropore walls and the crystal growth pressure. Since water diffusion between the micropores and the adjacent capillary pore is very short, the hindered water establishes thermodynamic equilibrium with the capillary water. Therefore, the disjoining pressure responds almost instantly to changes in capillary pressure and surface tension, as does the microprestress (mechanism 2 – b)) [145]. The microprestress is independent of the applied macroscopic stress but is influenced by temperature and moisture changes, which affect the chemical potential of adsorbed water in the nanopores. Therefore, it is also responsible for the transitional thermal creep associated with temperature changes (mechanism 3 – b)).

The creep mechanism starts with overstressing a creep site at the cement gel, which leads to a bond breakage in the water molecules between C-S-H. Each bond breakage and restoration at one creep site relaxes the shear stress at that site. As the stress is redistributed, a chain reaction occurs, leading to the overstressing of a new creep site and consequent new bond breakage. The progressive relaxation of the shear stresses at several creep sites and exhaustion of the available overstressed creep sites cause the creep rate under a constant applied load to decline with time, justifying the long-term part of the ageing creep [65]. The higher the microprestress acting in the cement gel, the easier and more pronounced this breakage and restoration phenomenon will occur [145].

Bažant et al. [141] proposed a multiaxial model for the numerical simulation of total creep based on the microprestress-solidification theory. Fig. 22 shows the creep model formulated by the microprestress-solidification theory.

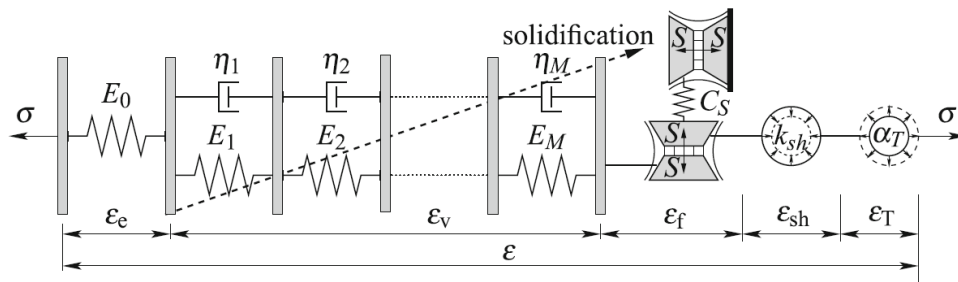


Fig. 22 – Rheologic scheme of complete microprestress-solidification theory: serial coupling of an elastic spring, solidifying Kelvin chain, flow element affected by microprestress relaxation, and units corresponding to free shrinkage and thermal expansion (adapted from [65]).

Bažant et al. [145] proposed a flow element coupled in series with the solidifying Kelvin Chain to simulate the drying creep. The flow element is subjected to two stresses:

- i) the macroscopic stresses that occur horizontally in the figure and cause the shear slip;
- ii) the microprestress S , which occurs vertically in Fig. 22 and affects the viscosity modulus of the flow element (the microprestress relaxation is simulated by a Maxwell element

(spring plus dashpot) tied to the viscosity modulus of the dashpot representing the flow creep ε_f , and connected to the solidifying Kelvin Chain representing the viscous creep ε_v).

The flow creep compliance was already introduced by Equation (2.94), with the viscosity dependent on the concrete age. In the microprestress-solidification theory, the flow strain is described by a dashpot with a viscosity modulus dependent on the microprestress, S .

$$\dot{\varepsilon}_f = \frac{\sigma}{\eta(S)} \quad (2.108)$$

where $\dot{\varepsilon}_f$ is the flow strain rate, σ is the macroscopic stress, and $\eta(S)$ is the effective viscosity modulus which is a decreasing function of the microprestress.

The microprestress theory requires the quantification of the microprestress over time. Bažant et al. [145] proposed that the relaxation of the microprestress be simulated by a Maxwell element, which consists of the connection in series between an elastic spring with the stiffness C_S , and a dashpot with the viscosity of $\eta(S)$ (vertical elements connected to the flow strain dashpot in Fig. 22). Therefore, the model for microprestress relaxation is given by:

$$\frac{\dot{S}}{C_S} + \frac{S}{\eta(S)} = \dot{s} \quad (2.109)$$

where S is the microprestress, $\dot{S}$ is the derivative of microprestress in order to time, and $\dot{s}$ is the rate of instantaneous microprestress induced by the changes in capillary tension, surface tension and crystal growth pressure.

The viscosity modulus $\eta(S)$ should be self-similar concerning changes in the scale by which microprestress S is measured. Bažant et al. [145] proposed the following relationship:

$$\frac{1}{\eta(S)} = c \cdot p \cdot S^{p-1} \quad (2.110)$$

where c and p are positive constants, and $p > 1$.

The microprestress built up during cement hydration due to the volume growth that generates disjoining pressures between hydrated cement grains [65]. While a quantitative relationship for this development remains absent in the literature, the precise microprestress development during cement hydration holds minor importance due to the absence of external loading during this period, which typically corresponds to the hours immediately following casting. Consequently, given the substantial creep strains and high microprestress values expected during this period, precise quantification of microprestress at this stage is not essential. After hydration ceases, the microprestress is mainly affected by the changes in the capillary tension and surface tension and can be formulated by an equation similar to the Kelvin equation (Equation (2.26)). Bažant et al. [145] proposed to calculate the rate of instantaneous microprestress induced by changes in the capillary pressure, surface tension and crystal growth as:

$$\dot{s} = -c_1 \frac{\dot{h}}{h} \quad (2.111)$$

where c_1 is a constant and h is the relative humidity.

Combining Equation (2.109) with Equation (2.111), one obtains:

$$\dot{S} + c_0 \cdot S^p = -c_1 \frac{\dot{h}}{h} \quad (2.112)$$

where $c_0 = C_s \cdot c \cdot p$ is a constant value.

The long-term ageing of flow viscosity is simply a consequence of the relaxation of the microprestress. For the special case of constant moisture content, Equation (2.112) is equal to:

$$\dot{S} = -c_0 \cdot S^p \quad (2.113)$$

Equation (2.113) is a first-order differential equation that governs the evolution of microprestress. The solution of this equation must provide the viscosity of the flow strain of model B3/B4 (Equation (2.94)).

$$\eta(t) = \frac{t}{q_4} \quad (2.114)$$

where q_4 is the parameter of model B3/B4 that controls long-term creep.

Combining Equation (2.110) and Equation (2.114), the microprestress for constant moisture content is given by:

$$S(t) = \left(\frac{q_4}{c \cdot p \cdot t} \right)^{1/(p-1)} \quad (2.115)$$

and the initial condition for microprestress $S(t_0) = S_0$ is given by:

$$S_0 = \left(\frac{q_4}{c \cdot p \cdot t_0} \right)^{1/(p-1)} \quad (2.116)$$

where t_0 is the onset of drying time.

By differentiation of Equation (2.115) with respect to time, one obtains:

$$\dot{S}(t) = -\frac{1}{p-1} \left(\frac{q_4}{p \cdot c} \right)^{1/(p-1)} t^{-p/(p-1)} \quad (2.117)$$

Equation (2.117) must be consistent with Equation (2.113). Replacing Equation (2.53) into Equation (2.113) and comparing it to Equation (2.117), Bažant and Jirásek [65] concluded that the equations are only valid for all the times t if:

$$\frac{p \cdot c}{(p-1)c_0} = q_4 \quad (2.118)$$

Equation (2.118) provides the connection between the parameters p , c and c_0 of the microprestress theory and the parameter q_4 of model B3/B4. Equation (2.118) may be reformulated as:

$$c = \frac{p-1}{p} c_0 \cdot q_4 \quad (2.119)$$

Combining Equation (2.57) into Equation (2.48), one obtains:

$$\frac{1}{\eta(S)} = (p-1)c_0 \cdot q_4 \cdot S^{p-1} \quad (2.120)$$

Combining Equation (2.120) and Equation (2.114), the microprestress for constant moisture content is given by:

$$S(t) = \left[\frac{1}{(p-1)c_0 \cdot t} \right]^{\frac{1}{p-1}} \quad (2.121)$$

The parameter $p = 2$ shows a good agreement with test data [145, 165]. Therefore, the final formulation of the microprestress theory for the particular case of constant moisture content is given by:

$$\frac{1}{\eta(S)} = c_0 \cdot q_4 \cdot S \quad (2.122)$$

and,

$$S(t) = \frac{1}{c_0 \cdot t} \quad (2.123)$$

If the pore pressure changes rapidly due to a huge humidity drop ($\dot{h} \rightarrow \infty$), Bažant and Jirásek [65] concluded that the term $c_0 S^p$ in the Maxwell element is negligible compared to the rate of the microprestress. For this particular case, Equation (2.112) can be simplified to:

$$\dot{S} = -c_1 \frac{\dot{h}}{h} \quad (2.124)$$

Integrating Equation (2.124) leads to $S = -c_1 \ln h + \text{const.}$

The moisture and temperature may affect the mechanism related to the flow creep. Similar to the equivalent age concept, Bažant [103] proposed the use of two transformed times:

- i) the reduced time t_r , which characterises the changes in the rate of bond breakages and restoration on the microstructural level;
- ii) the reduced microprestress time t_s .

In sealed conditions ($h \approx 0.98$) at room temperature $T_0 = 20^\circ\text{C}$, the transformed times are equal to the concrete age t . The equations describing the phenomena associated with the microstructure evolution should be written in terms of the transformed times. Therefore, the flow strain presented in Equation (2.108) is given by:

$$\frac{d\varepsilon_f}{dt_r} = \frac{\sigma}{\eta(S)} \quad (2.125)$$

and the relaxation of microprestress presented in Equation (2.109) is given by:

$$\frac{dS}{dt_s} + c_0 \cdot S^P = \frac{dS}{dt_s} \quad (2.126)$$

The reduced time t_r and the reduced microprestress time t_s are related to the concrete age t through coefficients that account for the temperature and relative humidity change, ψ_r and ψ_s :

$$dt_r/dt = \psi_r = \beta_{rT}(T) \cdot \beta_{rh}(h) \rightarrow dt_r = \psi_r \cdot dt \quad (2.127a)$$

$$dt_s/dt = \psi_s = \beta_{sT}(T) \cdot \beta_{sh}(h) \rightarrow dt_s = \psi_s \cdot dt \quad (2.127b)$$

where $\beta_{rT}(T)$ and $\beta_{rh}(h)$ are coefficients that account for the temperature T and relative humidity h effects on the reduced time. The parameters $\beta_{rT}(T)$ and $\beta_{rh}(h)$ are coefficients that account for the temperature T and relative humidity h effects in the reduced microprestress time. The parameters $\beta_{rT}(T)$ and $\beta_{sT}(T)$ are presented in subchapter 2.5.4 (a chapter related to the effects of temperature on hydration, moisture diffusion, shrinkage, and concrete creep). The parameter $\beta_{rh}(h)$ and $\beta_{sh}(h)$ are given by:

$$\beta_{rh}(h(t)) = \alpha_r + (1 - \alpha_r)h^2 \quad (2.128a)$$

$$\beta_{sh}(h(t)) = \alpha_s + (1 - \alpha_s)h^2 \quad (2.128b)$$

where α_r and α_s are empirical parameters, which can both be considered as 0.1 [103].

By replacing the reduced microprestress time t_s in Equation (2.126), by the respective relationship with the concrete age t presented in Equation (2.127b), one obtains the general form of microprestress relaxation as:

$$\dot{S} + \psi_s \cdot c_0 \cdot S^P = \dot{S} \quad (2.129)$$

By differentiation of the capillary stress given by Equation (2.26), and assuming that the density of the liquid water is constant, Bažant and Jirásek [65] obtained:

$$\dot{p}_c = -\frac{\rho_l R}{M_w} \frac{d}{dt} (T \cdot \ln h) \quad (2.130)$$

The change in surface tension and crystal growth pressure is given by an equation similar to Equation (2.130) with a different proportional constant. Therefore, the rate of instantaneous microprestress induced by changes in the capillary pressure, surface tension and crystal growth pressure, $\dot{s}$ can be described by the following equation:

$$\dot{s} = -\frac{c_1}{T_0} \frac{d}{dt} (T \cdot \ln h) = -\frac{c_1}{T_0} \left(\dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right) \quad (2.131)$$

where c_1 is a constant parameter that accounts for the constants in the capillary pressure, surface tension and crystal growth pressure at room temperature T_0 . Bažant and Jirásek [65] consider the combination of the c_1 and T_0 constants in $k_1 = c_1/T_0$.

Combining Equation (2.131) into Equation (2.129), Bažant and Jirásek [65] defined the general form of the microprestress evolution as:

$$\dot{S} + \psi_s \cdot c_0 \cdot S^P = -k_1 \left(\dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right) \quad (2.132)$$

Cusatis [166] and Bažant et al. [165] concluded that negative increments of the relative humidity h (drying) or positive increments of temperature T (heating) in Equation (2.132) lead to an increase in the microprestress and, therefore, an increase in the slip rate and creep flow. In contrast, in wetting or cooling, the right-hand side of Equation (2.132) changes the sign, and the microprestress relaxation is accelerated, reducing the creep rate temporarily and deactivating the current creep sites. However, new creep sites will form at other locations that were not stressed. Therefore, Cusatis [166] and Bažant et al. [165] suggested considering the right-hand side of Equation (2.132) always positive. The authors acknowledge that such an approach does not capture the temporary decrease of creep rate right after a change of sign of the rate of moisture and temperature; nevertheless, it reflects the most straightforward way that the overall increase of creep rate is likely to occur. Equation (2.132) should be replaced by:

$$\dot{S} + \psi_s \cdot c_0 \cdot S^P = k_1 \left| \dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right| \quad (2.133)$$

2.4.3.2 Microprestress-solidification theory formulation in order to viscosity

Jirásek and Havlásek [147] found that the microprestress parameter S can be omitted, if the relaxation equation is formulated in order to the viscosity $\eta(S)$. Such approach simplifies and optimizes the implementation of the microprestress-solidification theory. Recalling Equation (2.121) and differentiating the equation with respect to time, the authors obtained:

$$\dot{S} = -\left(\frac{1}{c_0 \cdot q_4} \right)^{\frac{1}{p-1}} \left[\frac{1}{(p-1)\eta} \right]^{\frac{p}{p-1}} \dot{\eta} \quad (2.134)$$

By replacing in Equation (2.133) the terms S and $\dot{S}$ by Equation (2.120) and Equation (2.134), the authors obtained:

$$\dot{\eta} + k_1 [c_0 \cdot q_4 (p-1)^p]^{p-1} \left| \dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right| \eta^{\frac{p}{p-1}} = \frac{\psi_s}{q_4} \quad (2.135)$$

For the commonly used value $p = 2$, Jirásek and Havlásek [147] obtained:

$$\dot{\eta} + k_1 \cdot c_0 \cdot q_4 \left| \dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right| \eta^2 = \frac{\psi_s}{q_4} \quad (2.136)$$

Equation (2.136) is a nonlinear first-order differential equation for viscosity and can be solved directly without introducing the microprestress variable. For constant temperature and humidity, the relation for flow viscosity is given by Equation (2.94).

Since parameters k_1 and c_0 are dependent on microprestress and can not be determined separately, Jirásek and Havlásek [147] proposed a new variable μ_s , that accounts for the effect of microprestress, as:

$$\mu_s = c_0 \cdot T_0^{p-1} \cdot k_1^{p-1} \cdot q_4 (p-1)^p \quad (2.137)$$

Jirásek and Havlásek [147] rewrite Equation (2.135) as:

$$\dot{\eta} + \frac{1}{u_s \cdot T_0} \left| \dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right| (u_s \cdot \eta)^{\frac{p}{p-1}} = \frac{\psi_s}{q_4} \quad (2.138)$$

For the commonly used value $p = 2$, the authors obtained:

$$\dot{\eta} + \frac{u_s}{T_0} \left| \dot{T} \cdot \ln h + T \frac{\dot{h}}{h} \right| \eta^2 = \frac{\psi_s}{q_4} \quad (2.139a)$$

$$u_s = c_0 \cdot T_0 \cdot k_1 \cdot q_4 = c_0 \cdot c_1 \cdot q_4 \quad (2.139b)$$

The numerical model becomes complete by establishing an initial condition for the viscosity $\eta(t_0)$, which is given by Equation (2.94):

$$\eta(t_0) = \frac{t_0}{q_4} \quad (2.140)$$

2.4.3.3 Extended microprestress-solidification theory

Bažant et al. [167] found that the microprestress-solidification theory failed to accurately simulate the size effect of creep in drying specimens since an excessive time delay for additional drying creep strains was observed. To overcome these problems, Rahimi-Aghdam et al. [124] proposed the extended microprestress-solidification theory (XMPS), which is an updated version of the microprestress-

solidification theory (MPS). The XMPS is centred on the results of Vandamme et al. [168] and Sinko et al. [169], [170] regarding molecular dynamics simulations. They showed that the rate of relative slip of parallel planar walls of C-S-H sheets increases in the presence of a water layer between the walls, and the rate of slip between the solid surfaces increases when the water layer moves. By analogy, the creep viscosity decreases in both mechanisms, increasing the creep at the macroscale. Fig. 23 shows the sliding between the C-S-H sheets.

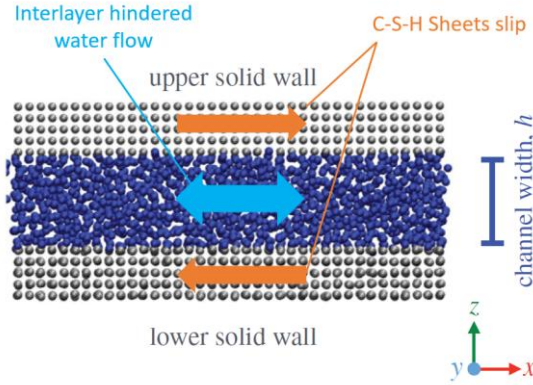


Fig. 23 – Sliding between the C-S-H sheets (adapted from [169])

The water flow between the C-S-H sheets accelerates the sliding between the C-S-H sheets independently of the direction of the flow (drying or wetting). This effect can be understood as the water movement being a source of acceleration of the bond breakage and restorations predicted in MPS. This phenomenon contributes to macroscopic creep and is omitted in the traditional MPS theory. Since any source of the thermodynamic imbalance, such as relative humidity change, influences the microprestress, the additional creep due to this phenomenon can be formulated based on the microprestress rate. Fig. 24 shows the new XMPS model for flow strain.

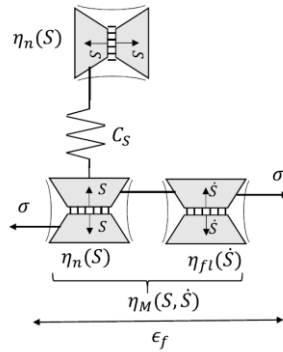


Fig. 24 – Flow strain in the extended microprestress-solidification theory (adapted from [124]).

The model divides the macroscale viscosity $\eta_M(S, \dot{S})$, into the sum of the nanoscale viscosity $\eta_n(S)$ (similar to older MPS), and the new term for the viscosity due to the water flow or the rate of any other phenomenon causing thermodynamic imbalance in nanopores $\eta_{flow}(\dot{S})$. The $\eta_{flow}(\dot{S})$ should account for the decrease in viscosity due to the water flow or rate of other phenomena, which may cause a thermodynamic imbalance in nanopores.

The macroscale viscosity can be described through the sum of the contributions of the two dashpots.

$$\frac{1}{\eta_M} = \frac{1}{\eta_n(S)} + \frac{1}{\eta_{flow}} = a \cdot S + b \cdot |\dot{S}| \quad (2.141)$$

where a and b are coefficients for the microprestress creep ($a = c_0 \cdot q_4$ in MPS).

The XMPS model accounts for the evolution of the microstructure of concrete through the concept of degree of hydration. The macroscopic flow can be rewritten as:

$$\frac{1}{\eta_M} = \frac{\alpha_u}{\alpha} (a \cdot S + b \cdot |\dot{S}|) \quad (2.142)$$

where α_u is the ultimate degree of hydration (for full cement hydration), and α is the current degree of hydration.

The model considers that before a certain degree of hydration $\alpha < 0.6 \cdot \alpha_u$, the microprestress should be assumed constant and equal to $S = S_0 = c_0 q_4$, as a simplification of the growing phase that occurs during the curing period.

The microprestress relaxation follows the behaviour of the rheological Maxwell fluid model as in the previous MPS theory (subchapter 2.4.3.1). The XMPS proposed changes to the rate of instantaneous microprestress induced by changes in the capillary pressure, surface tension and crystal growth, $\dot{S}$. The objective was to account for the effect of temperature on the relative humidity variation. Rahimi-Aghdam et al. [124] proposed to replace Equation (2.133) by:

$$\dot{S} = k_1 \left| \dot{T} \cdot \ln h + \frac{T}{h} \dot{h} + \frac{T}{h} \frac{\partial h}{\partial T} \dot{T} \right| \quad (2.143)$$

Furthermore, the XMPS proposed an update to the parameter $\beta_{sh}(h)$ in Equation (2.127b):

$$\beta_{sh}^{XMPS}(h) = p_0 + \frac{1 - p_0}{1 + \left(\frac{1 - h}{1 - h^*} \right)^{n_h}} \quad (2.144)$$

where the empirical constants of the equation can be assumed as $p_0 = 0.5$; $h^* = 0.75$; $n_h = 2$.

Fig. 25 compares the relative humidity coefficient in the MPS and the XMPS.

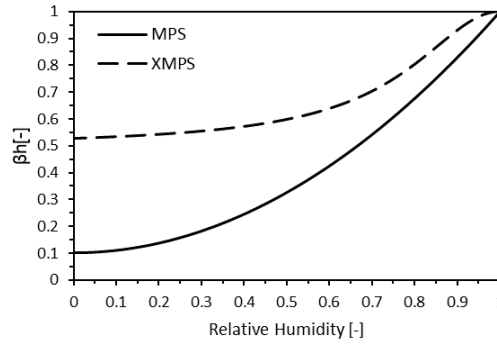


Fig. 25 – Comparison between the relative humidity influence on the microprestressing for the MPS and XMPS. The effect of relative humidity on the reduced microprestressing time is less accentuated in the XMPS than in the older MPS model.

2.4.3.4 Improved microprestressing-solidification theory

Yu et al. [148] proposed an alternative update to the microprestressing-solidification theory to account for the size effect of drying creep. Yu et al. [148] proposed to write the microprestressing relaxation according to the following equation:

$$\frac{\dot{S}_k}{C_s} + \frac{\psi_s(T, h) \cdot S_k}{\eta_s} = \frac{\dot{S}_k}{C_s} \quad (2.145)$$

where $S_k = S/S_0$, S_0 is the initial value of microprestressing, and

$$\dot{S}_k = \frac{\dot{S}}{S_0} = \frac{1}{T_0} \cdot \left| k_{TS} \cdot h^{\alpha_h} \cdot T - k_{hs} \cdot T_0 \frac{\dot{h}}{h} \right| \quad (2.146)$$

where $k_{TS} = k_T \cdot T_0/S_0$ and $k_{hs} = k_h \cdot T_0/S_0$.

The reformulation of MPS in order to introduce the new variable S_k avoids the requirements behind the quantification of microprestressing S and the initial value of microprestressing S_0 . Additionally, Yu et al. [148] proposed a new formulation for the viscosity modulus given by:

$$\eta_s = a_0 (-\ln(S_k))^{p_s} \quad (2.147)$$

where $a_0 = t/q_4$ and p_s is an empirical parameter.

2.4.3.5 Burger mechanical model for drying creep

In the Burger mechanical model [87, 149-151], the additional creep due to simultaneous drying $\dot{\epsilon}_{dc}$ is given by an additional dashpot with a non-linear viscosity modulus η_{dc} :

$$\dot{\varepsilon}_{dc} = \frac{1}{\eta_{dc}} \boldsymbol{\sigma} \cdot \langle \dot{h} \rangle \quad (2.148)$$

where,

$$\langle \dot{h} \rangle = \begin{cases} \dot{h} & \text{if } \dot{h} < 0 \text{ and } h(t) < \min_{\tau \in [0, t]} h(\tau) \\ 0 & \text{otherwise} \end{cases} \quad (2.149)$$

Equation (2.148) considered the total stress tensor and should be seen as an additional element to be added to the Burger rheological model presented in Fig. 21.

Benboudjema et al. [149] found that Equation (2.148) failed to calibrate the experimental results of Granger [114]. They proposed a new constitutive law for the drying creep by replacing the initial dashpot with a Kelvin-Voigt model with a non-linear viscosity modulus $\eta_{dc}/\theta|\dot{h}|$ and stiffness k_{dc} .

$$\eta_{dc} \cdot \dot{\varepsilon}_{dc} + \theta \cdot |\dot{h}| \cdot k_{dc} \cdot \varepsilon_{dc} = \theta \cdot |\dot{h}| \cdot \boldsymbol{\sigma} \quad (2.150)$$

In contrast with Equation (2.102) and Equation (2.105), the drying creep strains obtained from Equation (2.150) are not recoverable due to the nonlinearity of the Kelvin-Voigt element dashpot.

2.4.4 SIMULATION OF CONCRETE CREEP

Numerical simulation of the viscoelasticity of concrete is typically performed using rheological models. This chapter presents some numerical strategies commonly used in the literature to simulate concrete creep.

2.4.4.1 Initial considerations

2.4.4.1.1 Variable stress histories and the principle of superposition

The principle of superposition, first proposed by Boltzmann [171] for nonaging phenomena and later generalised by Volterra [172], states that the increment of strain due to variable stress can be evaluated as the sum of the responses obtained through each stress increment individually. Bazănt [107] showed that the principle of superposition is not precise when a substantial stress variation occurs at an instant t_1 greater than t_0 . However, since a linear viscoelastic behaviour is commonly assumed, the principle of superposition yields approximate results and has advantages in numerical implementation. For the case of a continuously variable stress function applied to a viscoelastic material, the respective strain variation can be evaluated by the integral of Riemann:

$$\varepsilon_{c\sigma}(t) = J(t, t') \cdot \sigma_c(t') + \int_{t'}^t J(t, \tau) \cdot \frac{\partial \sigma(\tau)}{\partial \tau} d\tau \quad (2.151)$$

Discretising the stress history into stress increments $\Delta\sigma_c$, Equation (2.151) becomes:

$$\varepsilon_{c\sigma}(t) = J(t, t') \cdot \sigma_c(t') + \sum_{i=1}^n J(t, \tau_i) \cdot \Delta \sigma_c(\tau_i) \quad (2.152)$$

2.4.4.1.2 Generalised mid-point rule

The analytical evaluation of the integrals is only possible for simple histories of prescribed stress or strain histories. The generalised mid-point rule is frequently adopted to simulate creep in transient nonlinear analyses [65, 173]. From Equation (2.151), the increment of strain from concrete age t to the concrete age $t + \Delta t$ can be expressed as:

$$\Delta \varepsilon_{c\sigma} = \int_0^t (J(t + \Delta t, \tau) - J(t, \tau)) \mathbf{C} \dot{\sigma}_c(\tau) d\tau + \int_t^{t+\Delta t} J(t + \Delta t, \tau) \mathbf{C} \dot{\sigma}_c(\tau) d\tau \quad (2.153)$$

For the numerical implementation into finite element analyses, Equation (2.153) must be rearranged to express the stress increment regarding the strain increment at the current step and the stress relaxation due to previous creep strains. Adopting the generalised mid-point rule ($t \leq t^* \leq t + \Delta t$) and assuming linear behaviour over the time step, the stress-strain incremental relationship is given by:

$$\Delta \sigma_c = \tilde{E}(t^*) \mathbf{C}^{-1} \Delta \varepsilon_{c\sigma} + \tilde{\sigma}_c(t) \quad (2.154)$$

where $\tilde{E}(t^*)$ is the equivalent stiffness that resembles the average elastic modulus value at the current time step, and is given by:

$$\frac{1}{\tilde{E}(t^*)} = \frac{1}{\Delta t} \int_t^{t+\Delta t} J(t + \Delta t, \tau) d\tau \quad (2.155)$$

The variable $\tilde{\sigma}_c(t)$ expresses the stress relaxation due to creep strains that occur at the time t for the entire loading history and is given by:

$$\tilde{\sigma}_c(t) = -\tilde{E}(t^*) \int_0^t (J(t + \Delta t, \tau) - J(t, \tau)) \dot{\sigma}_c(\tau) d\tau \quad (2.156)$$

2.4.4.2 Kelvin chain model

The Kelvin chain model is recurrently used to simulate concrete creep [174, 175]. The model consists of associating several Kelvin-Voigt elements in series. A Kelvin-Voigt element is a parallel association of a spring and a dashpot. For a constant load applied at an instant τ , the dashpot will initially sustain all the stresses since the spring deformation remains null at the loading time. The Kelvin-Voigt element strain increases over time due to the viscous behaviour of the dashpot and the respective transference of stresses from the dashpot to the spring. In the long term, the strain of the element will asymptotically approach the elastic strain, which would be obtained by an isolated spring. Fig. 26 shows the behaviour of the Kelvin-Voigt element.

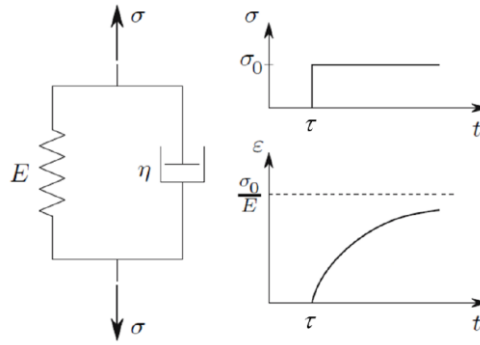


Fig. 26 – Kelvin-Voigt element and deformation under constant stress.

The mechanical response of the spring and dashpot must be equal, and the total stress flowing in the element, σ , is given by the sum of the contributions of the stresses in the spring and dashpot. The constitutive law for the Kelvin-Voigt element is given by:

$$\sigma = E \cdot \varepsilon + \eta \cdot \dot{\varepsilon} \quad (2.157)$$

where E is the elasticity of the spring and η is the viscosity of the dashpot.

Equation (2.157) is a first-order differential equation. The solution of Equation (2.157) gives the strain as:

$$\varepsilon = \frac{\sigma_0}{E} + C \cdot e^{-\frac{E}{\eta}t} \quad (2.158)$$

where C is a constant of integration. The parameter C can be determined considering the initial conditions $\varepsilon = 0$ for $t = t_0$. Equation (2.158) can be rewritten as:

$$\varepsilon = \frac{\sigma_0}{E} \left[1 - e^{-\frac{(t-\tau)}{\lambda}} \right] \quad (2.159)$$

where λ is the retardation time given by $\lambda = \eta/E$.

Equation (2.159) describes the strain function in order to time illustrated in Fig. 26. The shape of the function depends on the adopted retardation time. The presented function shows similarities with concrete creep compliance. However, a single Kelvin element is generally insufficient to describe the full creep compliance accurately. Therefore, several Kelvin-Voigt elements are connected in series with different retardation times to ensure the correct fit of the numerical model to the creep compliance. Usually, an isolated spring is added to the chain to simulate the instantaneous elastic deformation of concrete. Fig. 27 illustrates a typical framework of the Kelvin-Chain model for simulating concrete creep.

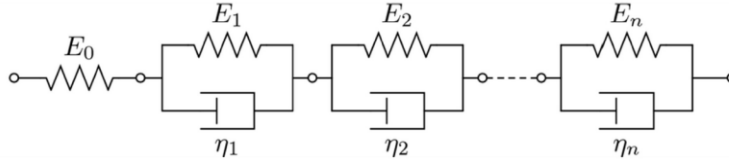


Fig. 27 - Kelvin-Chain model

Hardy and Riesz [176] developed the Kelvin Chain consisting of n Kelvin-Voigt elements as a Dirichlet series:

$$J(t, \tau) = \frac{1}{E_0(\tau)} + \sum_{\alpha=1}^n \frac{1}{E_{\alpha}(\tau)} \left(1 - e^{-\frac{t-\tau}{\lambda_{\alpha}}} \right) \quad (2.160)$$

where each Kelvin-Voigt element α is characterised by the retardation time λ_{α} and the modulus of elasticity $E_{\alpha}(\tau)$. The first term of the right-hand side of Equation (2.160) represents the single spring.

The Kelvin Chain parameters can be estimated through a curve fitting procedure applied between the compliance in Equation (2.160), J_{chain} , and the creep compliance provided by a creep model or experimental data, J_i . The least square method (LSM) is applied to m sampling ages in order to minimise the error given by:

$$error = \sum_{i=1}^m (J_{chain} - J_i)^2 \quad (2.161)$$

The number of Kelvin-Voigt elements to consider in the Kelvin Chain model depends on the duration of the analysis. Since each Kelvin-Voigt element contribution is delimited by the respective retardation time, it is essential to determine those so that the full coverage of the mechanical analysis is assured.

Considering the Kelvin Chain model given by Equation (2.160), the variable $\tilde{E}(t^*)$ is given by:

$$\frac{1}{\tilde{E}(t^*)} = \frac{1}{\Delta t} \sum_{\alpha=1}^n \int_t^{t+\Delta t} \frac{1}{E_{\alpha}(\tau)} \left(1 - e^{-\frac{t+\Delta t-\tau}{\lambda_{\alpha}}} \right) d\tau \quad (2.162)$$

and the stress relaxation due to creep strain and $\tilde{\sigma}_c(t)$ is given by:

$$\tilde{\sigma}_c(t) = -\tilde{E}(t^*) \sum_{\alpha=1}^n \int_0^t \frac{1}{E_{\alpha}(\tau)} \left(1 - e^{-\frac{\Delta t}{\lambda_{\alpha}}} \right) \cdot e^{-\frac{t-\tau}{\lambda_{\alpha}}} \tilde{\sigma}_c(\tau) d\tau \quad (2.163)$$

For a constant value of the stiffness $E_{\alpha}(\tau)$ during the time interval Δt , Equations (2.162) and Equation (2.163) can be integrated analytically. This approach is valid if an appropriate discretisation of the time scale is considered [177]. Subsequently, Equation (2.162) can be rewritten as:

$$\frac{1}{\tilde{E}(t^*)} = \sum_{\alpha=1}^n \frac{1}{E_{\alpha}(t^*)} \left(1 - \frac{\lambda_{\alpha}}{\Delta t} \left(1 - e^{-\frac{\Delta t}{\lambda_{\alpha}}} \right) \right) \quad (2.164)$$

and Equation (2.163) can be rewritten as:

$$\tilde{\sigma}_c(t) = -\tilde{E}(t^*) \sum_{\alpha=1}^n \left(1 - e^{-\frac{\Delta t}{\lambda_\alpha}}\right) \cdot \tilde{\epsilon}_\alpha(t) \quad (2.165)$$

where:

$$\tilde{\epsilon}_\alpha(t) = \int_0^t \frac{1}{E_\alpha(\tau)} e^{-\frac{t-\tau}{\lambda_\alpha}} \dot{\sigma}_c(\tau) d\tau \quad (2.166)$$

The internal variable $\tilde{\epsilon}_\alpha(t)$ stores the influence of the complete strain-stress history and allows the calculation of the creep strain at each step based on the previous step results. Borst and Van den Boogaard [177] showed that this value might be computed as:

$$\tilde{\epsilon}_\alpha(t + \Delta t) = \int_0^t \frac{1}{E_\alpha(\tau)} e^{-\frac{t+\Delta t-\tau}{\lambda_\alpha}} \dot{\sigma}_c(\tau) d\tau + \int_t^{t+\Delta t} \frac{1}{E_\alpha(\tau)} e^{-\frac{t+\Delta t-\tau}{\lambda_\alpha}} \dot{\sigma}_c(\tau) d\tau \quad (2.167)$$

which is approximately given by:

$$\tilde{\epsilon}_\alpha(t + \Delta t) = e^{-\frac{\Delta t}{\lambda_\alpha}} \tilde{\epsilon}_\alpha(t) + \frac{\lambda_\alpha}{E_\alpha(t^*) \Delta t} \Delta \sigma \left(1 - e^{-\frac{\Delta t}{\lambda_\alpha}}\right) \quad (2.168)$$

2.4.4.3 Maxwell chain model

An alternative approach for the simulation of relaxation problems is the Maxwell Chain [65]. The Maxwell chain is formed by the parallel coupling of Maxwell elements, which consist of a spring coupled in series with a dashpot. Fig. 28 shows the Maxwell chain.

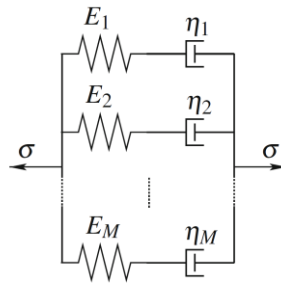


Fig. 28 – Maxwell Chain (adopted from [65])

The Maxwell Chain compliance can be formulated based on the same principles employed in the Kelvin Chain. The general form of relaxation compliance provided by the Maxwell model is described by a Dirichlet series:

$$R(t, \tau) = \sum_{\alpha=1}^M E_\alpha(\tau) \cdot e^{-\frac{t-\tau}{\lambda_\alpha}} \quad (2.169)$$

where $R(t, \tau)$ is the relaxation compliance, and M is the number of Maxwell elements.

2.4.4.4 Second-order exponential approach

The Kelvin chain model presented in subchapter 2.4.4.2 is based on the solution of the first-order differential equation in order to strain. Bažant and Jirásek [65] obtained additional accuracy without any extra mathematical cost by considering a second-order exponential approach. The following equation expresses the Kelvin-Voigt element evaluated as the sum of the elastic and viscoelastic contributions of stress:

$$\sigma_e + \sigma_v = \sigma \quad (2.170)$$

where $\sigma_e = E\varepsilon$ is the elastic stress and $\sigma_v = \eta\dot{\varepsilon}$ is the viscoelastic stress.

By applying a derivation regarding time to Equation (2.170), the authors obtained:

$$\dot{\sigma}_e + \dot{\sigma}_v = \dot{\sigma} \quad (2.171)$$

The elastic stress can be related to the viscoelastic stress by the following equation:

$$\dot{\sigma}_e = E \cdot \dot{\varepsilon} = E \frac{\sigma_v}{\eta} = \frac{\sigma_v}{\tau} \quad (2.172)$$

where $\tau = \eta/E$ is the retardation time.

Combining Equation (2.172) and Equation (2.171), the authors obtained:

$$\frac{\sigma_v}{\tau} + \dot{\sigma}_v = \dot{\sigma} \quad (2.173)$$

Considering time step Δt , the stress rate can be approximated by a constant $\Delta\sigma$ and Equation (2.173) becomes:

$$\frac{\sigma_v}{\tau} + \dot{\sigma}_v = \frac{\Delta\sigma}{\Delta t} \quad (2.174)$$

The approximation in Equation (2.174) is exact if the stress rate, $\dot{\sigma}$, is constant, i.e., if the stress history is linear within the time step Δt . Equation (2.174) is a first-order differential equation, similar to Equation (2.157), derived from the Kelvin Voigt element but expressed in terms of viscoelastic stress. The analytical solution of Equation (2.174) is given by:

$$\sigma_v^{j+1} = \tau \frac{\Delta\sigma^j}{\Delta t^j} + \left(\sigma_v^j - \tau \frac{\Delta\sigma^j}{\Delta t^j} \right) e^{-\Delta t^j / \tau} \quad (2.175)$$

where the index j refers to the time step.

Bažant and Jirásek [65] proposed to evaluate the increment of viscous stress as:

$$\Delta\sigma_v^j = \sigma_v^{j+1} - \sigma_v^j = (1 - \beta^j) \left(\tau \frac{\Delta\sigma^j}{\Delta t^j} - \sigma_v^j \right) = \lambda^j \cdot \Delta\sigma^j - (1 - \beta^j) \sigma_v^j \quad (2.176)$$

where,

$$\beta^j = e^{-\frac{\Delta t^j}{\tau}} \quad (2.177a)$$

$$\lambda^j = (1 - \beta^j) \frac{\tau}{\Delta t^j} \quad (2.177b)$$

Bažant and Jirásek [65] introduced the coefficient β^j and λ^j for numerical purposes. Both parameters should vary between 1 and 0 according to the relationship between $\Delta t^j/\tau$. When the value of $\Delta t^j/\tau$ is too large, the parameter β^j will asymptotically approximate to 0, which may cause computational overflow and $\beta^j = 0$ must be imposed. In contrast, when $\Delta t^j/\tau$ is much smaller than 1, the value of β^j becomes 1 and $\lambda^j = 0$, which is a numerical error, and Equation (2.177b) should be replaced by a Taylor series:

$$\lambda = 1 - \frac{1}{2} \left(\frac{\Delta t^j}{\tau} \right) + \frac{1}{6} \left(\frac{\Delta t^j}{\tau} \right)^2 - (\dots) \quad (2.178)$$

The strain increment at the current step is given by:

$$\Delta\varepsilon^j = (1 - \lambda^j) \frac{\Delta\sigma^j}{E} + (1 - \beta^j) \frac{\sigma_v^j}{E} \quad (2.179)$$

The first part of the right-hand side of Equation (2.179) gives the elastic stress, while the second part gives the contribution of the creep strain.

Similar to the Kelvin-Voigt element, the second-order exponential approach allows the computation of creep strains without storing all stress history. In this model, the stress history is stored through the computation of the viscoelastic stress, which should be updated at each step. For the particular case of a non-ageing Kelvin-Voigt element, the viscoelastic stress can be directly determined in each step as the difference between the current stress state and the current elastic stress, and, in this particular case, there is no need to store the viscoelastic stress. The second-order algorithm is more accurate than the original Kelvin-Voigt model [65]. The previous deduction is applied to only one Kelvin-Voigt element, but it can also be employed in a Kelvin Chain model.

2.5 TEMPERATURE EFFECTS ON HYDRATION, MOISTURE DIFFUSION AND CREEP

The temperature influences cement hydration and may lead to important structural deformations [5, 178, 179]. An adequate heat transference model is necessary to accurately evaluate the concrete elements' temperature fields. The temperature evolution depends on the heat transfer inside the concrete and

between the concrete element and the environment. Three principal heat transfer mechanisms can be defined [5]:

- i) conduction, which is the transference of heat by microscopic collisions of particles and movement of electrons in the element;
- ii) convection, which resembles the heat transference associated with a flow;
- iii) radiation, which is associated with energy emissions due to high temperatures.

Theoretically, the convection may occur inside the concrete element due to liquid and gas matter flux. Bažant and Jirásek [65] show that internal convection can be discarded due to the pore gas's low mass density and the moisture transport's slow nature. Therefore, heat conduction is considered the primary and most important mechanism concerning heat transference inside the concrete element, at least for temperatures below 100°C, while convection and radiation are the main mechanisms that govern heat transferences at the element's boundary. Fig. 29 shows an illustration of these three mechanisms.

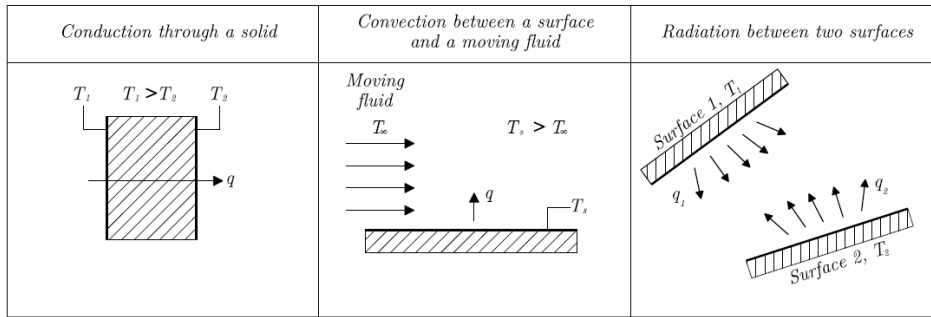


Fig. 29 – Modes of heat transfer (adapted from [5])

The heat equation is based on the first law of thermodynamics or energy conservation law, where the increase in total energy is equal to the sum of supplied work and heat. Assuming some simplifications in the energy balance equation, one can obtain the heat equation postulated by the Fourier law:

$$\rho c \dot{T} = \nabla \cdot (k \cdot \nabla T) + \dot{Q} \quad (2.180)$$

where ρ is the mass density, c is the effective specific heat capacity of concrete per unit mass, T is the temperature, k is the thermal conductivity and $\dot{Q}$ is the heat released by cement hydration given by $\dot{Q} = d\alpha/dt Q_{max}$.

De Schutter and Taerwe [180] observed that the effective specific heat capacity c , and the thermal conductivity k vary in time owing to the microstructure evolution of concrete. Azenha [5] shows that considering these values as constants simplifies the numerical computations without losing numerical precision in the simulation of experimental tests.

2.5.1 TEMPERATURE EFFECTS ON HYDRATION

The chemical reactions occurring during hydration are thermally activated [181]. Therefore, higher temperatures will increase the ratio of chemical reactions. This effect is simulated by the equivalent age concept based on the Arrhenius equation.

$$dt_e/dt = \psi_e = \beta_{eT}(T) \cdot \beta_{eh}(h) = \left(\exp \left[\frac{Q_e}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \right) \cdot \frac{1}{1 + [\alpha_e(1-h)]^4} \quad (2.181)$$

where $\beta_{eT}(T)$ is the equation that accounts for the effect of temperature on the concrete age t , Q_e is the thermal activation energy, R is the universal gas constant, T_0 is the initial temperature and T is the temperature.

To account for the temperature effects on hydration, the concrete age t in the numerical models presented in Chapter 2.1 must be replaced by the equivalent age t_e . For a constant temperature of $T = 20^\circ\text{C}$, the equivalent age is equal to the concrete age. Otherwise, higher temperatures will accelerate hydration, while lower temperatures will slow down the hydration.

2.5.2 TEMPERATURE EFFECTS ON MOISTURE DIFFUSION

To account for the temperature influences on the moisture transport, the evaporable water function, $w_e = \phi(h)$, should be replaced by a new variable that accounts for temperature effects $w_e = \phi(h, T)$. Bažant and Jirásek [65] rewrite equation (2.27) as:

$$\dot{w}_e = \frac{\partial \phi}{\partial h} \dot{h} + \frac{\partial \phi}{\partial T} \dot{T} \quad (2.182)$$

The relative humidity given by equation (2.24) depends on the partial pressure of the water vapour, p_v , and saturated vapour pressure, p_{sat} . Both of these quantities are dependent on the temperature. Consequently, reformulating the moisture transport regarding vapour pressure instead of relative humidity is advantageous when considering the effects of temperature on moisture transport. The relationship between the relative humidity and vapour pressure is given by:

$$\dot{h} = \frac{\partial}{\partial t} \left(\frac{p_v}{p_{sat}} \right) = \frac{\dot{p}_v}{p_{sat}} - \frac{p_v}{p_{sat}^2} \frac{dp_{sat}}{dT} \dot{T} \quad (2.183)$$

where p_{sat} depends on temperature and can be calculated as [182]:

$$p_{sat}(T) = p_{atm} \cdot \exp \left(\frac{11.9515(T - 373.15 \text{ K})}{T - 39.724 \text{ K}} \right) \quad (2.184)$$

where p_{atm} is the atmospheric pressure and can be considered $p_{atm} = 101.325 \text{ kPa}$.

Combining Equation (2.182) and Equation (2.183) into Equation (2.48), Bažant and Jirásek [65] obtained the general equation for the temperature-dependent moisture transport in terms of the vapour pressure:

$$\frac{1}{p_{sat}} \frac{\partial \phi}{\partial h} \dot{p}_v + \left(\frac{\partial \phi}{\partial T} - \frac{p_v}{p_{sat}^2} \frac{dp_{sat}}{dT} \frac{\partial \phi}{\partial h} - \frac{dw_d}{dT} \right) \dot{T} = -\nabla(\Phi_{dif} + \Phi_{per} + \Phi_{con}) - \frac{\partial w_s}{\partial t} - q \quad (2.185)$$

where w_d is the dehydrated water at high temperatures (usually null for $T < 100$ °C [183-185]) and the function $\phi(h, T)$ is the sorption isotherm at high temperatures [186-188].

Equations (2.179) and (2.185) should be solved as a system of two partial differential equations dependent on each other. Bažant and Jirásek [65] observed that the numerical differences between using the coupled system of Equation (2.185) and Equation (2.180) instead of the uncoupled system of Equation (2.48) and Equation (2.180) are negligible for temperatures $T < 100$ °C.

2.5.3 TEMPERATURE EFFECTS ON SHRINKAGE

Shrinkage can be summarised as the sum of basic and drying shrinkage (see Chapter 2.3). The basic shrinkage is associated with cement hydration, which depends on the temperature mentioned in Chapter 2.5.1. Therefore, the equivalent age time should replace the concrete age in the basic shrinkage equation. Bažant and Jirásek [65] state that drying shrinkage depends on the moisture content and the shrinkage coefficient. Since temperature affects moisture transport (Chapter 2.5.2), the temperature will also affect the drying shrinkage. Therefore, in the presence of an adequate and accurate model for moisture diffusion, the temperature effects are implicitly included in the drying shrinkage model given by Equation (2.74). For the relationship between drying shrinkage and relative humidity presented by Equation (2.75), it should be noticed that the shrinkage coefficient k_{sh}^* is dependent on the sorption isotherm, which may also be affected by the temperature (see Chapter 2.5.2).

2.5.4 TEMPERATURE EFFECTS ON CONCRETE CREEP

According to the MPS theory, concrete creep depends on the solidified material volume, the viscous processes at the microstructural level and the microprestress. To consider the temperature effects on concrete creep, Bažant and Jirásek [65] proposed to replace the concrete age, t , in the creep model by the respective transformed times:

- i) the *equivalent age* t_e , which characterises the changes in the rate of hydration;
- ii) the *reduced time* t_r , which characterises the changes in the rate of bond breakages and restoration on the microstructural level associated with viscous processes;
- iii) the *reduced microprestress time* t_s .

The transformed time variables may affect the different sources of creep distinctly. For example, the basic creep (without the flow strain) is dependent on the hydration, and for this case, the authors proposed to replace the concrete age t by the equivalent age t_e . The flow strain is dependent on the viscous process at the microstructural level, and for this case, the authors proposed to replace the concrete age by the reduced time t_r . The microprestress relaxation is a different mechanism influencing the transient part of concrete creep, and for this case, the authors proposed to replace the concrete age t

by the reduced microprestress time t_s . The following equation summarises the approach for considering the temperature effects and relative humidity on creep:

$$dt_i/dt = \psi_i = \beta_{iT}(T) \cdot \beta_{ih}(h) \quad (2.186)$$

where i is an index that indicates the transformed time for the rate of hydration, e , or for the rate of bond breakages and restoration on the microstructural level associated with viscous processes, r , or microprestress, s . $\beta_{ih}(h)$ is a function of the moisture presented in Equation (2.66), Equation (2.128a) and Equation (2.128b), respectively. The function $\beta_{iT}(T)$ accounts for the temperature effect on the transformed time variables. The equations that describe the influence of temperature for the three transformed times present a similar form. For the case of the equivalent age, the equation has been presented in Chapter 2.5.1. The following equations present the effect of temperature on the reduced time t_r and reduced microprestress time t_s :

$$\beta_{rT}(T(t)) = \exp \left[\frac{Q_r}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \quad (2.187a)$$

$$\beta_{sT}(T(t)) = \exp \left[\frac{Q_s}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \quad (2.187b)$$

where T is the absolute temperature (in Kelvin), R is the universal gas constant, and Q_r and Q_s are the activation energies for the viscous processes and microprestress relaxation, respectively.

Despite the mechanisms that influence creep may show different responses due to temperature effects, in the absence of further information, Bažant and Jirásek [65] proposed considering the activation energy of the three mechanisms equal. The Q_i/R ratio may vary in the range of 2700 K to 5000 K. Model B4 recommends the use of $Q_i/R = 4000$ K.

2.6 CONCRETE FRACTURE

Cracking occurs when the local tensile strain capacity of the concrete is exceeded [189]. Designers should ensure that cracking does not affect the structure's function, durability or aesthetics. The design crack widths w_d must be less than or equal to the nominal limit value of the crack width w_{lim} . The exposure classes and the nominal concrete cover influence the crack width limits. The standards specify the nominal crack widths, but in relevant cases, nominal crack widths may be agreed with the client.

2.6.1 CRACKING IN REINFORCED CONCRETE STRUCTURES

Report 22 from the Concrete Society [190] divides cracks into two groups:

- a) the cracks generated by loading in reinforced concrete structures;
- b) the intrinsic cracks, which are categorised as plastic, early thermal contraction and long-term drying shrinkage.

The cracks generated by loading are a structural response of the material to the design loads or accidental overloading. Cracks due to design loads are normal in reinforced concrete structures, and they do not present any structural issues as long as they are within the crack width limits established at the design stage. In some demanding cases, prestressed concrete may be used to avoid cracking. The intrinsic cracks are associated with physical phenomena and can manifest from casting to the long term. Fig. 30 shows several examples of intrinsic cracks on reinforced concrete elements.

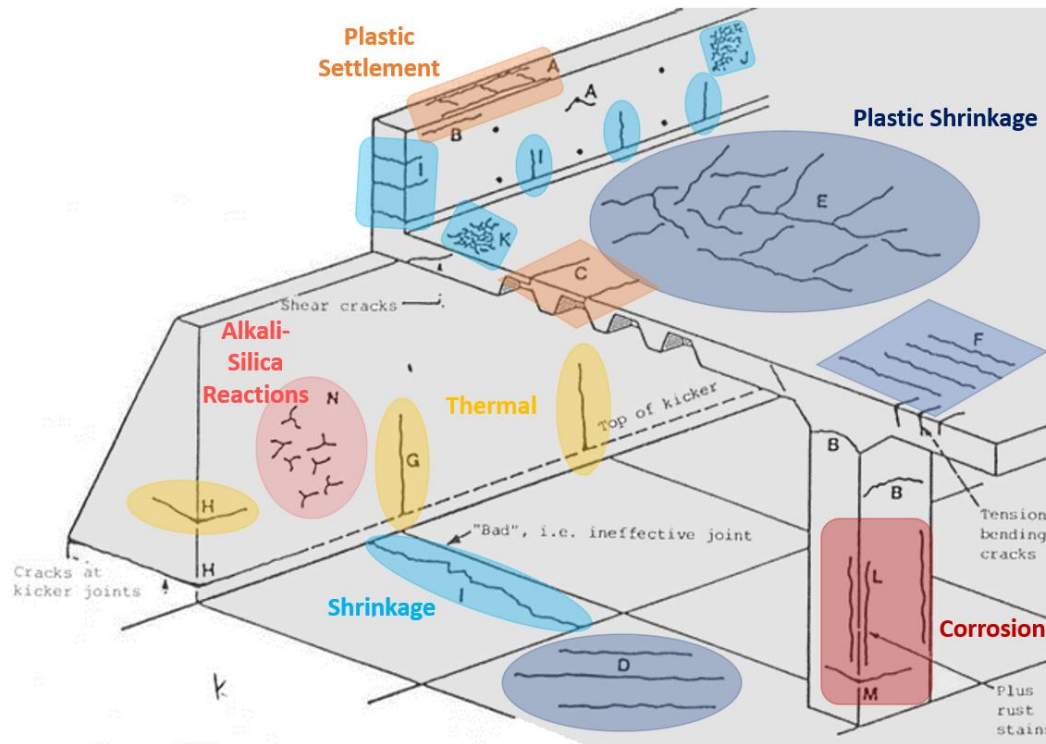


Fig. 30 – Example of intrinsic cracks on reinforced concrete (adapted from [190])

The intrinsic cracks can be divided into cracks that occur before hardening, like plastic cracks, and cracks that occur after hardening, like thermal cracks, shrinkage cracks, crazing, corrosion cracks, and alkali-silica-reaction (ASR) cracks [190]. The plastic cracks occur while the concrete is in a plastic state, typically within minutes to a few hours after casting. The plastic cracks are categorised into plastic settlement cracks and plastic shrinkage cracks. The plastic settlement cracks occur over obstructions like reinforcement bars in deep sections, arching over column tops or changes in slab depth. Their primary cause is excess bleeding (water separating from the mix) or a change in the depth of the baffle slabs. They result from the settlement of solids in the plastic concrete due to gravity and water movement. Plastic settlement cracks can be mitigated by reducing bleeding or settlement by incorporating small quantities of fibres or air-entraining admixtures into the mix, reducing restraint by rearranging the tie bolts or increasing the cover for the reinforcement fixed at the top of a deep section and by revibration of concrete, which can improve its properties and strength.

The plastic shrinkage cracks are primarily caused by rapid early drying of the concrete surface, where the rate of evaporation exceeds the rate of bleeding water, which can rise to the surface. They are common in the exposed surfaces of slabs but can also occur in the exposed top faces of walls or other elements. Plastic shrinkage cracks can be mitigated by improving the early curing conditions to reduce

the rate of surface evaporation. Other strategies include mix design adjustments, including eliminating admixtures with retarding effects, incorporating air-entraining admixtures and the use of fibres.

The early thermal contraction cracks are typically observed in thick walls or where there is external or internal restraint to the concrete thermal strains. These cracks are typically caused by excessive heat generation during cement hydration. The heat generated during cement hydration leads to a temperature rise during the hardening phase and subsequent cooling in a stiffer phase. The cooling down results in a contraction of the structural element, which may lead to cracking in the presence of external and/or internal restraints (in the case of large temperature gradients within the concrete element). The early thermal contraction cracks appear within the first 24 hours to two or three weeks after casting. The early thermal contraction cracks can be mitigated by reducing the heat generation through mix design adjustments, which include using blended cement with pulverised fuel ash (PFA) or GGBS and/or reducing the cement content or using other admixtures and additives that may help reduce the temperature rise during cement hydration, changes to the insulation of the concrete by design formwork to facilitate heat dissipation, design joints and reinforcement to accommodate thermal movement [191], minimize the restraint from surrounding elements and formwork and by controlling the temperature rise and cooling rates [192].

Long-term drying shrinkage cracks appear in slabs and walls, particularly at points where there are insufficient joints. They are caused by the excess water content in the concrete mixture (water not used in cement hydration) and the moisture transport of this water, driven by pressure or concentration gradients (see Chapter 2.2). The lower relative humidity in the environment sets the moisture transport, leading to drying shrinkage. Depending on the ratio of volume to exposed surface, these cracks can develop over several weeks to decades. Long-term drying shrinkage cracks are more commonly observed in thin elements due to the high ratio of volume to exposed surface and the slow characteristics of drying processes in concrete. Nevertheless, they may occur in any element size as long as drying continues. The long-term drying shrinkage cracks can be mitigated by reducing drying shrinkage or reducing the restraint of the structural element. Reducing drying shrinkage is possible by designing the concrete mixture to include additives for such purposes, increasing aggregate content and maximum aggregate size and/or decreasing the mixture's water or workability. Nevertheless, caution is required since some of the strategies to reduce drying shrinkage may increase the other types of shrinkage or concrete contraction that may lead to cracking. Additional solutions include providing adequate curing to exposed surfaces, eliminating external restraints as much as possible by setting movement joints where applicable and/or setting sufficient reinforcement for crack control. Even without external restraint, drying may lead to cracks due to the internal restraint. The fast drying occurring at the element's surface, in contrast with the slower drying a few millimetres in-depth of the element, leads to the generation of self-equilibrated stresses, which may lead to the appearance of microcracks. Microcracking is used to denote cracks hardly visible to the naked eye, smeared over the most superficial layer of concrete, that do not progress in depth. It has been found that cracks thinner than 0.02 mm are hardly visible to the naked eye [193, 194]. Wu et al. [195] investigated the influence of microcracks and related size effects on mass transport properties. They concluded that the drying-induced microcracks would have a minor influence on the durability of most ordinary concrete structures.

Crazing is the formation of a fine network of cracks that appear on the surface layer of concrete. Crazing generally occurs in floated or trowelled surface layers of concrete slabs and formed surfaces of cast stone and concrete. Environmental conditions like low humidity, high temperature, and wind contribute to crazing. These cracks generally appear one to seven days after casting through, sometimes later. Crazing occurs due to a high moisture concentration gradient and/or discontinuity in composition near the exposed surface. Crazing can be avoided by focusing on improving curing and finishing techniques, with recommendations including avoiding over-rich or excessively wet mixes, ensuring adequate compaction, avoiding excessive finishing or any procedure which will depress coarse aggregate and produce a concentration of cement paste and fines at the surface, and applying adequate and continuous curing as soon as finishing has been completed.

Other types of cracks may include cracks due to chlorides and corrosion of the reinforcement and Alkali-silica reaction (ASR) cracks. The cracks due to chlorides and corrosion of the reinforcement are associated with a lack of adequate concrete cover or excess calcium chloride within the concrete. When the steel corrodes, the resulting rust occupies a larger volume, creating expansive forces that crack the surrounding concrete. These cracks usually appear two years after casting. Chloride and corrosion of the reinforcement can be mitigated by reducing the chloride content in the mix, ensuring sufficient concrete cover over the reinforcement and using good-quality concrete. The ASR cracks result from a deleterious chemical reaction between reactive silica in the aggregate and alkalis in the cement when moisture is present. This reaction forms a gel that absorbs water and expands, leading to internal stresses and cracking. The ASR cracks typically occur more than two years after casting. The risk of the appearance of ASR cracks can be minimised by using aggregate with a long history of satisfactory performance, testing the aggregate for reactive silica, testing the cement aggregate combination for reactive silica, placing an alkali limit on the concrete or the cement and using a blended cement.

2.6.1.1 Experimental investigation on early-age cracking in concrete elements

The cracks associated with early thermal contraction are commonly observed in thick concrete elements, like dams and thick walls or slabs, due to the almost adiabatic conditions observed in the core of these types of elements. Due to the exothermic characteristics of cement hydration, the temperature rises during the first hours to days after casting. Over time, the hydration reactions will slow, and the temperature will decrease due to heat conduction. In a restrained concrete element, the temperature increase during the hardening phase results in the appearance of compressive stresses. In contrast, the contraction of concrete due to the cooling down occurs in a stiffer phase, resulting in tensile stresses. The tensile stresses are a consequence of the evolution of the stiffness of the concrete element correlated with the concrete creep. Creep is highly pronounced in the early ages, substantially decreasing over the first days owing to maturity effects related to the ongoing cement hydration. Since the compressive loading occurs first owing to the rising temperature, the compressive creep strains are much higher than the tensile creep strains that occur later owing to the temperature drop, resulting in tensile stresses after the drop in temperature. The maximum temperature reached, and the later the temperature dropped, the

higher the risk of early thermal contraction cracking. Additionally, autogenous shrinkage and the temperature effects on the acceleration of hydration contribute to worsening this problem.

Fairbairn and Azenha [179] recently edited a state-of-the-art report about thermal cracking in massive structures. They identified the structural mechanisms, monitoring techniques, regulations, and numerical models for assessing and controlling early-age cracking. Several experimental setups have been developed to investigate the restraint effects since casting. Fig. 31 shows the adjustable restraining frame (ARF) developed at the Technical University of Graz (TU Graz) [196] and the Temperature-stress-testing-machine (TSTM) developed at the Norwegian University of Science and Technology (NTNU) [197].



a)



b)

Fig. 31 – Experimental setups to access early-age cracking: a) the adjustable restraining frame from TU Graz (adapted from [196]; b) the Temperature-Stress-Testing-Machine from NTNU (adapted from [197]).

Both experimental setups are based on a rigid frame where the temperatures and the restraint forces are measured from the casting time. However, the concrete specimen is not thick enough to generate high temperatures in these experimental setups. In the ARF, insulations can provide semi-adiabatic conditions with temperature histories similar to those observed in thick concrete elements. The temperatures are continuously monitored at the core and surface of the concrete element. In contrast, the TSTM allow the application of a specific temperature history. The ARF system is passively restrained with a constant stiffness, resulting in a variation in the degree of restraint over time. In a later stage, one of the edges of the ARF system can become movable, allowing additional deformation to be imposed. In the TSTM, the restraint is applied as an imposed deformation. The system controls the degree of restraint by prescribing the imposed deformation based on the free deformation of a companion specimen exposed to the same temperature history. The present experimental setups allowed the investigation of the evolution of the stress history at an early age due to cement hydration temperature histories, with practical guidance for the cracking risk and control of cracking in thick concrete elements [196-199].

2.6.1.2 Experimental investigation on cracking patterns in thick concrete elements

In thick concrete elements, cracking control is usually limited to the surface region of the concrete elements. The objective is to ensure that the design crack widths at the surface or at the reinforcement position comply with the limit values, whilst larger crack widths are tolerated at the core of the element.

The reinforcement configuration at the element's surface prompts crack patterns distinct from the ones observed in thin concrete elements [200]. Fig. 32 shows the typical crack patterns observed in thick restrained concrete walls.

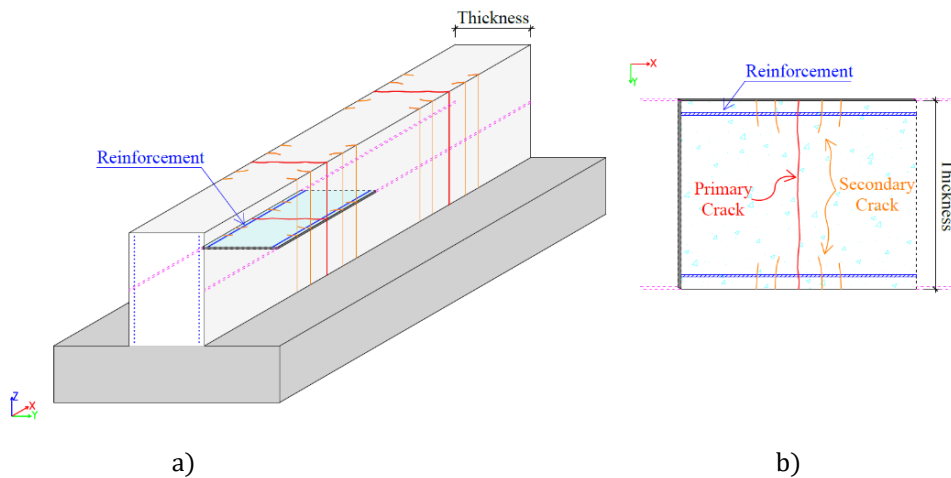


Fig. 32 - Primary and secondary cracks in a thick, axially restrained RC wall: a) 3D view of the wall; b) slice view (adapted from [201]).

Two types of cracks can be identified:

- i) primary cracks, which fully penetrate through the element thickness;
- ii) secondary cracks, which are formed in the vicinity of the primary ones but do not cross the entire member thickness.

Secondary cracks result from the transference of the steel force in the reinforcement at the primary crack into the concrete surface region in the vicinity of the primary crack. From the structural point of view, secondary cracks are beneficial in cracking control once the deformation is redistributed by those superficial cracks instead of being concentrated in a single primary crack [202].

Schlicke et al. [203] developed the Modified Frame (MF) to investigate the cracking patterns of a reinforced concrete panel. Fig. 33 shows the modified frame.



Fig. 33 – Modified frame from TU Graz (adapted from [196]).

The experimental campaign consists of a short-term test where a reinforced concrete panel is subjected to an imposed deformation that will lead to cracking. The concrete panel is cast outside the frame and

installed at a later stage. The restraint force, the elongation and the crack widths are continuously monitored. The experiment shows crack patterns similar to those shown in Fig. 32 b). Additionally, Schlicke et al. [203] verified that the sum of the crack widths at the surface from primary and secondary cracks matches the crack width of the primary crack in the core of the specimen, to which secondary cracks do not propagate.

2.6.1.3 Experimental investigation of the combined effect of bending and axial restraint in slab-like specimens

The cracks due to design loads and intrinsic cracks may occur in conjunction. In concrete buildings, the axial contraction of RC slabs due to shrinkage is typically restrained by their interaction with bracing systems, such as building cores, shear walls, and foundations. This restraint leads to the development of axial forces in the slabs, which can influence their serviceability performance in terms of steel stresses, crack widths, and deformation. Gomes et al. [204] conducted an experimental campaign to understand the complex interactions between self-imposed deformations (particularly due to drying shrinkage), concrete viscoelasticity and external loads in the crack development process in reinforced concrete elements. The experimental campaign was performed within the scope of the IntegraCrete research project. The new experiment method consists of a restraining device to constrain slab-like specimens' axial deformation while simultaneously allowing them to endure bending. The experimental program consisted of the long-term testing of slabs over 15 months in a controlled environment room. Fig. 34 shows the experimental slabs of the IntegraCrete project.

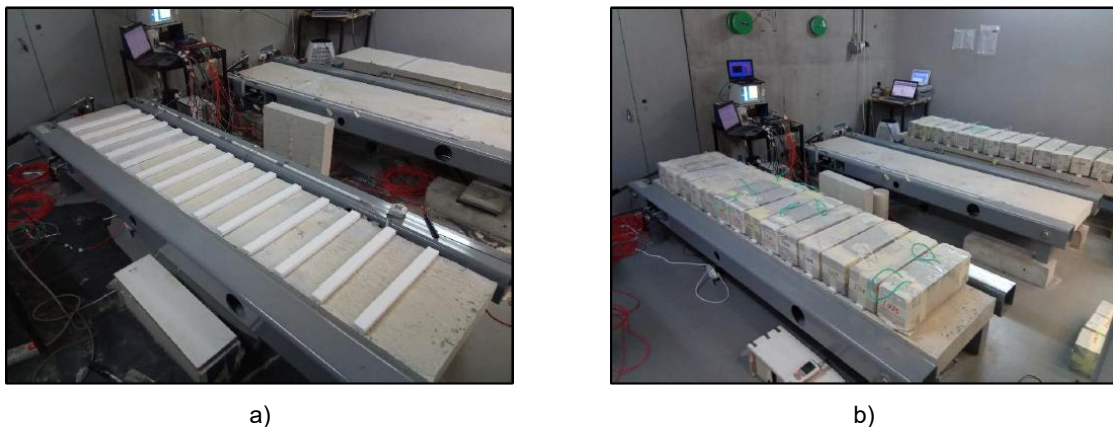


Fig. 34 – Experimental slabs of the IntegraCrete project: a) before applying vertical loading; b) after applying vertical loading.

The experimental campaign included a material characterisation of the concrete mixture and the comparison between three experimental slabs cast with different configurations:

- SLAB1 – Combined restrained shrinkage and vertical loads (slab at the left of Fig. 34);
- SLAB2 – Restraining shrinkage and self-weight (slab in the middle of Fig. 34);
- SLAB3 – Vertical loads only (slab at the right of Fig. 34);
- Dummy specimens – Two unrestrained plain concrete specimens to determine the exact free deformations due to drying shrinkage (shown between SLAB1 and SLAB2 in Fig. 34).

The test setup consists of a restraining device designed to simulate a stretch of a continuous one-way slab. The axial restraint is achieved by two hydraulic actuators connected to the steel rods embedded in one slab extremity, allowing for progressive adjustment of the axial force while controlling deformation in a pre-defined central control region (1.4 m long). Load cells measure the applied axial load. The slabs are 2.6 m long, 10 cm thick, and 0.5 m wide. They are reinforced with 8 mm rebars spaced every 100 mm in both the top and bottom layers. The secondary transverse reinforcement consists of 6 mm rebars spaced by 250 mm. Fig. 35 shows the IntegraCrete slab configuration.

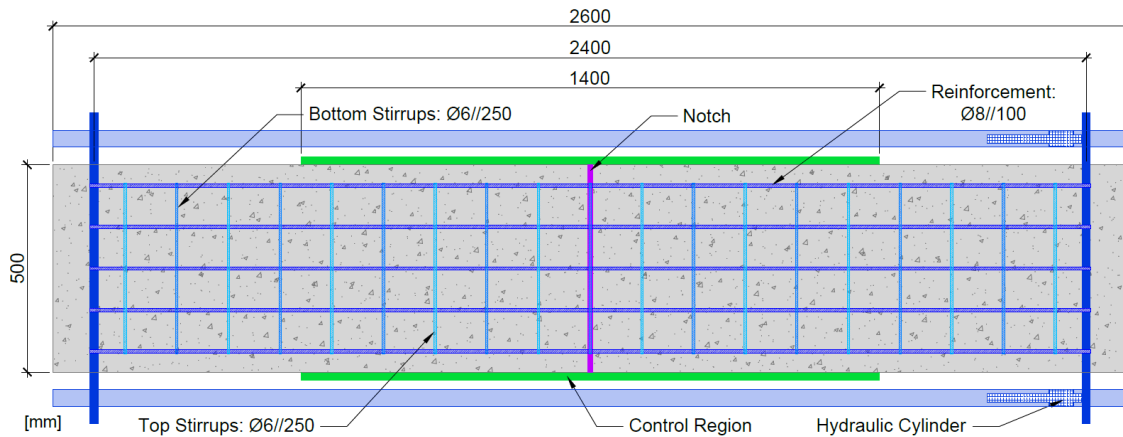


Fig. 35 – IntegraCrete slab configuration.

The concrete is cast in a single batch. The formwork was removed at 7 days, after which the slabs were subjected to drying and self-weight effects. The vertical load is applied at 50 days in SLAB1, and SLAB3 consists of concrete blocks to simulate the quasi-permanent load (Fig. 34 b).

The research highlights the need for a deeper understanding of how self-imposed deformations (like drying shrinkage) and external loads influence crack development in RC slabs. It shows that the level of axial restraint affects the slab behaviour. The restrained SLAB1 and SLAB2 show multiple bottom-surface cracks aligned with reinforcement spacing. In contrast, the unrestrained SLAB3 formed a single central crack only after applying the vertical load at 50 days. The crack width of the cracks of SLAB1 is wider than the crack width of the cracks in the other two slabs, especially after load application at 50 days. Although axial restraint reduced stiffness by inducing cracks, it also generated a geometric nonlinearity that limited vertical deflection. Therefore, SLAB1 and SLAB3 exhibit very similar long-term deflection. Overall, the results show a complex material behaviour involving the combination of design loads and drying shrinkage cracks.

2.6.2 NUMERICAL SIMULATION OF CONCRETE CRACKING

The importance of cracking in the durability of concrete structures and the continuous improvement of computational power have led to the development of sophisticated numerical strategies to simulate and predict cracking. Two main approaches are used for the simulation of cracking in nonlinear finite element analysis [173]:

- i) discrete cracking models [205, 206];

- ii) smeared crack models [207].

The discrete cracking models simulate cracking explicitly based on a discontinuity in the geometry between the old node and the new one.

The smeared crack models are based on a continuity model, where after cracking, the notions of stress and strain continue to apply. The fracture behaviour is included in the stress-strain relations [208], which commonly replaces the initial isotropic stress-strain relationship with an orthotropic stress-strain relationship. Unlike the discrete models, the topology of the original finite element mesh remains preserved in the smeared models, bringing flexibility to the numerical simulations. The smeared crack models can be categorised into rotating or fixed crack concepts. In the rotating concept, the orientation of the crack plane rotates aligned with the principal directions, while in the fixed concept, the orientation of the crack plane is fixed at the cracking threshold. There are several smeared crack models available in the literature:

- i) the total strain cracking models, which are based on continuous material behaviour even after cracking and are controlled by the total strain at each integration point [208, 209];
- ii) the scalar damage cracking models, where the concrete fracture is simulated by a scalar damage variable that reduces the previous isotropic stress-strain relationship [210];
- iii) the smeared cracking models with strain decomposition, as the fixed or multi-directional fixed smeared crack models, where the crack strains are explicitly separated from the concrete strains [211-214];
- iv) the plasticity cracking models, which are based on the consideration of cracking within the framework of plasticity models [215, 216].

Several teams have recently employed thermo-hygro-mechanical models incorporating time-dependent properties and concrete fracture simulations to study cracking-related issues [35, 36, 64, 114, 217-223]. Such approaches have allowed the performance of research investigations like assessing long-term crack widths considering minimum reinforcement used in the reinforced concrete design [224] or the best configurations for experimental setups like the ring test, considering axial or radial drying conditions [225]. The numerical smeared crack models based on the total strain approach and strain decomposition selected for the numerical model implemented during this PhD work are presented in detail in Chapter 3.8.

3

POINTWISE THERMO-HYGRO-MECHANICAL MODEL FOR THE NUMERICAL SIMULATION OF CONCRETE

3.1 JUSTIFICATIONS AND OBJECTIVES

Concrete structures undergo significant volumetric changes over their lifetime, which can result in excessive deflections or cracking. These issues may compromise the structural function, reduce durability, or necessitate costly strengthening interventions. In the context of striving for a sustainable society, substantial efforts have been made to prevent or predict such damage, extend the service life of existing structures, and minimise the frequency of interventions required over time. One effective approach involves the use of numerical analyses as a predictive tool to support risk assessment and management of reinforced concrete structures [226, 227]. However, to enhance the effectiveness of numerical analysis as a decision-making tool, it is crucial to accurately model relevant physical processes, many of which are challenging to implement using conventional numerical methods. Advances in numerical computation have enhanced the simulation of concrete multiphysics behaviour at the macroscale through THM models [35, 36, 64, 114, 217-223]. This methodology involves the numerical prediction of the temperature and relative humidity profiles, which directly influence the mechanical response of concrete elements by affecting the development of the concrete microstructure, leading to volumetric deformations and changes in stiffness and strength [22, 24, 31, 65, 99-103, 181, 228]. In structural analysis using THM models, the concrete properties and maturity are established based on a pointwise constitutive model associated with local hygrothermal profiles. This pointwise material model includes the simulation of thermal and hygral strains [65, 117, 123, 138], as well as creep strains associated with ageing, drying creep and transitional thermal creep [34, 65, 109, 139-144]. Several creep models have been used in the pointwise modelling approaches, e.g. the microprestress solidification theory (MPS), originally published by Bažant et al. [145], [146] and improved by Rahimi-Aghdam et al. [124], Jirásek and Havlásek [147], Yu et al. [148], and a spherical and deviatoric creep strains splitting model, later called Burger concrete model [87, 149-152].

The self-induced strains associated with nonlinear hygrothermal phenomena often exceed the local tensile strain capacity of the concrete, requiring the implementation of a suitable cracking model. The smeared crack concept is advantageous for concrete damage simulation in pointwise THM models [211-

213]. Prominent models include scalar damage models [210], strain-decomposition models [229], and total strain models [209, 230-236]. Although total strain models were popular for cracking simulation in the 1990s, they have been replaced by scalar damage models with a more straightforward implementation [210]. Despite this advantage, scalar damage models do not explicitly compute crack directions at each integration point, presenting a notable limitation when compared to crack models with strain decomposition.

The pointwise THM model presented in this chapter intends to overcome two limitations associated with the numerical approach that averages the concrete behaviour through the element cross-section, and it is commonly used in current engineering practices:

- I. the material model based on averaged cross-section properties is not, strictly speaking, a material model because it varies depending on the geometry of the element considered and the boundary conditions;
- II. the numerical results of an averaged cross-section approach provide an approximate simulation of the overall structural response, as the model simplifies the local concrete behaviour by averaging properties over a broader region rather than capturing detailed local variations. Consequently, the results are not fully accurate for analysing localised behaviour and can only be considered a representation of the general response.

Regarding the first limitation, the numerical models based on the average response of the material's cross-section are calibrated for a specific morphology that experiences a particular hygrothermal distribution over time. In numerical analysis, one can argue that a previously calibrated model based on this approach may fail to reproduce the correct behaviour of a concrete element if the geometric conditions or boundary conditions are slightly changed, which results in different hygrothermal distributions in the cross-section. Consequently, material models based on the average response of a material's cross-section must be calibrated using empirical parameters linked to the size effect, resulting in a geometry-dependent material model [2, 50, 51]. The pointwise THM model should be independent of the structure morphology, avoiding the use of size effect calibration parameters by establishing constitutive laws affected by the local hygrothermal profiles.

The second limitation is related to the ability to calculate the pointwise self-equilibrated stresses along the cross-section and, consequently, capture localised cracking. The average cross-section approach neglects the microcracking generated due to the self-equilibrated stresses. Since macrocracking results from the progressive localisation of cracking strains, the average cross-section approach fails to simulate cracking in the presence of substantial hygrothermal self-equilibrated stresses.

Ferreira et al. [224] proposed a THM model known as the layered approach, in which the finite element (FE) mesh is subdivided into layers or groups of finite elements, with material properties assigned based on their temperature and relative humidity histories. This method allows for capturing hygrothermal effects at the finite element level. However, the layered approach requires the calibration of a new material for each layer, making the process extensive and time-demanding, mainly when dealing with complex hygrothermal phenomena and refined meshes. Moreover, small changes in hygrothermal properties or mesh structure require complete recalibration of the material model for each layer.

The innovative contributions of the pointwise THM model presented in this chapter are the implementation, revision and interoperability of hygrothermal time-dependent models, including maturity, viscoelasticity, eigenstrains, and fracture at the integration point. While some of these models have been developed and validated by other authors (as shown and discussed in Chapter 2), their combination, direct dependence on local hygrothermal properties at the integration point and their validation for application to macroscale analysis of civil engineering structures represent a novel contribution.

Another novelty of the present THM model relies on combining the thermo-hygral framework with the total strain cracking models. Other published THM models account for cracking simulation using scalar damage or strain-decomposition models [35, 36, 64, 114, 217-223]. The total strain models present advantages relative to the alternatively used cracking models: the former explicitly compute the cracking directions (similar to the strain-decomposition models), and allow the implementation of the rotating and fixed crack concepts, providing a seamless transition between them. These features are valuable for modelling different cracking states, from microcracking, where a rotating crack model may be preferable, to macrocracking, where the fixed crack concept is more appealing. Both these situations are essential for correctly simulating structural elements sensitive to hygrothermal imbalances.

3.2 GENERAL ASPECTS OF THE NUMERICAL THM FRAMEWORK

The thermo-hygro-mechanical framework comprises a staggered approach subdivided into two stages:

- a thermo-hygral analysis;
- a mechanical analysis.

The thermo-hygral analysis is performed using the 3D finite element software developed by Azenha [5], and implemented in MATLAB. Some programming changes are required to the original software to satisfy interoperability, version update and input requirements of the mechanical analysis:

- reader routines have received updates for compatibility with data files from the DIANA Interactive Environment V10.6. This update addresses compatibility issues arising from the data input previously generated using the FEMGEN and FEMVIEW services. These services were discontinued and are no longer included in the DIANA FEA software licence;
- output routines now enable the presentation of temperature evolution in the temperature table and relative humidity evolution in the concentration table. These modifications replace the previous version's approach of input shrinkage strains and temperature variations in the temperature table. Additionally, the maturity table that relates concrete age to the equivalent age was removed from the output files since these effects will be accounted for in the pointwise mechanical model;
- a new routine has been developed to enhance interoperability between the mesh of representative structural sections simulated in the thermo-hygral software and the mesh of the model for mechanical analysis. Since most common thermo-hygral scenarios are based on 2D or 1D flows, only a representative structural section needs to be analysed to obtain the thermo-

hygral profiles for the mechanical analysis, i.e. only a finite element column with the slab thickness is required to obtain the thermo-hygral profiles for the mechanical analysis of a regular structural slab. The objective of this routine is to replace the numbering of the nodes from the thermo-hygral mesh with the corresponding group of nodes which are supposed to be represented in the mechanical mesh. The routine automates this process so the output tables are ready to be used in the mechanical analysis without further post-processing requirements.

The outputs of the thermo-hygral analysis are utilised as inputs for the mechanical analysis conducted in DIANA FEA. Fig. 36 shows the schematic representation of this integrated thermo-hygro-mechanical framework.

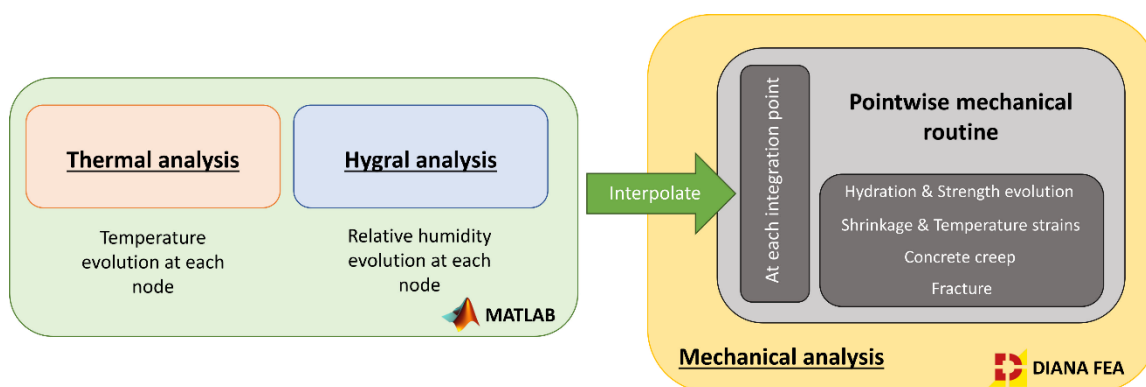


Fig. 36 – Schematic representation of the adopted numerical framework.

The mechanical analysis is performed using the pointwise mechanical routine, which simulates the chemical reactions and the mechanical behaviour of concrete based on constitutive laws dependent on local temperatures and relative humidities. The pointwise mechanical routine is developed in FORTRAN language and implemented in the finite element package DIANA FEA V10.6 through a user-supplied material subroutine.

3.3 HYGROTHERMAL MODEL

The hygrothermal model is simulated by solving the moisture transport and heat conduction equations. As shown in Chapters 2.2.7 and 2.5, the hygral results may affect the microstructure evolution, affecting the heat conduction parameters, while the temperature may affect the moisture transport. Nevertheless, the numerical complexity involved in these approaches can be dismissed when considering good curing conditions and temperatures below 100 °C (which covers most ordinary structural cases). Therefore, the current hygrothermal model solves the moisture transport and heat conduction equations in a decoupled way. Convergence in one step is only achieved when both moisture transport and heat conduction equations have converged [5].

3.3.1 NUMERICAL SIMULATION OF MOISTURE TRANSPORT IN CONCRETE

The moisture transport is given by Equation (2.51), hereby recalled:

$$\frac{\partial w}{\partial h} \frac{\partial h}{\partial t} = \nabla \cdot (D(h) \nabla h) + \dot{h}_s \quad (3.1)$$

Equation (3.1) combines the derivative of time, the second derivative of space and an extra parameter that accounts for the water consumption due to hydration, $\dot{h}_s = \partial h_s / \partial t$. The equation takes the form of a combined system between partial differential equations (PDE) and an ordinary differential equation (ODE). The equation can be solved using numerical methods that involve discretising time and space into 1D, 2D or 3D. The numerical methods used to solve PDE equations are:

- Finite Differences Method (FDM) - space divided into lines;
- Finite Volume Method (FVM) - space divided into volumes;
- Finite Element Method (FEM) - space divided into elements.

The solution of the combined system of PDE and ODE is typically performed by a predictor-corrector method. In structural analysis, the FEM and the FDM are commonly used for solving thermal and moisture transport problems, whereas the FVM is generally more common in Computational Fluid Dynamics (CFD). Table 6 shows a comparison between the advantages and disadvantages of FDM and the FEM.

Table 6 – Comparison between the finite differences method and the finite element method

Finite differences method	Finite element method
“strong form” : states the conditions at every point over a domain that a solution must satisfy	“weak form” : states the conditions that the solution must satisfy in an integral sense
Mainly used with regular grids, complex for irregular grids	Straightforwardly adaptable for irregular grids
Explicit method of integration applicable in space and time discretisations	Explicit method of integration applicable only in time discretisations
Less computational costs	Higher computational costs
Less memory is required for storing data	Higher memory is required for storing data
Large discretisation for reaching good solutions	Can reach good approximations with lower discretisation
Easy implementation	Complex implementation

The FDM can be a useful tool for proceeding to the initial calibration of the hygral model to experimental data due to its low computational costs and easy implementation. Nevertheless, the FEM model provides improved accuracy and flexibility regarding mesh discretisation and boundary conditions.

Lewis and Schrefler [60], Benboudjema [87] and Azenha [5] modelled fluid flow in porous media using the FEM. This chapter presents the numerical implementation of the FEM for solving the moisture transport problem, as implemented by Azenha [5] and utilised in the present pointwise THM framework. The FEM is based on the simulation of flux transport, discretising the space into finite elements. Fig. 37 shows the discretisation of a solid body in 3D, where Ω represents the volume of the solid and Γ represents the boundary surface.

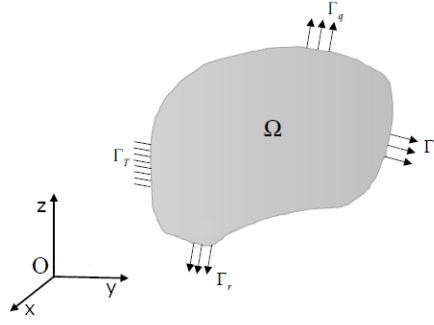


Fig. 37 – Solid body for finite element simulations.

Recalling the moisture transport problem described by Equation (3.1), for a 3D space, the relative humidity field equation can be rewritten as:

$$\frac{\partial w}{\partial h} \frac{\partial h}{\partial t} = \left(\frac{\partial}{\partial x} \left(D_h \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_h \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(D_h \frac{\partial h}{\partial z} \right) \right) + \frac{\partial h_s}{\partial t} \quad (3.2)$$

where $D_h = D(h)$.

Equation (3.2) represents an exact solution to the moisture transport problem in the solid body. For a “weak form” approach, an approximate solution is determined within a convergence limit. Hence, the real relative humidity value h must be replaced by the approximate relative humidity $\tilde{h}$, and Equation (3.2) can be rewritten in a short form as:

$$\frac{\partial w}{\partial \tilde{h}} \frac{\partial \tilde{h}}{\partial t} - \nabla \cdot (D_h \nabla \tilde{h}) - \dot{h}_s = R(\tilde{h}) \quad (3.3)$$

The FEM will provide a satisfactory solution based on the weighted residual method given by the following equation:

$$\int_{\Omega} W \cdot R(\tilde{h}) d\Omega = 0 \quad (3.4)$$

where W is a virtual weight function and $R(\tilde{h})$ is the residual function, which can be given by Equation (3.3).

To fully characterise the moisture transport, boundary conditions must be described to account for the moisture transfer between the solid body and the exterior. Chapter 2.2.5 presents the theoretical background of boundary conditions in moisture transport. Recalling Equation (2.61) and assuming a constant surface emissivity coefficient h_m one obtains the following discretization at the boundary of the body element:

$$-(D_h \nabla h) \cdot \hat{\mathbf{n}} = q_m = h_m(h - h_{env}) \quad \forall x, y, z \in \Gamma \quad (3.5)$$

where $\hat{\mathbf{n}}$ is the outward-pointing unit normal at each point of the boundary Γ , q_m is the flux of moisture dissipated through the boundary. Equation (3.5) is also known as the Neumann boundary condition. Equation (3.5) is related to Equation (2.61) by assuming $q_m = \mathbf{j}_w \cdot \mathbf{n}$ and $h_m = \eta_e^*$.

Combining Equation (3.3) and Equation (3.5), one obtains the residual function as:

$$R(\tilde{h}) = \frac{\partial w}{\partial \tilde{h}} \frac{\partial \tilde{h}}{\partial t} - \nabla \cdot (D_h \nabla \tilde{h}) - \dot{h}_s - [-(D_h \nabla \tilde{h}) \cdot \hat{\mathbf{n}} - q_m] \quad (3.6)$$

Applying Equation (3.4) to Equation (3.6), one obtains:

$$\int_{\Omega} \mathbf{W} \left[\frac{\partial w}{\partial \tilde{h}} \frac{\partial \tilde{h}}{\partial t} - \nabla \cdot (D_h \nabla \tilde{h}) - \dot{h}_s \right] d\Omega - \int_{\Gamma} \mathbf{W} [-(D_h \nabla \tilde{h}) \cdot \hat{\mathbf{n}} - q_m] d\Gamma = 0 \quad (3.7)$$

In the Bubnov-Galerkin formulation, the weighting function is equal to the interpolation function, i.e., $\mathbf{W} = \mathbf{N}$. Equation (3.7) can be rewritten as:

$$\int_{\Omega} \mathbf{N}^T \left[\frac{\partial w}{\partial \tilde{h}} \frac{\partial \tilde{h}}{\partial t} - \nabla \cdot (D_h \nabla \tilde{h}) - \dot{h}_s \right] d\Omega - \int_{\Gamma} \mathbf{N}^T [-(D_h \nabla \tilde{h}) \cdot \hat{\mathbf{n}} - q_m] d\Gamma = 0 \quad (3.8)$$

For convenience, discretising all the terms of Equation (3.8), one obtains:

$$\int_{\Omega} \mathbf{N}^T \frac{\partial w}{\partial \tilde{h}} \frac{\partial \tilde{h}}{\partial t} d\Omega - \int_{\Omega} \mathbf{N}^T [\nabla \cdot (D_h \nabla \tilde{h})] d\Omega - \int_{\Omega} \mathbf{N}^T \dot{h}_s d\Omega + \int_{\Gamma} \mathbf{N}^T [(D_h \nabla \tilde{h}) \cdot \hat{\mathbf{n}}] d\Gamma + \int_{\Gamma} \mathbf{N}^T q_m d\Gamma = 0 \quad (3.9)$$

Considering the integral relation:

$$\int f g' = \int (f g)' - \int f' g \quad (3.10)$$

and assuming $f = \mathbf{N}^T$ and $g = D_h \nabla \tilde{h}$, the second term on the left-hand side of Equation (3.9) is given by:

$$\int_{\Omega} \mathbf{N}^T [\nabla \cdot (D_h \nabla \tilde{h})] d\Omega = \int_{\Omega} [\nabla \cdot (\mathbf{N}^T (D_h \nabla \tilde{h}))] d\Omega - \int_{\Omega} (\nabla \cdot \mathbf{N}^T) D_h \nabla \tilde{h} d\Omega \quad (3.11)$$

The divergence theorem states that the surface integral of a vector flux in a closed surface equals the volume integral of the divergence over the region inside these surfaces. For the volume element Ω in the closed surface Γ , the divergence theorem for a general function f is given by:

$$\int_{\Omega} (\nabla \cdot f) d\Omega = \int_{\Gamma} (f \cdot \hat{\mathbf{n}}) d\Gamma \quad (3.12)$$

Considering $f = \nabla \cdot (\mathbf{N}^T (D_h \nabla \tilde{h}))$ and applying the divergence theorem, one obtains:

$$\int_{\Omega} [\nabla \cdot (\mathbf{N}^T (D_h \nabla \tilde{h}))] d\Omega = \int_{\Gamma} \mathbf{N}^T [(D_h \nabla \tilde{h}) \cdot \hat{\mathbf{n}}] d\Gamma \quad (3.13)$$

The term presented on the right-hand side of Equation (3.13) is equal to the fourth term presented on the left-hand side of Equation (3.9). Replacing Equation (3.13) into (3.11) and replacing those in Equation (3.9), the fourth term of Equation (3.9) vanishes, and one obtains:

$$\int_{\Omega} \mathbf{N}^T \frac{\partial w}{\partial h} \frac{\partial \tilde{h}}{\partial t} d\Omega + \int_{\Omega} (\nabla \cdot \mathbf{N}^T) D_h \nabla \tilde{h} d\Omega - \int_{\Omega} \mathbf{N}^T \dot{h}_s d\Omega + \int_{\Gamma} \mathbf{N}^T [h_m (\tilde{h} - h_{env})] d\Gamma = 0 \quad (3.14)$$

Following the standard discretisation used in FEM, the approximate relative humidity is given by:

$$\tilde{h} = \mathbf{N} \cdot \hat{\mathbf{h}} \quad (3.15)$$

where $\mathbf{N}$ is the interpolation matrix and $\hat{\mathbf{h}}$ is the relative humidity at the nodes of a finite element with the volume Ω .

Applying Equation (3.15) to Equation (3.14), one obtains:

$$\int_{\Omega} \mathbf{N}^T \frac{\partial w}{\partial \tilde{h}} \mathbf{N} d\Omega \frac{\partial \hat{\mathbf{h}}}{\partial t} + \int_{\Omega} (\nabla \cdot \mathbf{N})^T D_h \nabla \mathbf{N} d\Omega \hat{\mathbf{h}} + \int_{\Gamma} \mathbf{N}^T h_m \mathbf{N} d\Gamma \hat{\mathbf{h}} = \int_{\Omega} \mathbf{N}^T \dot{h}_s d\Omega + \int_{\Gamma} \mathbf{N}^T h_m h_{env} d\Gamma \quad (3.16)$$

Equation (3.16) can be rewritten in a short form as:

$$\mathbf{C}^e \left(\frac{\partial \hat{\mathbf{h}}}{\partial t} \right) + \mathbf{G}^e \hat{\mathbf{h}} = \mathbf{F}_s^e + \mathbf{F}_b^e \quad (3.17)$$

where,

$$\mathbf{C}^e = \int_{\Omega} \mathbf{N}^T \frac{\partial w}{\partial \tilde{h}} \mathbf{N} d\Omega \quad (3.18a)$$

$$\mathbf{G}^e = \int_{\Omega} (\nabla \cdot \mathbf{N})^T D_h \nabla \mathbf{N} d\Omega + \int_{\Gamma} \mathbf{N}^T h_m \mathbf{N} d\Gamma \quad (3.18b)$$

$$\mathbf{F}_s^e = \int_{\Omega} \mathbf{N}^T \dot{h}_s d\Omega \quad (3.18c)$$

$$\mathbf{F}_b^e = \int_{\Gamma} \mathbf{N}^T h_m h_{env} d\Gamma \quad (3.18d)$$

The first term of Equation (3.17) is a differential equation in order to time, and therefore it must be discretised. Some discretisation methods for first-order differential equations are the forward Euler method (explicit method), the backward Euler method and the Crank-Nicolson method (both implicit methods) [237]. A general form for the time discretisation of Equation (3.17) is given by:

$$\left(\frac{\mathbf{C}^e}{\Delta t} + \alpha \mathbf{G}^e\right) \hat{\mathbf{h}}^{j+1} = (1 - \alpha)(\mathbf{F}_s^e + \mathbf{F}_b^e)^j + \alpha(\mathbf{F}_s^e + \mathbf{F}_b^e)^{j+1} + \left(\frac{\mathbf{C}^e}{\Delta t} - (1 - \alpha)\mathbf{G}^e\right) \hat{\mathbf{h}}^j \quad (3.19)$$

where $\alpha = 0$ applies the forward Euler method, $\alpha = 1/2$ applies the Crank-Nicolson method, and $\alpha = 1$ applies the backward Euler method. The term $j + 1$ is relative to the next time step variable, which means $j + 1 = t + \Delta t$, and the term j is relative to the actual time step. The forward Euler method in FEM has a stability criterion to ensure a real solution is obtained.

The moisture capacity, $\partial w / \partial \tilde{h}$, and the diffusion coefficient, D_h , are dependent on the relative humidity, $\tilde{h}$. Therefore, for the backward Euler method or the Crank-Nicolson method, the numerical procedure becomes nonlinear since the terms $\mathbf{C}^e$ and $\mathbf{G}^e$ become dependent on the solution of the problem, $\hat{\mathbf{h}}^{j+1}$. For those methods, the Newton-Raphson method is used to solve Equation (3.19). For simplicity, consider Equation (3.19) as:

$$\mathbf{K}^{j+1} \hat{\mathbf{h}}^{j+1} = \mathbf{F}^{j,j+1} \quad (3.20a)$$

$$\mathbf{K}^{j+1} = \left(\frac{\mathbf{C}^e}{\Delta t} + \alpha \mathbf{G}^e\right) \quad (3.20b)$$

$$\mathbf{F}^{j,j+1} = (1 - \alpha)(\mathbf{F}_s^e + \mathbf{F}_b^e)^j + \alpha(\mathbf{F}_s^e + \mathbf{F}_b^e)^{j+1} + \left(\frac{\mathbf{C}^e}{\Delta t} - (1 - \alpha)\mathbf{G}^e\right) \hat{\mathbf{h}}^j \quad (3.20c)$$

Azenha [5] used the FEM backward Euler approach for thermo-hygral analysis. Box 3.1 shows the FEM algorithm applied to the non-linear moisture transport.

Box 3.1 - Finite Elements Algorithm for the moisture transport (adapted from [5])

INPUT: j , $\hat{\mathbf{h}}^j$, Δt , t_{end} , TOLER

OUTPUT: $\hat{\mathbf{h}}^{j+1}$

i) Update time $t^{j+1} = t^j + \Delta t$

Is $t^{j+1} > t_{end}$?

NO: Go to step (ii)

YES: Go to step (x)

ii) Initialise the iteration loop $k = 0$ and set $\Delta \hat{\mathbf{h}}^{j+1,k} = 0$.

iii) Set $\hat{\mathbf{h}}^{j+1,k} = \hat{\mathbf{h}}^j + \Delta \hat{\mathbf{h}}^{j+1,k}$

iv) Compute or update $\mathbf{K}^{j+1,k}$ and $\mathbf{F}^{j,j+1,k}$.

v) Compute residual vector $\boldsymbol{\psi}^{j+1,k} = \mathbf{F}^{j,j+1,k} - \mathbf{K}^{j+1,k} \hat{\mathbf{h}}^{j+1,k}$

vi) Check convergence:

Is $\|\boldsymbol{\psi}^{j+1,k}\| \leq \text{TOLER}$?

NO:	Go to step (vii)
YES:	Go to step (ix)
vii)	Compute $\Delta \hat{h}^{j+1,k+1} = \Delta \hat{h}^{j+1,k} + [K^{j+1,k}]^{-1} \psi^{j+1,k}$
viii)	Update iteration counter $k = k + 1$. Go to (iii)
ix)	Update the step counter $j = j + 1$. Go to (i)
x)	End.

3.3.2 NUMERICAL SIMULATION OF HEAT CONDUCTION IN CONCRETE

The numerical simulation of heat conduction in concrete is governed by Equation (2.180) [5], hereby recalled in the 3D discretisation form:

$$\rho c \frac{\partial T}{\partial t} = \left(\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) \right) + \dot{Q} \quad (3.21)$$

Azenha [5] implemented the solution of Equation (3.21) through the FEM. The numerical procedure follows the same steps as the implementation of the moisture transport problem presented in Chapter 3.3.1. Table 7 shows the corresponding entities in the implementation of the numerical model.

Table 7 – Corresponding entities between the moisture field and the temperature field.

Moisture Field	Temperature Field
h	T
D_h	k
$\partial w / \partial h$	ρc
h_m	h_{cr}
h_{env}	T_{env}
$\dot{h}_s$	$\dot{Q}$

3.4 ARCHITECTURE OF THE POINTWISE MECHANICAL MODEL

In FE software, the pointwise mechanical model operates at the stress calculation level, incorporating a set of subroutines that interact with each other. Fig. 38 presents a schematic representation of the architecture of the pointwise mechanical model.

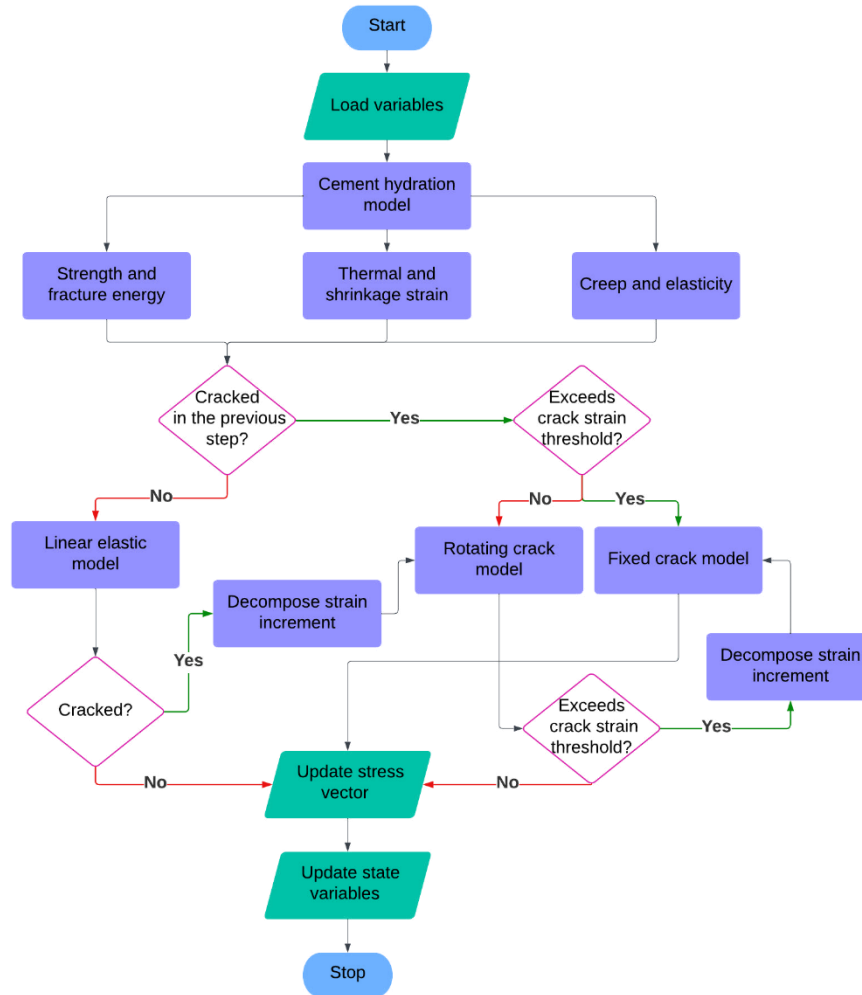


Fig. 38 – Schematic representation of the pointwise mechanical model.

The pointwise mechanical routine starts with the cement hydration model. The transformed times approach is adopted to account for the effects of temperature and relative humidity on microstructure development [92, 103, 228]. Subsequently, the concrete strength properties and fracture energy are evaluated through time-controlled equations [49]. Shrinkage and thermal strains are determined through local constitutive models [55, 65, 74].

Creep strains and the current incremental elastic modulus are evaluated according to the MPS theory [124, 145-147]. The outputs of the three subsequent subroutines are utilised in the stress calculation model, which includes three approaches:

- i) the linear elastic model assuming a linear isotropic incremental approach;
- ii) the rotating crack model, i.e. the total strain model with rotating cracks; and

- iii) the fixed crack model, i.e. the total strain model with fixed cracks or the single-crack model with strain decomposition.

Model selection is governed by integer indicators, which account for different continuum states in each integration point. The numerical procedure begins with the linear elastic model. Once the linear tensile strain capacity is exceeded, the strain increment is split into the linear part that extends the stress and strain into the tensile strength capacity and the remaining strain increment. For the remaining strain increment, the total strain model with rotating cracks is used until a user-defined total strain threshold is reached. If the total strain threshold is exceeded, the total strain increment is divided into the rotating strain component, which extends the total strain towards the threshold limit, and the remaining strain increment that will be used in the fixed crack model. In the rotating crack model, the crack directions rotate aligned with the principal strain directions. In contrast, the fixed crack model assumes that crack directions, once established at the initiation of cracking, remain constant throughout the analysis. The total strain threshold defines the transition point between the two models.

The total strain model with rotating cracks can also simulate linear elastic behaviour, though it is more computationally demanding than the linear elastic model. There is no reversibility in the stress calculation models: once the fixed crack model is activated, it remains active throughout the analysis.

The final step of the pointwise routine involves updating and storing the state variables necessary for subsequent steps. The main output of the pointwise routine to the nonlinear FE software is the updated stress state for the current iteration.

3.5 CEMENT HYDRATION

3.5.1 CONTEXTUAL INTRODUCTION

The cement hydration model aims to simulate the chemical reactions that occur in concrete, as explained in Chapter 2.1, which influence the evolution of the mechanical properties. Fig. 39 presents a layout of the cement hydration model.

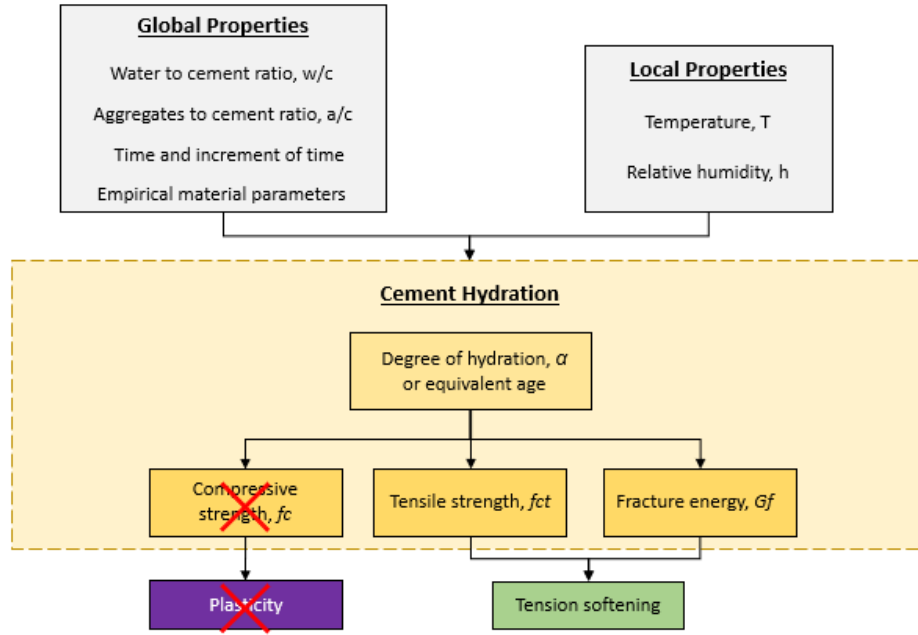


Fig. 39 – Layout of the cement hydration routine.

Two different cement hydration models are implemented for use in the numerical simulation of cement hydration:

- Transformed times model: This model evaluates the cement hydration based on the transformed times, replacing the concrete age with the equivalent age affected by parameters dependent on the temperature and relative humidity.
- Degree of hydration model: This model evaluates the degree of hydration based on the cement hydration of a single particle of alite as initially proposed by Rahimi-Aghdam et al. [24] and hereby debugged.

3.5.2 IMPLEMENTATION DETAILS

3.5.2.1 Transformed times model

The transformed times model replaces the concrete age time with the transformed times that account for the temperature and relative humidity effects on concrete (see Chapters 2.5.1 and 2.5.4). The temperature and the relative humidity at the current time-step are computed according to the following equation:

$$\begin{cases} T^{t+\Delta t/2} = T^t + \frac{\Delta T}{2} \\ h^{t+\Delta t/2} = h^t + \frac{\Delta h}{2} \end{cases} \quad (3.22)$$

where $T^{t+\Delta t/2}$ and $h^{t+\Delta t/2}$ represent the average temperature and relative humidity at the middle of the current step, T^t and h^t represent the temperature and relative humidity at the concrete age t , and ΔT and Δh represent the total increment of temperature and relative humidity during the current step.

As mentioned in Chapter 2.5.4, there are three transformed times: the equivalent age, t_e , the reduced time, t_r , and the microprestress reduced time, t_s . The effects of temperature in the transformed times are simulated by equations (2.181) and (2.187a), hereby recalled:

$$\beta_{eT}(T) = \left(\exp \left[\frac{Q_e}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \right) \quad (3.23a)$$

$$\beta_{rT}(T) = \left(\exp \left[\frac{Q_r}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \right) \quad (3.23b)$$

$$\beta_{sT}(T) = \left(\exp \left[\frac{Q_s}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \right) \quad (3.23c)$$

where β_{eT} , β_{rT} and β_{sT} are the temperature functions for the equivalent age, reduced time and reduced microprestress time, respectively, R is the universal gas constant and Q_e , Q_r and Q_s are the activation energies for hydration, viscous processes and microprestress relaxation, respectively.

The effects of relative humidity in the transformed times are simulated by equations (2.66) and (2.128a), hereby recalled:

$$\beta_{eh}(h) = \frac{1}{1 + [\alpha_e(1 - h)]^4} \quad (3.24a)$$

$$\beta_{rh}(h) = \alpha_r + (1 - \alpha_r) \cdot h^2 \quad (3.24b)$$

$$\beta_{sh}(h) = \alpha_s + (1 - \alpha_s) \cdot h^2 \quad (3.24c)$$

where β_{eh} , β_{rh} and β_{sh} are the relative humidity functions for the equivalent age, reduced time and reduced microprestress time, respectively, h is the relative humidity and α_e , α_r and α_s are empirical parameters.

For the other numerical models in the pointwise mechanical subroutine, the following transformed time functions are required:

$$\psi_e^{t+\Delta t/2} = \beta_{eh}(h^{t+\Delta t/2}) \cdot \beta_{eT}(T^{t+\Delta t/2}) \quad (3.25a)$$

$$\psi_r^t = \beta_{rh}(h^t) \cdot \beta_{rT}(T^t) \quad (3.25b)$$

$$\psi_r^{t+\Delta t} = \beta_{rh}(h^{t+\Delta t}) \cdot \beta_{rT}(T^{t+\Delta t}) \quad (3.25c)$$

$$\psi_s^{t+\Delta t/2} = \beta_{sh}(h^{t+\Delta t/2}) \cdot \beta_{sT}(T^{t+\Delta t/2}) \quad (3.25d)$$

The increments of equivalent time and reduced time can be calculated according to the following equations:

$$\Delta t_e = \psi_e^{t+\Delta t/2} \cdot \Delta t \quad (3.26a)$$

$$\Delta t_r = \frac{(\psi_r^t + \psi_r^{t+\Delta t})}{2} \cdot \Delta t \quad (3.26b)$$

where Δt_e is the increment of the equivalent age and Δt_r is the increment on the reduced time.

The variables Δt_e , Δt_r and $\psi_s^{t+\Delta t/2}$ are required for the subsequent models. The equivalent time at the end of the step is calculated according to the following equation:

$$t_e^{t+\Delta t} = t_e^t + \Delta t_e \quad (3.27)$$

The reduced time, $t_r^{t+\Delta t}$, and the microprestress reduced time, $t_s^{t+\Delta t}$, at the end of the step, can be obtained by replacing the equivalent times in equation (3.27), by the respective transformed times.

For the evaluation of the mechanical properties and the solidified material volume within the step increment, the mid-point rule is adopted by using the value $t_e^{t+\Delta t/2} = t_e^t + \Delta t_e/2$ rather than $t_e^{t+\Delta t}$.

3.5.2.2 Cement hydration of a single particle controlled by diffusion through barrier shells of C-S-H

Rahimi-Aghdam et al. [24] proposed a model for the simulation of cement hydration based on water transport from capillary pores through barrier shells towards the interface with anhydrous cement. The model considers an idealised spherical cement particle representing the average hydration evolution in the cement paste. Such an approach allows for evaluating the degree of hydration at each integration point based on the cement paste composition and properties, and the local temperature and relative humidity field. The implemented model is based on the algorithms described by Rahimi-Aghdam et al. [24] and Rahimi-Aghdam et al. [124], revised with the required modifications fully described and justified below.

In the first step, the volume fraction for the concrete compounds must be determined. Rahimi-Aghdam et al. [24] proposed to evaluate the volume of cement (V_c^0), water (V_w^0) and aggregates (V_a^0) as a fraction of the unit volume of concrete ($V_c^0 + V_w^0 + V_a^0 = 1 \text{ m}^3/\text{m}^3$).

$$V_c^0 = \frac{\rho_a \rho_w}{\rho_a \rho_w + \rho_c \rho_w a/c + \rho_c \rho_a w/c} \quad (3.28a)$$

$$V_w^0 = \frac{\rho_a \rho_c w/c}{\rho_a \rho_w + \rho_c \rho_w a/c + \rho_c \rho_a w/c} \quad (3.28b)$$

$$V_a^0 = \frac{\rho_c \rho_w a/c}{\rho_a \rho_w + \rho_c \rho_w a/c + \rho_c \rho_a w/c} \quad (3.28c)$$

where ρ_w is the water density ($\rho_w = 1000 \text{ kg/m}^3$), ρ_c is the cement density ($\rho_c = 3150 \text{ kg/m}^3$) and ρ_a is the density of the aggregates (Rahimi-Aghdam et al. [24] proposed to consider $\rho_a = 1600 \text{ kg/m}^3$ for gravel and sand combined, in the absence of the laboratory characterisation of the material).

In the second step, Rahimi-Aghdam et al. [24] proposed to determine the average cement particle size (initial cement particle radius) a_0 , and the number of cement particles per unit volume of cement n_g according to the following equations:

$$a_0 = 6.5(\mu\text{m}) \frac{350}{f_{bl}} \quad (3.29a)$$

$$n_g = \frac{V_c^0}{\frac{4}{3}\pi(a_0)^3} \quad (3.29b)$$

where f_{bl} is the Blaine fineness of cement, corresponding to $f_{bl} = 350 \text{ m}^2/\text{kg}$ for a cement particle with a radius of $a_0 = 6.5 \mu\text{m}$.

Subsequently, Rahimi-Aghdam et al. [24] proposed to evaluate the hydration degree at the setting time α_{set} which represents the reactions approximately related to the end of the dormant period, and the critical hydration degree α_c , which represents the hydration degree for which a complete gel barrier will fulfil the entire cement particle radius and switches the hydration rate mechanics from the nucleation-growth process to diffusion-controlled hydration. For a cement particle with $a_0 = 6.5 \mu\text{m}$ and $w/c = 0.3$ at room temperature $T = 20 \text{ }^\circ\text{C}$, one can consider $\alpha_{set}^0 = 0.05$ and $\alpha_c^0 = 0.36$. For different concrete mixtures, the authors proposed to calculate an approximation to these parameters using the following equations:

$$\alpha_c = \alpha_c^0 f_1(a) f_2(w/c) \beta_{eT}(T) \leq 0.65 \quad (3.30a)$$

$$f_1(a) = \frac{a_0^n}{a} (\mu\text{m}/\mu\text{m}) \quad (3.30b)$$

$$f_2(w/c) = 1 + 2.5(w/c - 0.3) \quad (3.30c)$$

$$\frac{\alpha_{set}}{\alpha_{set}^0} = \frac{\alpha_c}{\alpha_c^0} \quad (3.30d)$$

In Equation (3.30b), the representation of the variable a is ambiguous. Rahimi-Aghdam et al. [24] describe a as the radius of the anhydrous cement particle, which varies throughout the analysis. Equations (3.30) are formulated to calculate the parameter α_c and α_{set} , which are intended to be constant. Therefore, the parameter a in Equation (3.30b) should be more accurately defined as the initial cement particle radius, a_0 . Accordingly, Equation (3.30a) and Equation (3.30b) have been reformulated as follows:

$$\alpha_c = \alpha_c^0 f_1(a_0) f_2(w/c) \beta_{eT}(T) \leq 0.65 \quad (3.31a)$$

$$f_1(a_0) = \frac{6.5}{a_0} (\mu\text{m}/\mu\text{m}) \quad (3.31b)$$

The present model will initiate at the setting time. Since the degree of hydration at the setting time is not zero ($\alpha_{set} > 0$), the volume of cement V_c^{set} , portlandite V_{CH}^{set} and gel (C-S-H) V_g^{set} at the setting time needs to be updated. Rahimi-Aghdam et al. [24] developed the model based on the cement hydration governed by the stoichiometry of the Alite compound. Therefore, they proposed to consider the volume ratios for the gel and portlandite reaction as $\zeta_{CSH,c} = 1.52$ and $\zeta_{CH,c} = 0.59$, respectively. The volume of cement, V_c^{set} , portlandite, V_{ch}^{set} . and gel, V_{gel}^{set} , at the setting time can be calculated according to the following equations:

$$V_c^{set} = (1 - \alpha_{set})V_c^0 \quad (3.32a)$$

$$V_{CH}^{set} = \zeta_{CH,c} \alpha_{set} V_c^0 \quad (3.32b)$$

$$V_{gel}^{set} = \zeta_{CSH,c} \alpha_{set} V_c^0 \quad (3.32c)$$

The radius of the cement particle and the outer radius of the C-S-H barrier at the setting time are given by:

$$a^{set} = \left(\frac{V_c^{set}}{4/3 \pi n_g} \right)^{1/3} \quad (3.33a)$$

$$z^{set} = \left(\frac{V_c^{set} + V_g^{set}}{4/3 \pi n_g} \right)^{1/3} \quad (3.33b)$$

Once all the previous parameters are determined, one can start the loop to determine the hydration degree at each time increment $t + \Delta t$. Rahimi-Aghdam et al. [24] proposed a forward Euler approach where the relative humidity and the previous hydration degree are used for calculating the water diffusivity through the barrier shells, B_{eff} :

$$B_{eff}^t = B_0 \cdot f_0 \left(h_p^{t+\frac{\Delta t}{2}} \right) \cdot f_4(\alpha^t) \quad (3.34a)$$

where $B_0 = 1.0 \times 10^{-11} \text{ m}^2/\text{day}$ for alite specimens and $B_0 = 1.1 \times 10^{-11} \text{ m}^2/\text{day}$ for cement specimens, and:

$$f_0(h_p^{t+\Delta t/2}) = c_f + \frac{1 - c_f}{1 + \left(\frac{1 - h_p^{t+\Delta t/2}}{1 - h^*} \right)^{n_h}} \quad (3.34b)$$

where $h_p^{t+\Delta t/2}$ is the relative humidity at the capillary pore obtained in Equation (3.22), $n_h = 8$, $h^* = 0.88$, $c_f = 0$. Rahimi-Aghdam et al. [124] proposed that $f_4(\alpha^t)$ should be evaluated according to:

$$\begin{cases} f_4(\alpha^t) = \gamma \cdot \exp(-\gamma) & \text{for } \alpha^t \leq \alpha^* \\ f_4(\alpha^t) = (\beta/\alpha_s)^m \cdot \exp[(\beta/\alpha_s)^m] & \text{for } \alpha^t > \alpha^* \end{cases} \quad (3.34c)$$

with:

$$\gamma = (\alpha^t / \alpha_{max})^m, \quad \beta = \alpha^t - \alpha^* + \alpha^* \alpha_s / \alpha_{max} \quad (3.34d)$$

where $\alpha_s = 0.3$, $\alpha_{max} = \alpha_c / 2$, $\alpha^* = 0.75 \cdot \alpha_c$ and $m = 1.8$.

Even though Rahimi-Aghdam et al. [24] state that Equation (3.34a) should be continuous at α^* , the formulation presented in [24] and [124] is not continuous at α^* . This occurs due to a possible typo in the signal of the value in the exponential of the $f_4(\alpha^t)$ for $\alpha^t > \alpha^*$. Therefore, in this PhD it is proposed to replace the second term of Equation (3.34c) and Equation (3.34d) by the following one, which is continuous at α^* :

$$\begin{cases} f_4(\alpha^t) = \gamma \cdot \exp(-\gamma) & \text{for } \alpha^t \leq \alpha^* \\ f_4(\alpha^t) = \beta \cdot \exp(-\beta) & \text{for } \alpha^t > \alpha^* \end{cases} \quad (3.35a)$$

with:

$$\gamma = (\alpha^t / \alpha_{max})^m, \quad \beta = \left(\frac{\alpha^t - \alpha^* + \alpha^* \alpha_s / \alpha_{max}}{\alpha_s} \right)^m \quad (3.35b)$$

where $\alpha_s = 0.3$, $\alpha_{max} = \alpha_c / 2$, $\alpha^* = 0.75 \cdot \alpha_c$ and $m = 1.8$.

Fig. 40 shows the continuity of Equation (3.35a) for $\alpha_c = 0.36$.

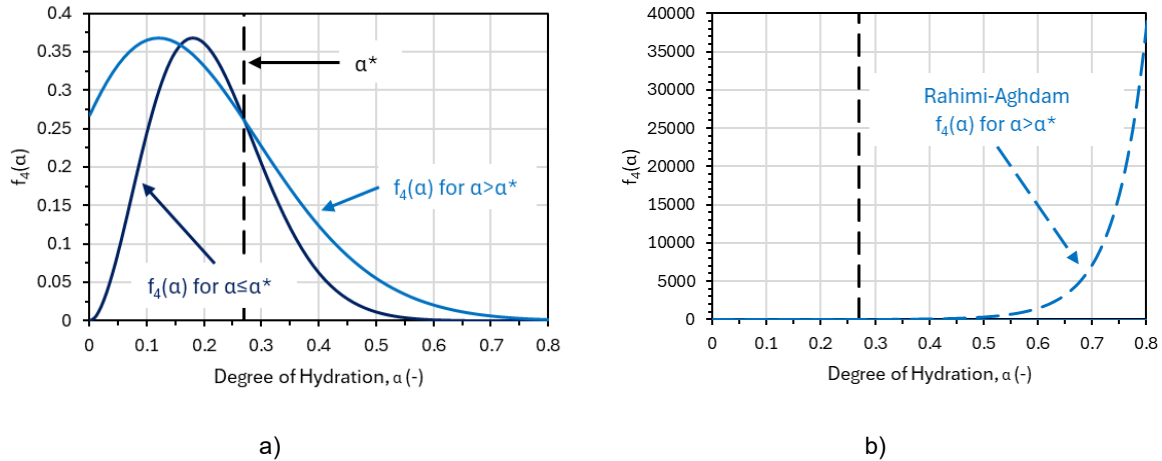


Fig. 40 – Continuity of the function $f_4(\alpha^t)$ for $\alpha_c = 0.36$: a) proposed model using Equation (3.35); b) deviations of Rahimi-Aghdam (3.35a) $f_4(\alpha^t)$ for $\alpha^t > \alpha^*$ using Equation (3.34c).

Equation (3.34c) for $\alpha^t > \alpha^*$ is not visible in the Fig. 40a), since it starts in values above 0.4 and is equal to 16.5 at α^* . Fig. 40b) shows that Equation (3.34c) for $\alpha^t > \alpha^*$ continuous to grow with the increasing of the degree of hydration while the inverse is supposed to happen, strengthening the idea that the equation has a typo.

Rahimi-Aghdam et al. [124] proposed to account for the reduction of the contact-free surface due to cement grains contact by replacing the actual shell radius z , by the equivalent radius of the contact-free C-S-H shells $\hat{z}$ evaluated according to the following equation:

$$\hat{z}^t = \frac{z^t}{1 + \left(6.4 \frac{z^t - a_0}{a_0}\right)^5} \quad (3.36)$$

In each time increment $t + \Delta t$, Rahimi-Aghdam et al. [124] proposed to evaluate the water discharge Q^t according to the following equation:

$$Q^t = 4 \pi a^t z^t B_{eff}^t(\alpha^t, h_p^{t+\Delta t}) \frac{h_p^{t+\Delta t} - h_c}{z^t - a^t} \left(\frac{(\hat{z}^t)^2}{(z^t)^2} \right) \quad (3.37)$$

where h_c is the relative humidity at the interface between the shell barrier and the anhydrous cement grain for which hydration ceases, and can be considered equal to $h_c = 0.78$ for $T = 20^\circ\text{C}$ (the value can change according to the admixtures used [67]).

In each time increment $t + \Delta t$, Rahimi-Aghdam et al. [24] proposed to calculate the increment of anhydrous cement volume $dV_c^{t+\Delta t}$, portlandite $dV_{CH}^{t+\Delta t}$ and cement gel $dV_{gel}^{t+\Delta t}$ using the calculated water discharge Q^t . The following equations may be applied for the calculation of the volume of each compound:

$$V_c^{t+\Delta t} = V_c^t + dV_c^t = V_c^t - n_g Q^t \zeta_{cw} dt \quad (3.38a)$$

$$V_{gel}^{t+\Delta t} = V_{gel}^t + dV_{gel}^t = V_{gel}^t + n_g Q^t \zeta_{gw} dt \quad (3.38b)$$

$$V_{CH}^{t+\Delta t} = V_{CH}^t + dV_{CH}^t = V_{CH}^t + n_g Q^t \zeta_{CHw} dt \quad (3.38c)$$

The parameter ζ_{cw} is the ratio between the variation in the volume of anhydrous cement and the water consumed. Rahimi-Aghdam et al. [24] consider that water consumption during cement hydration is not restricted to chemical reactions, and some water becomes hindered in the growing hydration products. Therefore, they considered that water consumption should be affected by porosity and the increase in gel volume. Rahimi-Aghdam et al. [24] divided the cement paste porosity φ_p into the sum of the inter-particle porosity (capillary porosity) φ_{cap} and the gel porosity φ_{gel} ($\varphi_p = \varphi_{cap} + \varphi_{gel}$). The hindered water is located at the gel porosity, which includes pores with dimensions below 5.6 nm [238]. However, Rahimi-Aghdam et al. [24] mentioned that the Kelvin equation can only be applied to pores larger than 3 nm. Therefore, they divided the gel porosity into the porosity in which the Kelvin equation applies φ_{Kp} and the porosity of the nanopores φ_{np} where it doesn't ($\varphi_{gel} = \varphi_{Kp} + \varphi_{np}$). The water in the gel pores for which Kelvin equation applies is dependent on the saturation degree at the cement gel pores S_{Kp} , which they assumed to be equal to the saturation degree in the inter-particle pores (capillary pores). Consequently, they proposed the water consumption to be calculated according to the following equation:

$$dV_w^t = \frac{n_w M_w}{\rho_w} + dV_g^t (\varphi_{np} + \varphi_{Kp} \cdot S_{Kp}) \quad (3.39)$$

where dV_w is the water consumed, n_w is the number of particles, M_w is the molar mass of water and ρ_w is the density of the water.

The gel porosity φ_{gel} , the gel porosity for which the Kelvin equation is valid φ_{Kp} and the gel porosity at the nanopores φ_{np} are parameters difficult to determine and highly dependent on the concrete matrix [24]. Rahimi-Aghdam et al. [24] proposed that the gel porosity may be considered $\varphi_{gel} = 0.32$, out of which 33% follow the Kelvin equation ($\varphi_{Kp} = 33\% \varphi_{gel}$). One would obtain the value of $\zeta_{wc} = 1.26$ at full saturation, decreasing until $\zeta_{wc} = 1.10$. However, the parameter proposed by Rahimi-Aghdam et al. [24] is $\zeta_{wc,0} = 1.21$ at full saturation, decreasing until $\zeta_{wc} = 1.13$, which would correspond to the porosity in the gel of $\varphi_{gel} = 0.29$, out of which 19% follow the Kelvin equation ($\varphi_{Kp} = 19\% \varphi_{gel}$). Therefore, the $\varphi_{gel} = 0.29$, out of which 19% follow the Kelvin equation ($\varphi_{Kp} = 19\% \varphi_{gel}$) were considered in the implemented model. The other volume fractions are obtained as $\zeta_{cw} = 1/\zeta_{wc}$, $\zeta_{gw} = \zeta_{gc}\zeta_{cw}$ and $\zeta_{CHw} = \zeta_{CHc}\zeta_{cw}$.

Based on the results of the variation of the cement volume dV_c , Rahimi-Aghdam et al. [24] proposed to calculate the decrease in the anhydrous cement particle radius, $a^{t+\Delta t}$, the hydration degree, $\alpha^{t+\Delta t}$, and the increment of the gel barrier, $z^{t+\Delta t}$ according to the following equations:

$$a^{t+\Delta t} = a^t + da^t = a^t + \frac{1}{4\pi a_0^2 n_g} dV_c^t \quad (3.40a)$$

$$\alpha^{t+\Delta t} = \alpha^t + d\alpha^t = \alpha^t - \frac{3}{4\pi a_0^3 n_g} dV_c^t \quad (3.40b)$$

$$z^{t+\Delta t} = z^t + dz^t = z^t + \frac{dV_g^t + dV_c^t}{4\pi (\hat{z}^t)^2}, \quad \text{for } \alpha^t > \alpha_c \quad (3.40c)$$

Equation (3.40c) leads to unrealistic increases in the gel barrier. Comparing Equation (3.40a) with Equation (3.40c), it is clear that Equation (3.40c) is missing the parameter n_g in the denominator. Therefore, Equation (3.40c) presented in [24, 124], was replaced by the following equation:

$$z^{t+\Delta t} = z^t + dz^t = z^t + \frac{dV_g^t + dV_c^t}{4\pi (\hat{z}^t)^2 n_g}, \quad \text{for } \alpha^t > \alpha_c \quad (3.41)$$

Rahimi-Aghdam et al. [24] also proposed a formulation to evaluate the self-desiccation $dh_s^{t+\Delta t}$. For that purpose, the saturation degree variation and the capillary porosity are required. The saturation degree can be estimated using a desorption isotherm law, $dh^t = K_h dS_{cap}^t$, while the capillary porosity is given by:

$$\varphi_{cap}^{t+\Delta t} = \varphi_{cap}^t + d\varphi_{cap}^t = \varphi_{cap}^t - (dV_g^t + dV_{CH}^t + dV_c^t) \quad (3.42)$$

The self-desiccation can be estimated according to the following equation:

$$dh_s^{t+\Delta t} = K_h \left(\frac{-n_g Q^t dt - d\varphi_{cap} S_{cap}^{t+\Delta t}}{\varphi_{cap}^{t+\Delta t}} \right) \quad (3.43)$$

In the absence of more detailed information, Rahimi-Aghdam et al. [24] proposed to evaluate the desorption isotherm parameter as $K_h = 1 - w/c$. Rahimi-Aghdam et al. [124] proposed to evaluate the ultimate degree of hydration α_u according to the following equation:

$$\alpha_u = 0.4 + 1.45 \cdot (w/c - 0.17)^{0.8} \quad (3.44)$$

The present model evaluates the degree of hydration evolution in a pointwise THM analysis. The mechanical properties can be evaluated according to Equation (2.15). Nevertheless, there are some inconveniences when connecting the model to the mechanical analysis:

- many parameters are not easily quantified and are challenging to calibrate when dealing with the simulation of experiments with only experimental data available at the macroscale (e.g. reaction ratios, cement particle sizes, discharge properties, porosity properties, etc);
- the degree of hydration is calculated based on a forward Euler approach, which is dependent on the time discretisation. To ensure accuracy in numerical models, very small time increments are essential, but this generates large output files that can quickly consume significant memory, especially when models incorporate many finite elements.

For these reasons, the transformed times model is more efficient and stable in the pointwise THM analysis. The cement hydration model, when active, will only provide a prediction of the degree of hydration, while the transformed times models are still used for the mechanical properties. Further investigations are required to improve the use of the present model in THM analysis.

3.6 HYGROTHERMAL STRAINS

3.6.1 CONTEXTUAL INTRODUCTION

The objective of this subroutine is to numerically simulate volumetric strains due to hygrothermal variations, hereafter referred to as eigenstrains. Eigenstrains are deformations not caused by external mechanical stresses. In the current pointwise THM model, the use of this term is limited to hygrothermal strains at the integration point, representing the sum of free shrinkage and the local thermal strain. Fig. 41 shows the layout of the eigenstrains subroutine.

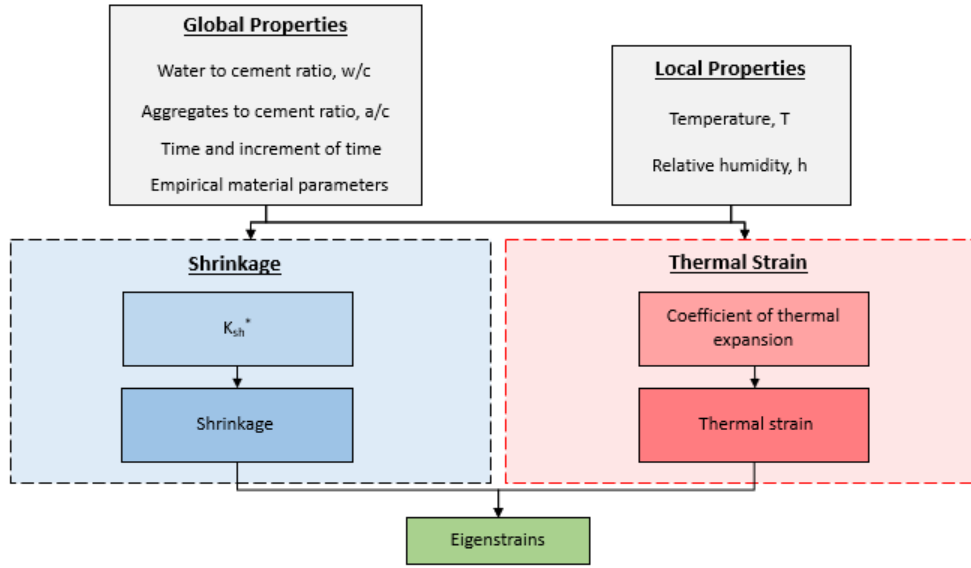


Fig. 41 - Layout of the shrinkage and thermal strain subroutine.

The eigenstrains subroutine calculates both free shrinkage strains and thermal strains. Free shrinkage strains occur due to changes in relative humidity, whereas thermal strains are associated with temperature variations. The free shrinkage and thermal strains are evaluated based on their scalar value at the integration point. Each scalar value is stored in a separate state variable accessed in the post-processing to manage local deformation due to hygrothermal variations in the numerical analysis. Within the pointwise THM model framework, these free shrinkage and thermal strains are summed to form the eigenstrains vector, which is the primary output of this subroutine employed in the mechanical analysis.

3.6.2 IMPLEMENTATION DETAILS

3.6.2.1 Shrinkage model

The free shrinkage strain due to relative humidity is given by the following equation:

$$\dot{\epsilon}_{sh} = \left[\frac{\partial w}{\partial h} \right] k_{sh} \cdot \dot{h} \quad (3.45)$$

where $\dot{\epsilon}_{sh}$ is the free shrinkage rate, $\left[\frac{\partial w}{\partial h} \right]$ is the moisture capacity and k_{sh} is the shrinkage coefficient.

The analysis of desorption curves in Chapter 2.2.2 shows that moisture capacity is often nearly constant in drying scenarios. Additionally, according to Fig. 18, the shrinkage coefficient k_{sh} can be considered constant. Such approach would result in a linear relationship between the free shrinkage rate and the relative humidity rate. However, a nonlinear relationship may provide better predictions for modern concrete mixtures or wetting conditions. Two approaches considering a non-linear shrinkage relationship are investigated. The first is derived from the Kwak equation [123], equation (2.79), as follows:

$$\frac{\partial \varepsilon_{sh}}{\partial t} = \frac{\partial (\varepsilon_{sh,ult} \cdot [0.97 - 1.895 \cdot (h(t) - 0.2)^3])}{\partial t} \rightarrow \dot{\varepsilon}_{sh} = \left[\frac{\partial w}{\partial h} \right] k_{sh} \cdot \dot{h} \quad (3.46)$$

which results in:

$$k_{sh} \cdot \left[\frac{\partial w}{\partial h} \right] = c_1 \cdot (h - c_2)^{c_3} \quad (3.47)$$

where $c_1 = 5.685 \cdot \varepsilon_{sh,ult}$, $c_2 = 0.2$ and $c_3 = 2$ returns the Kwak equation. The Kwak equation in this derived form is hereby called the dKwak equation.

The second option is to adapt the Bažant and Najjar [89] equation for the diffusion processes, equation (2.53) (hereby labelled as BN equation), for the description of the moisture capacity as follows:

$$\left[\frac{\partial w}{\partial h} \right] = c_{BN,1} + \frac{1 - c_{BN,1}}{1 + \left(\frac{1 - h}{1 - c_{BN,2}} \right)^{c_{BN,3}}} \quad (3.48)$$

where $c_{BN,i}$ are calibration parameters.

The experimental desorption data from Van den Heede et al. [231] are analysed to determine which equation best fits the moisture capacity. Van den Heede et al. [239] investigated sorption in three different mixtures to assess the effect of fly ash on sorption curves. The composition of these mixtures is presented in the following table.

Table 8 – Mixture properties of the experimental campaign of Van den Heede et al.

	Mixture 1	Mixture 2	Mixture 3
Strength class	C35/45	C50/60	C25/30
w/c	0.5	0.4	0.4
Cement	350 kg/m ³	400 kg/m ³	200 kg/m ³
Fly ashes	-	-	200 kg/m ³
Aggregates	1834 kg/m ³	1831 kg/m ³	1760 kg/m ³
Water	175 kg/m ³	160 kg/m ³	160 kg/m ³
Superplasticizer	-	1.9 ml/kg cem	2.5 ml/kg cem

Fig. 42 shows the desorption isotherm for the three concrete mixtures.

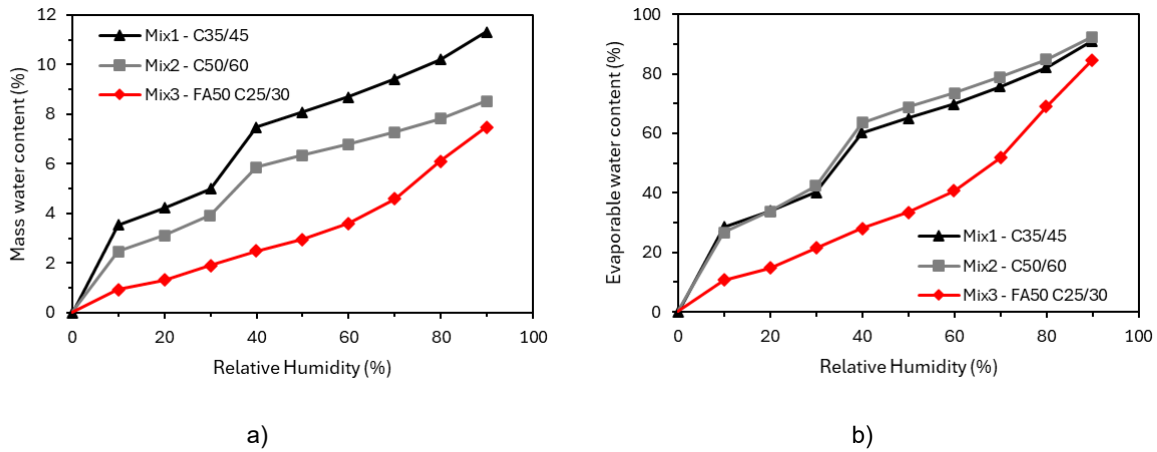


Fig. 42 - The desorption curves for the three mixtures: a) as % of the mass of water content; b) as % of the evaporable water content.

The analysis of the experimental data reveals a distinct difference in behaviour between the concrete mixtures without fly ash and Mixture 3, which contains fly ash. The moisture capacity is considered as the derivative of the desorption data presented in Fig. 42b). The following parameters are used in the calibration of the equation: for the dKwak equation, $c_1 = 5.685$, $c_2 = 0.2$ and $c_3 = 2$; for the BN equation, $c_1 = 0$, $c_2 = 0.65$ and $c_3 = 8$. Fig. 43 shows the adjustment of dKwak equation and BN equation to the moisture capacity evolution.

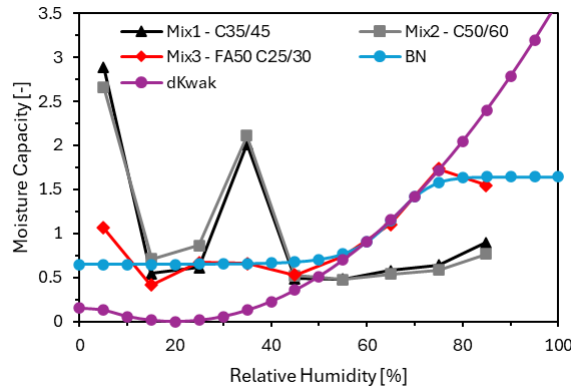


Fig. 43 – Moisture capacity fit to experimental data using dKwak and B-N-s equations.

Analysis of the figure reveals two distinct behaviours. For relative humidities above 40%, concrete mixtures without fly ash exhibit an almost linear moisture capacity, whereas the mixture containing fly ash shows a more nonlinear response. The moisture capacity of Mixture 3 is better captured by nonlinear equations such as the dKwak or the BN equation. For relative humidities below 40%, Mixtures 1 and 2 present nonlinear moisture capacity behaviour, while Mixture 3 exhibits more constant moisture capacity behaviour.

Bissonnette et al. [115] show that the shrinkage coefficient can be considered constant for the investigated concrete mixtures shown in Fig. 18. Nevertheless, no evidence confirms that this holds true for modern concretes. In the numerical simulation of concrete shrinkage using the pointwise mechanical model, it is not strictly necessary to characterise moisture capacity and the shrinkage coefficient separately. Instead, the nonlinearities associated with moisture capacity and potential variations in the

shrinkage coefficient can be mutually addressed by combining both parameters into the equivalent shrinkage coefficient, $k_{sh}^* = [\partial w / \partial h] \cdot k_{sh}$. Nonlinearities in moisture capacity, the shrinkage coefficient, or both will be reflected in the behaviour of the equivalent shrinkage coefficient. Therefore, the dKwak and BN equations can be directly applied to determine the equivalent shrinkage coefficient without the need to quantify the moisture capacity and the shrinkage coefficient separately. The free shrinkage is computed in the mechanical pointwise model according to the following equation:

$$\Delta \varepsilon_{sh} = k_{sh}^* \cdot \Delta h \quad (3.49)$$

Regardless of the chosen equation for the equivalent shrinkage coefficient, special attention is required when the relative humidity drops below 40% or during wetting cycles due to the hysteresis behaviour of sorption curves. This PhD study focuses on cases with relative humidity above 40% and drying scenarios, which are most relevant for structural applications in civil engineering. Future research should address these limitations, if needed.

The implemented rate equation simulates the combined effects of drying and basic shrinkage. Both drying and basic shrinkage are expressed by the relative humidity history obtained in the hygrometric analysis. Drying shrinkage is linked to the moisture transport, while basic shrinkage is simulated by the relative humidity drop associated with self-desiccation. In the present THM framework, a self-desiccation model is implemented based on the basic shrinkage equation of MC2010 (Equation (2.68)). The present self-desiccation model converts the basic shrinkage strains into the equivalent relative humidity drop. Box 3.2 shows the algorithm used for the self-desiccation model implemented in the hygrometric model presented in Chapter 3.3.1.

Box 3.2 - Algorithm for the self-desiccation model based on basic shrinkage.

1. Calculate the equivalent age:

$$\frac{\Delta t_e}{\Delta t} = \beta_{eT} \cdot \beta_{eh}$$

2. Calculate the basic shrinkage according to the MC2010 equation:

$$\varepsilon_{cbs}(t) = \varepsilon_{cbs0} \cdot [1 - \exp(n_{cbs,1} \cdot (t_{eq})^{n_{cbs,2}})]$$

where ε_{cbs0} is the asymptotic basic shrinkage, $n_{cbs,1}$ and $n_{cbs,2}$ are calibration parameters. Considering $n_{cbs,1} = -0.2$ and $n_{cbs,2} = 0.5$ returns the MC2010 basic shrinkage equation.

3. Calculate the relative humidity drop according to the following equation:

$$\dot{h}_{bs} = \frac{\dot{\varepsilon}_{cbs}}{k_{sh}^*} \rightarrow \Delta h_{bs} = \frac{\varepsilon_{cbs}(t_e + \Delta t_e) - \varepsilon_{cbs}(t_e)}{k_{sh}^*}$$

where $k_{sh}^* = [\frac{\partial w}{\partial h}] k_{sh}$ is dependent on the shrinkage model selected, which could be constant, dKwak equation or BN equation.

4. Update the relative humidity at the current step (increment):

$$\hat{h}^{j+1,k} = \hat{h}^j + \Delta \hat{h}^{j+1,k} - \hat{h}_{bs}$$

3.6.2.2 Thermal strains model

The thermal strains are evaluated according to the following Equation.

$$\Delta \varepsilon_T = \alpha_T \cdot \Delta T \quad (3.50)$$

where $\Delta \varepsilon_T$ is the scalar value of the thermal strain increment, α_T is the coefficient of thermal expansion and ΔT is the temperature variation.

Zahabizadeh et al. [55] demonstrated that the coefficient of thermal expansion of concrete, α_T , varies during the early ages. However, this parameter stabilizes few days after casting and can be considered constant over the long term. In the current implementation, the effects of microstructural evolution on the shrinkage coefficient and the coefficient of thermal expansion have not been included. This decision was made due to the difficulty of accurately quantifying these changes at early ages across the various concrete mixtures investigated. Moreover, variations in these parameters occur rapidly within a few hours after setting, during which substantial loading is generally not expected, except in studies involving restrained elements from the time of casting. However, in such cases, the structural response is also influenced by the evolution of stiffness, which is likewise challenging to quantify. Future work should address the implementation of a time-dependent coefficient of thermal expansion and its connection to the implemented cement hydration models, if needed.

3.6.2.3 Eigenstrains computation

The scalar values of the shrinkage and thermal strain are then combined to describe the volumetric deformation at the global coordinate system in a single strain vector:

$$\Delta \varepsilon_{eigen} = (\Delta \varepsilon_{sh} + \Delta \varepsilon_T) \cdot \mathbf{e} \quad (3.51)$$

where $\mathbf{e}$ is the eigenvector given by $\mathbf{e} = [1,1,1,0,0,0]$.

3.7 CONCRETE CREEP AND ELASTICITY

3.7.1 CONTEXTUAL INTRODUCTION

The proposed model delineates three distinct contributions: firstly, an elastic contribution, ε_e , associated with the static modulus of elasticity; secondly, a viscous contribution, ε_v , correlated with the basic creep and modelled through the solidifying Kelvin Chain; and thirdly, a flow contribution, ε_f , associated with the drying creep and conceptualised using the microprestress theory. Fig. 44 shows a schematic presentation of the implemented model.

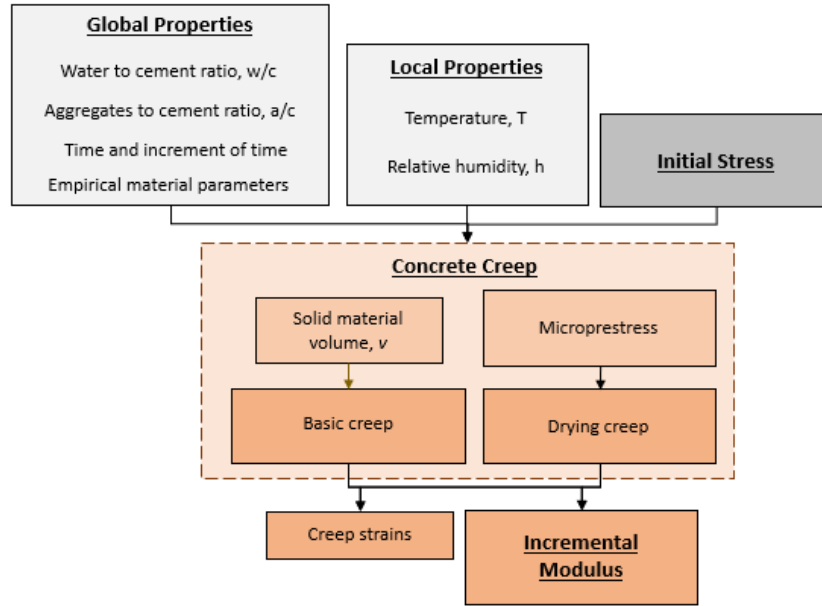


Fig. 44 – Layout of the concrete creep model.

The MPS theory was utilised for the creep model in the present implementation due to its theoretically grounded robustness and compatibility with Models B3/B4. The original formulation of the MPS method is implemented in the pointwise mechanical model presented here, with the recommended empirical parameters applied. Additional details on the generic formulation can be found in Chapter 2.4 [65, 145, 154]. The creep compliance is given by:

$$J(t, t') = q_1 + J_v(t, t') + J_f(t, t') \quad (3.52)$$

where q_1 is the instantaneous strain due to unit stress, also known as asymptotic compliance, $J_v(t, t')$ is the compliance function for the viscoelastic part of creep and $J_f(t, t')$ is the compliance function for the flow part of creep.

The numerical computation process is divided into several subroutines, each addressing distinct tasks of the overall computation:

- evaluate the inverse of the solidifying material volume;
- apply the Post-Widder approach to determine the non-ageing Kelvin Chain parameters;
- calculate the parameters β and λ (Equation (2.177)), essential for the viscoelastic formulation of creep;
- evaluate the flow strain according to the microprestress theory;
- calculate the incremental modulus of elasticity and creep strains at the current step.

3.7.2 IMPLEMENTATION DETAILS

3.7.2.1 Solidified material volume

The viscoelastic part of the creep $J_v(t, t')$ is given by a solidifying Kelvin chain model [154]:

$$J_v(t, t') = \frac{1}{v(t)} \cdot J_0 \quad (3.53)$$

where $v(t)$ is the solidified material volume and J_0 is the non-ageing creep compliance.

The ageing characteristics of concrete creep are addressed by the evolution of the solidified material volume $v(t)$. According to [155, 156], the inverse of the solidifying material volume can be described using a power-law function:

$$\frac{1}{v(t)} = \left[1 + \frac{q_2}{q_3} \left(\frac{1}{t} \right)^{0.5} \right] \quad (3.54)$$

where q_2 and q_3 are model B3/B4 parameters and t is the time in days.

Table 4 shows the relationship between the parameters q_2 and q_3 . The following equation shows this relationship:

$$\frac{1}{a_v} = \frac{q_2}{q_3} = \frac{1}{p_3 \cdot \left(\frac{a/c}{6} \right)^{p_{3a}} \cdot \left(\frac{w/c}{0.38} \right)^{p_{3w}}} \quad (3.55)$$

Equation (3.55) shows that the solidified material volume depends on the cement type and mixture proportions. Fig. 45 shows the evolution of the inverse of the solidified material volume for the model B3/B4 calibration parameters of $a/c = 6$ and $w/c = 0.38$, and a normal concrete hardening with $p_3 = 39.3 \times 10^{-3}$.

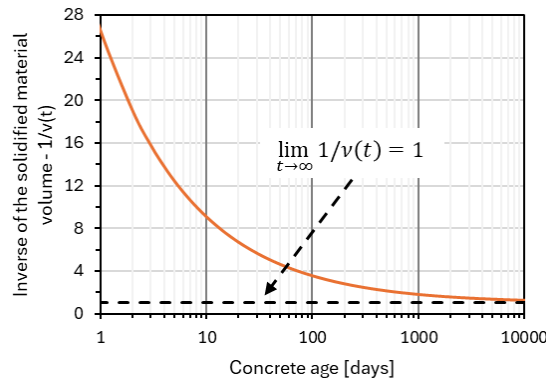


Fig. 45 – Inverse of the solidified material volume

Fig. 45 shows that the inverse of the solidified material volume decreases over time to the asymptotic value of 1. As shown by Equation (3.53), the viscoelastic part of creep is determined by multiplying the non-ageing creep compliance by the inverse of the solidified material volume. The present evolution of the inverse of the solidified material volume shows that creep compliances are increased at early ages. However, over the long term, the inverse of the solidified material volume tends to 1, which means that the viscoelastic part of creep will tend towards non-ageing creep compliance. Nevertheless, reaching the asymptotic value of 1 requires that the solidified material volume continues to increase over time, i.e. the inverse of the solidified material to decrease over time. Since the solidified material volume is related

to the ongoing cement hydration, one should conclude that whenever cement hydration ceases, the evolution of the inverse of the solidified material volume should also halt. This effect is captured by replacing the concrete age in Equation (3.54) by the equivalent age (see Chapter 3.5.2.1). The function β_{eh} (varying between 1 for relative humidity equal to 1 and decreasing with the drying progression) will lead to the equivalent age developing slower than the concrete age, or even halting once the relative humidity is lower than a certain value. The equivalent age $t_e^{t+\Delta t/2}$ used to replace the concrete age t in Equation (3.54) is determined based on the midpoint rule:

$$t_e^{t+\Delta t/2} = t_e^t + \frac{\Delta t_e}{2} \quad (3.56)$$

where t_e^t is a state variable updated in each step using Equation (3.27) and Δt_e is given by Equation (3.26a).

Considering that cement hydration progresses at a much slower rate for a concrete age above 28 days, it is possible to expect long-term creep compliance to be around 4 to 8 times the non-ageing creep compliance. Future works should investigate the connection between the inverse of the solidified material volume and the degree of hydration to comply with the cement hydration model presented in Chapter 3.5.2.2.

The inverse of the solidifying material volume, $1/\nu(t_{eq}^{t+\Delta t/2})$, is stored and returned as output to the calling subroutine.

3.7.2.2 Post-Widder approach

The non-ageing creep compliance is characterised by Equation (2.88), hereby recalled:

$$J_0(t) = q_3 \cdot \ln(1 + (t - t')^{0.1}) \quad (3.57)$$

Equation (3.57) is simulated through a non-ageing Kelvin-Chain. For the implementation in the mechanical pointwise model, the Kelvin Chain parameters need to be determined to provide the creep compliance defined by Equation (3.57). The Least Squares Method (LSM) can be used to determine the Kelvin Chain parameters. However, Bažant and Jirásek [65] have suggested a more straightforward method utilising the retardation spectrum approach. Bažant and Jirásek [65] recommend employing the Post-Widder method with $k = 2$. This method achieves analytical fitting of Equation (3.57) with an error margin below 3%, which the authors consider negligible from an engineering perspective. The inverse of the modulus of elasticity of each Kelvin-Voigt element, calculated using the Post-Widder method proposed by Bažant and Jirásek [65] are given by:

$$\begin{cases} \frac{1}{E_1} = q_3 \cdot \left[\ln(1 + \tilde{\tau}_1) - \frac{\tilde{\tau}_1}{10 \cdot (1 + \tilde{\tau}_1)} \right], & \text{with } \tilde{\tau}_1 = \left(\frac{2 \cdot \tau_{1,days}}{\sqrt{10}} \right)^{0.1} \\ \frac{1}{E_\mu} = q_3 \cdot \ln 10 \cdot \frac{(0.9 + \tilde{\tau}_\mu) \tilde{\tau}_\mu}{10 \cdot (1 + \tilde{\tau}_\mu)^2}, & \text{with } \tilde{\tau}_\mu = (2 \cdot \tau_{\mu,days})^{0.1} \end{cases} \quad (3.58)$$

where $\tau_{i,days}$ are the retardation times [days].

Bažant and Jirásek [65] suggest enhancing accuracy by applying empirical factors to the retardation times and the modulus of elasticity rather than increasing the complexity of the Post-Widder approach. Alternatively, the Kelvin chain fit's accuracy can be improved by introducing calibration parameters, $c_{e,i}$, into Equation (3.58):

$$\begin{cases} \frac{1}{E_1} = c_{e,1} \cdot q_3 \cdot \left[\ln(1 + \tilde{\tau}_1) - \frac{\tilde{\tau}_1}{10 \cdot (1 + \tilde{\tau}_1)} \right], & \text{with } \tilde{\tau}_1 = \left(\frac{2 \cdot \tau_{1,days}}{\sqrt{10}} \right)^{0.1} \\ \frac{1}{E_\mu} = c_{e,\mu} \cdot q_3 \cdot \ln 10 \cdot \frac{(0.9 + \tilde{\tau}_\mu) \tilde{\tau}_\mu}{10 \cdot (1 + \tilde{\tau}_\mu)^2}, & \text{with } \tilde{\tau}_\mu = (2 \cdot \tau_{\mu,days})^{0.1} \end{cases} \quad (3.59)$$

where $c_{e,i}$ are the calibration parameters that, when set equal to 1, return Equation (3.58).

In the pointwise THM model, the retardation times and the number of Kelvin-Voigt elements are inputs in the data file. The default configuration includes 10 Kelvin-Voigt elements, with retardations starting at 5 seconds, according to a geometric sequence, $\tau_{\mu,seconds} = 5 \times 10^{\mu-1}$. An accurate fit of the non-ageing creep compliance without increasing the order of the Post-Widder formula is obtained by setting the parameters $c_{e,1}$ and $c_{e,10}$ to 1.15, while the remaining parameters $c_{e,2 \leq i \leq 9}$ are maintained equal to 1.0. Fig. 46 shows the Post-Widder fit of the Kelvin chain to the compliance of the non-ageing creep, J_0 , for loading applied at 1 day with $q_3 = 1$.

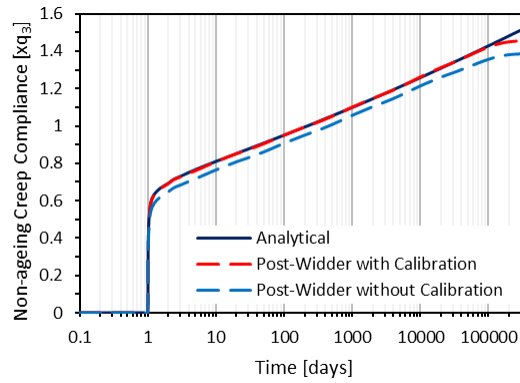


Fig. 46 – Post-Widder fit of the Kelvin chain to the analytical equation for the non-ageing creep compliance in the solidifying theory for loading at 1 day.

The fitting results indicate good agreement between the analytical equation and the Kelvin chain fit for up to 100 000 days, equivalent to approximately 250 years. This type of accuracy is enough for the numerical simulations of the serviceability of most structures.

3.7.2.3 Evaluation of the viscoelastic parameters

Implementing a Kelvin chain model requires the computation of state variables to store stress history effects on creep. The second-order exponential algorithm detailed by Bažant and Jirásek [65] and presented in chapter 2.4.4.4 is adopted in the pointwise THM model. The β_μ and λ_μ parameters are

determined for each Kelvin-Voigt element according to Equation (2.177), hereby recalled in vector form for all Kelvin-Voigt elements μ in the Kelvin chain:

$$\beta_\mu = e^{-\frac{\Delta t_r}{\tau_\mu}} \quad (3.60a)$$

$$\lambda_\mu = (1 - \beta_\mu) \frac{\tau_\mu}{\Delta t_r} \quad (3.60b)$$

where Δt_r is the reduced time given by Equation (3.26b) that replaces Δt in Equation (2.177) to account for the relative humidity and temperature in the viscoelastic creep compliance.

Bažant and Jirásek [65] remark that both parameters computed in Equations (3.60a) and (3.60b) should vary between 1 and 0. They observed that for excessively large values of $\Delta t_r/\tau_\mu$, the parameter β_μ tends to asymptotically approach 0. This scenario can lead to computational overflow and $\beta_\mu = 0$ must be imposed. In contrast, when $\Delta t_r/\tau_\mu$ is much smaller than 1, the value of β_μ approaches 1 and the determination of λ_μ by Equation (3.60b) becomes inaccurate. Therefore, for $\Delta t_r/\tau_\mu$ values much smaller than 1, Bažant and Jirásek [65] suggest replacing Equation (3.60b) with a Taylor series:

$$\lambda_\mu = 1 - \frac{1}{2} \left(\frac{\Delta t_r}{\tau_\mu} \right) + \frac{1}{6} \left(\frac{\Delta t_r}{\tau_\mu} \right)^2 - (\dots) \quad (3.61)$$

For the pointwise mechanical model, the upper and lower limits concerning the validity of Equations (3.60a) and (3.60b) were defined as, if $\Delta t_r > 20 \cdot \tau_\mu$, then $\beta_\mu = 0$ is used instead of Equation (3.60a) and if $\Delta t_r < 10^{-5} \cdot \tau_\mu$, then Equation (3.61) is used instead of Equation (3.60b). The coefficients β_μ and λ_μ are evaluated for each Kelvin-Voigt element μ and stored in two respective vectors β_μ and λ_μ that are returned as output to the calling subroutine.

3.7.2.4 Evaluate the flow strain

The flow part of the creep $J_f(t, t')$ is given by a dashpot with a nonlinear viscosity modulus $\eta(S)$ dependent on the microprestress relaxation [65, 124, 145, 146], in accordance with:

$$J_f(t, t') = \int_{t'}^t \frac{1}{\eta(S)} dr = \int_{t'}^t [c_0 \cdot q_4 \cdot S] dr \quad (3.62)$$

where S is the microprestress variable and c_0 is an empirical parameter.

The relaxation of the microprestress given by Equation (2.133) for the generic value $p = 2$ results in the following equation:

$$\dot{S} + \psi_s \cdot c_0 \cdot S^2 = k_1 \left| \dot{T} \cdot \ln h + T \cdot \frac{\dot{h}}{h} \right| \quad (3.63)$$

where ψ_s is the coefficient for the reduced microprestress time given by Equation (3.25d) and k_1 is an empirical parameter.

Equation (3.63) is a nonlinear differential equation, which cannot be solved analytically due to the inability to separate the time-dependent variables $\dot{S}$ and $\dot{s} = k_1 \left| \dot{T} \cdot \ln h + T \cdot \frac{\dot{h}}{h} \right|$. In finite element implementation, the right-hand side of Equation (3.63) can be linearised over each step increment. Bažant and Jirásek [65] showed that the linearization can be done according to the following equation:

$$\dot{s} = k_1 \left| \dot{T} \cdot \ln h + T \cdot \frac{\dot{h}}{h} \right| = k_1 \left| \frac{(T + \Delta T) \cdot \ln(h + \Delta h) - T \cdot \ln(h)}{T_0 \cdot \Delta t} \right| \quad (3.64)$$

The parameter $\dot{s}$ can now be handled as a constant. Equation (3.63) can be described in the following integral form:

$$\int_{S^t}^{S^{t+\Delta t}} \frac{1}{B^2 - A^2 \cdot S^2} dS = \int_t^{t+\Delta t} dt \quad (3.65)$$

where,

$$A = \sqrt{\psi_s^{t+\Delta t/2} \cdot c_0} \quad (3.66a)$$

$$B = \sqrt{k_1 \left| \frac{(T + \Delta T) \cdot \ln(h + \Delta h) - T \cdot \ln(h)}{T_0 \cdot \Delta t} \right|} \quad (3.66b)$$

Bažant et al. [146], Jirásek and Havlásek [147] and Bažant and Jirásek [65] presented an analytical solution to Equation (3.65). In the pointwise THM model, the following analytical equations were implemented for the solution of Equation (3.65):

$$S^{t+\Delta t} = -\frac{B}{A} \cdot \frac{1 + \tilde{e} \cdot \tilde{\mu}}{1 - \tilde{e} \cdot \tilde{\mu}} \quad (3.67)$$

where,

$$\tilde{\mu} = \frac{A \cdot S^j + B}{A \cdot S^j - B} \quad (3.68)$$

and

$$\tilde{e} = e^{2 \cdot A \cdot B \cdot \Delta t} \quad (3.69)$$

For the special case where the parameter $\tilde{e} < 10^{-6}$, the microprestress can be evaluated based on the non-drying formulation (see Chapter 2.4.3.1). In this particular case, the microprestress at the current step becomes:

$$S^{t+\Delta t} = \frac{S^t}{1 + c_0 \cdot S^t \cdot \Delta t} \quad (3.70)$$

Equations (3.67) to (3.70) are mathematically equivalent to the formulation presented by [65, 146, 147, 240]. The actual time increment Δt is used, since the temperature and relative humidity effects are accounted for in the variable $\psi_s^{t+\Delta t/2}$ that affects the microprestress relaxation function.

The viscosity modulus $\eta(S)$ depends on the microprestress at the current step given by Equation (3.70). Bažant and Jirásek [65] suggested determining the viscosity modulus η according to the following equation:

$$\eta^{t+\Delta t} = \frac{1}{c_0 \cdot q_4 \cdot S^{t+\Delta t} + b_{xmps} \cdot \frac{|S^{t+\Delta t} - S^t|}{\Delta t}} \quad (3.71)$$

where the parameters b_{xmps} results from the XMPS (see chapter 2.4.3.3).

In Equation (3.71), the original MPS formulation is obtained by setting $b_{xmps} = 0$. To account for the temperature and relative humidity effects, the viscosity modulus η should be replaced by the equivalent viscosity modulus $\tilde{\eta}$ given by the following equation:

$$\tilde{\eta}^{t+\Delta t} = \eta^{t+\Delta t} / \psi_r^{t+\Delta t} \quad (3.72)$$

where $\psi_r^{t+\Delta t}$ is given by Equation (3.25c).

Bažant and Jirásek [65] described the total increment of flow creep strains, $\Delta \epsilon_{c\sigma,f}$, according to the following equation:

$$\Delta \epsilon_{c\sigma,f} = \Delta \epsilon'_{c\sigma,f} + c_f \cdot \Delta \sigma \quad (3.73)$$

where $\Delta \epsilon'_{c\sigma,f}$ is the increment of flow creep strain that would occur under constant stress and c_f is the incremental flow modulus that accounts for the flow creep due to the stress increment occurring in the current step.

For the computation of the flow creep strains, it is required to determine the variation in the viscosity modulus during two subsequent steps according to the following equation:

$$\Delta \tilde{\eta} = \tilde{\eta}^{t+\Delta t} - \tilde{\eta}^t \quad (3.74)$$

Bažant and Jirásek [65] compute the increment of flow creep strains under constant stress and the incremental flow compliance according to the following formulation.

If $|\Delta \tilde{\eta}| > 10^{-4} \cdot \tilde{\eta}^t$, the increment of flow creep strains under constant stress and the incremental flow modulus are computed as:

$$\Delta \varepsilon'_{c\sigma,f} = \frac{\Delta t}{\Delta \tilde{\eta}} \cdot \ln \left(1 + \frac{\Delta \tilde{\eta}}{\tilde{\eta}^t} \right) \cdot \mathbf{C} \cdot \boldsymbol{\sigma} \quad (3.75a)$$

$$c_f = \frac{\Delta t}{\Delta \tilde{\eta}} \cdot \left(1 - \frac{\ln \left(1 + \frac{\Delta \tilde{\eta}}{\tilde{\eta}^t} \right)}{\frac{\Delta \tilde{\eta}}{\tilde{\eta}^t}} \right) \quad (3.75b)$$

else, to avoid numerical problems, the increment of flow creep strains under constant stress and the incremental flow modulus are computed as:

$$\Delta \varepsilon'_{c\sigma,f} = \frac{\Delta t}{\tilde{\eta}^t} \cdot \left(1 - \frac{1}{2} \cdot \frac{\Delta \tilde{\eta}}{\tilde{\eta}^t} + \frac{1}{3} \cdot \left(\frac{\Delta \tilde{\eta}}{\tilde{\eta}^t} \right)^2 \right) \cdot \mathbf{C} \cdot \boldsymbol{\sigma} \quad (3.76a)$$

$$c_f = \frac{\Delta t}{\tilde{\eta}^t} \cdot \left(\frac{1}{2} - \frac{1}{3} \cdot \frac{\Delta \tilde{\eta}}{\tilde{\eta}^t} \right) \quad (3.76b)$$

where the matrix $\mathbf{C}$ is given by:

$$\mathbf{C} = \begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1+\nu) & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(1+\nu) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1+\nu) \end{bmatrix} \quad (3.77)$$

where ν is Poisson's ratio.

The flow creep strains $\Delta \varepsilon'_f$ and the incremental flow modulus c_f are the outputs of the flow routine implemented in the creep model.

3.7.2.5 Incremental modulus of elasticity and creep strains

During each incremental time step in the viscoelastic analysis, creep strains are generated due to the current stress increment. Consequently, the elastic modulus E used in the linear-elastic stress-strain relationship must be replaced by the incremental modulus, $\tilde{E}$. The incremental modulus provides a measure of concrete stiffness in a viscoelastic analysis, and it is calculated using the midpoint rule applied to the inverse of the creep compliance. Bažant and Jirásek [65] proposed to evaluate the incremental modulus as follows:

$$\tilde{E} = \left[q_1 + \sum_{\mu=1}^n \frac{1}{\nu \left(t_{eq}^{t+\frac{\Delta t}{2}} \right)} \cdot \left[\frac{1-\lambda_\mu}{E_\mu} \right] + c_f \right]^{-1} \quad (3.78)$$

where q_1 is the static value of the elastic modulus according to model B3/B4, $\sum_{\mu=1}^n \frac{1}{v(t_{eq}^{t+\Delta t/2})} \cdot \left[\frac{1-\lambda_\mu}{E_\mu} \right]$ corresponds to the viscoelastic contribution to the incremental modulus, and c_f is the incremental flow modulus given by Equation (3.75b) or (3.76b).

The total increment of creep strains under constant stress is evaluated according to the following equation:

$$\Delta \epsilon_{c\sigma} = \Delta \epsilon_{c\sigma,vs} + \Delta \epsilon'_{c\sigma,f} \quad (3.79)$$

where $\Delta \epsilon_{c\sigma,vs}$ is the increment of viscoelastic creep strains and $\Delta \epsilon'_{c\sigma,f}$ is the increment of flow creep strains given by Equation (3.75a) or (3.76a).

Bažant and Jirásek [65] proposed to evaluate the increment of viscoelastic strains that would occur under constant stress, $\Delta \epsilon_{c\sigma,vs}$, according to the following Equation:

$$\Delta \epsilon_{c\sigma,vs} = \sum_{\mu=1}^n \frac{1}{v(t_{eq}^{t+\Delta t/2})} \cdot \frac{(1-\beta_\mu)}{E_\mu} \cdot \mathbf{C} \cdot \sigma_{v,\mu}^t \quad (3.80)$$

where $\sigma_{v,\mu}^t$ is the vector that stores the state variables for the viscoelastic stress of the Kelvin-Voigt element μ , defined in the vector form of the stress vector $\sigma_v = [\sigma_{v,x}, \sigma_{v,y}, \sigma_{v,z}, \sigma_{v,xy}, \sigma_{v,yz}, \sigma_{v,xz}]^T$, $1/v(t_{eq}^{t+\Delta t/2})$ is the inverse of the solidified material volume given by Equation (3.54), β_μ is the viscoelastic parameter determined by Equation (3.60a), E_μ is the modulus of elasticity of the Kelvin-Voigt element μ given by Equation (3.59) and the matrix $\mathbf{C}$ is given by Equation (3.77).

The state variables of the viscoelastic stress $\sigma_{v,\mu}$ need to be updated at the end of the current step. Bažant and Jirásek [65] proposed the following equation:

$$\sigma_{v,\mu}^{t+\Delta t} = \lambda_\mu \cdot \Delta \sigma^{t+\Delta t} + \beta_\mu \cdot \sigma_{v,\mu}^t \quad (3.81)$$

where $\sigma_{v,\mu}^{t+\Delta t}$ is the updated viscoelastic stress vector, λ_μ is the viscoelastic parameter determined by Equation (3.60b) and β_μ is the viscoelastic parameter determined by Equation (3.60a). The viscoelastic stress vectors $\sigma_{v,\mu}^{t+\Delta t}$ are saved in the columns of the viscoelastic stress matrix $\sigma_{v,[6 \times \mu]}^{t+\Delta t}$ which is stored in state variables and updated in each step.

3.8 CONTINUUM OR FRACTURE MODEL

3.8.1 CONTEXTUAL INTRODUCTION

The continuum or fracture model's principal objective is to compute the current stress state. The stress calculation represents the last step of the material pointwise THM model and directly or indirectly

interacts with the outputs of all the preceding subroutines. Fig. 47 shows the numerical framework adopted for the continuum or fracture model.

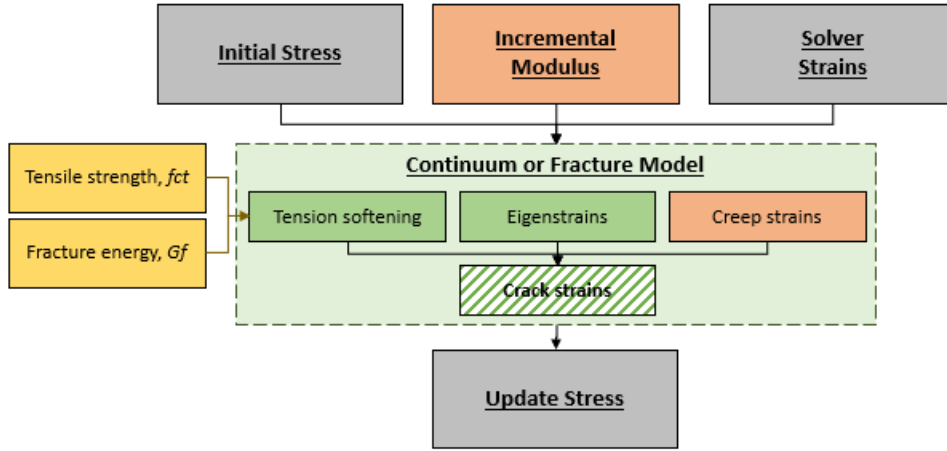


Fig. 47 – Layout of the continuum or fracture model.

The numerical evaluation of the stress state is performed using linear behaviour or a fracture model within the smeared crack concept [211-213]. Different fracture models were implemented for the simulation of cracking:

- total strain model – rotating and fixed crack approach;
- single fixed crack model with strain decomposition.

The selection of the cracking model in the pointwise THM model is performed according to an integer indicator specified in the data input. The integer indicator follows the following codification:

- -1 – the linear model is used and cracking is disabled in the pointwise THM model;
- 0 – the total strain model switching from rotating to fixed cracks is selected;
- 1 – the total strain model with rotating cracks is selected;
- 2 – the total strain model with fixed cracks is selected;
- 4 – the single fixed crack model with strain decomposition is used.

3.8.2 IMPLEMENTATION DETAILS

3.8.2.1 Linear behaviour

The linear model evaluates the stress using a linear incremental rate approach. The increment of stress $\Delta\sigma$ is determined based on the following formulation [65]:

$$\Delta\sigma = \tilde{E} \cdot \mathbf{D} \cdot (\Delta\epsilon - \Delta\epsilon_{eigen} - \Delta\epsilon_{creep}) \quad (3.82)$$

where $\tilde{E}$ is the incremental modulus given by Equation (3.78), $\Delta\epsilon_{eigen}$ is the eigenstrains vector due to temperature and relative humidity variations given by Equation (3.51), $\Delta\epsilon_{creep}$ is the increment of creep strains that would occur under constant stress obtained in the creep and elasticity model given by

Equation (3.80), $\Delta \epsilon$ is the strain increment obtained through the iterative process implemented in DIANA FEA, and $\mathbf{D}$ is the inverse of matrix $\mathbf{C}$ given by:

$$\mathbf{D} = \frac{1}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \quad (3.83)$$

where ν is Poisson's ratio.

The stress is updated according to the following Equation:

$$\sigma^{t+\Delta t} = \sigma^t + \Delta \sigma \quad (3.84)$$

where $\sigma^{t+\Delta t}$ is the stress vector at the current step and σ^t is the stress vector at the beginning of the analysis.

3.8.2.2 General aspects of the cracking models

Crack initiation is defined by a specific failure criterion. In the case of brittle materials like concrete, the Rankine criterion, also referred to as the maximum principal stress criterion, is commonly used. This criterion assumes that cracking occurs when the maximum principal stress at a point reaches the material's uniaxial tensile or compressive strength. When applying the Rankine criterion in cracking models, a tensile cut-off criterion must be specified to define the onset of cracking. The constant and linear tension cut-off models are widely used approaches in the simulation of concrete cracking [211, 230]. Fig. 48 shows the constant and linear tension cut-off models.

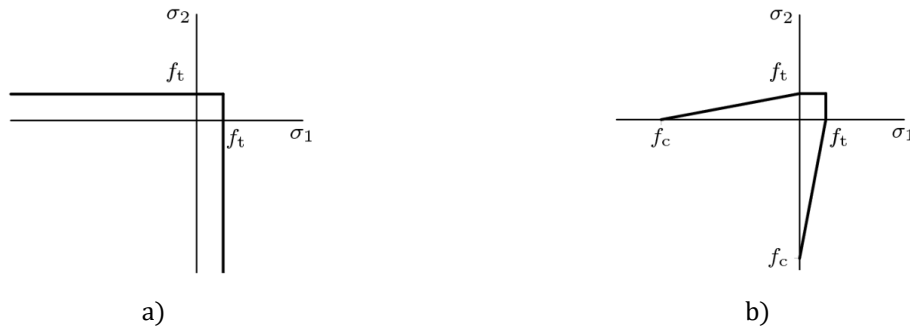


Fig. 48 – Tension cut-off model: a) constant; b) linear (adapted from [230]).

The pointwise THM model considers the constant tension cut-off model, which assumes that a crack initiates once one of the principal stresses, σ_1 or σ_2 , reaches the tensile strength of the material f_t . The verification is carried out according to the selected tension softening model through the following equation:

$$\begin{cases} \sigma_1 \leq f_{ct}(t) & \text{for the Hordijk Tension Softening} \\ \sigma_1 \leq 0.9 \cdot f_{ct}(t) & \text{for the MC2010 Bilinear Tension Softening} \end{cases} \quad (3.85)$$

where σ_1 is the maximum principal stress value and $f_{ct}(t)$ is the tensile strength at the concrete age t .

The evolution of the strength and fracture energy of concrete in tension due to the maturity of mechanical properties is reproduced through time-based equations [49, 241] of the form:

$$\begin{cases} f_i(t) = f_{i,28} \cdot \left(\exp \left[n_{i,1} \cdot \left(1 - \left(\frac{28}{t} \right)^{n_{i,2}} \right) \right] \right)^{n_{i,3}} \\ G_f(t) = G_{f,28} \cdot \frac{f_c(t)}{f_{c,28}} \end{cases} \quad (3.86)$$

where f_i is the tensile strength f_{ct} , or compressive strength f_c at time t , $f_{i,28}$ is the tensile or compressive strength at 28 days, $n_{i,1}$, $n_{i,2}$ and $n_{i,3}$ are model parameters for tensile or compressive strength evolution and $G_{f,28}$ is the fracture energy at 28 days.

The effect of temperature and relative humidity on the evolution of the mechanical properties in Equation (3.86) is obtained by replacing the concrete age t by the equivalent time $t_e^{t+\Delta t/2}$.

To decrease the number of nonlinearities in the cracking model, once a crack occurs in a specific integration point, the tensile strength and fracture energy are assumed to be constant in that integration point and equal to the value at cracking initiation for the remaining analysis time. Notice that in the uncracked integration points, the mechanical properties continue to be affected by the maturity model.

If the crack model indicator is >-1 and Equation (3.85) is not satisfied, the strain increment is divided into two components, $\Delta \boldsymbol{\varepsilon} = \Delta \boldsymbol{\varepsilon}_a + \Delta \boldsymbol{\varepsilon}_b$. The strain increment $\Delta \boldsymbol{\varepsilon}_a$ is the elastic part of the strain increment that would lead to an equality in Equation (3.85), while the strain increment $\Delta \boldsymbol{\varepsilon}_b$ is the inelastic part of the total strain increment computed in the fracture model. The determination of the $\Delta \boldsymbol{\varepsilon}_a$ and $\Delta \boldsymbol{\varepsilon}_b$ is performed according to the following equation:

$$\begin{cases} \Delta \boldsymbol{\varepsilon}_a = f_{lin} \cdot \Delta \boldsymbol{\varepsilon} \\ \Delta \boldsymbol{\varepsilon}_b = (1 - f_{lin}) \cdot \Delta \boldsymbol{\varepsilon} \end{cases} \quad (3.87)$$

where,

$$f_{lin} = \frac{f_{ct} - \sigma_1^t}{\sigma_{1,lin}^{t+\Delta t} - \sigma_1^t} \quad (3.88)$$

where $\sigma_{1,lin}^{t+\Delta t}$ is the principal stress that would result from the computation of the stress using the linear model and does not comply with Equation (3.85) ($\sigma_{1,lin}^{t+\Delta t} > f_{ct}$) and σ_1^t is the principal stress at the beginning of the current time step (before loading).

The strain increment $\Delta \boldsymbol{\varepsilon}_a$ is applied within the linear behaviour model presented in Chapter 3.8.2.1. The remaining strain increment $\Delta \boldsymbol{\varepsilon}_b$ is provided to the cracking model. When considering the fixed cracks models, the principal directions are determined and fixed for the stress state after applying $\Delta \boldsymbol{\varepsilon}_a$ ($\sigma_1 =$

f_{ct}) and before applying $\Delta\epsilon_b$. This process is important for correctly determining the fixed crack directions, especially when dealing with principal directions rotation due to the current step strain increment.

In the cracking model including switching from rotating to fixed cracks, it is necessary to assess whether the crack strain exceeds the crack strain switch threshold. This process can be done by comparing the maximum crack strain with the crack switching strain according to the following equation.

$$\max[\epsilon_{cr,nst}] \leq \epsilon_{cr,switch} \quad (3.89)$$

where $\epsilon_{cr,switch}$ is the crack strain for the switch from the total strain rotating model to the total strain fixed model.

If Equation (3.89) is not fulfilled, then the strain increment is divided into two components: one part used in the rotating model and the second used in the fixed crack model. The numerical process requires transposing the crack strain for switching from the rotating to the fixed crack model into the corresponding total strain $\epsilon_{t,switch}$. Formerly, the computation process is the same as used in Equation (3.87), but replacing the factor f_{lin} by the total strain switching factor f_{switch} given by:

$$f_{switch} = \frac{\epsilon_{cr,t,switch} - \epsilon_{t,1}^t}{\epsilon_{t,1}^{t+\Delta t} - \epsilon_{t,1}^t} \quad (3.90)$$

where $\epsilon_{t,switch}$ is the total strain that would lead to $\epsilon_{cr,switch}$, $\epsilon_{t,1}^t$ is the maximum principal strain for the total strain vector at the beginning of the step and $\epsilon_{t,1}^{t+\Delta t}$ is the maximum principal strain for the total strain vector at the end of the step.

When there is a change from the rotating crack model to the fixed crack model, the rotating model is used with the first strain increment that would bring the total strain to $\epsilon_{t,switch}$. Then, the principal directions of the current total strain vector, ϵ_{tot} , are determined and stored for the rest of the numerical analysis (in the total strain model, the principal directions of the stress and strain vector are the same). The total strain model with fixed cracks is used for the remaining part of the analysis. In the pointwise THM model, the crack models are irreversible, meaning that once the rotating crack model is activated, even if there is unloading, the rotating crack model will remain active. The same happens if the crack strain switch threshold is exceeded, even if unloading occurs to a total strain below the crack switch threshold or even linear behaviour, the fixed crack model will remain active.

3.8.2.3 Total strain crack model with rotating cracks

The total strain crack model is implemented in a rotating crack formulation based on the principle that the principal strain directions are the same as the principal stress directions and that three mutually orthogonal cracks can occur aligned with the principal or crack directions. The evaluation of the principal strains or stresses and respective principal directions is an important issue in any of the

implemented cracking models. Different numerical algorithms are commonly used to compute the principal vectors and directions, including :

- the polar formulation;
- the Jacobian method;
- the QR algorithm.

While these algorithms may yield satisfactory results in determining the principal values for general cases, they encounter challenges in specific cases, notably in the precise computation of principal directions in 3D tensors. Therefore, in the pointwise THM model, the principal values and directions were computed following a subroutine from the LAPACK library [242]. LAPACK includes a set of optimised routines designed for advanced linear algebra computations. The LAPACK's capability to accurately evaluate eigenvalues and eigenvectors of a symmetric matrix is particularly relevant in the present context. The LAPACK subroutine DSYEVX (D – Double precision, SY – symmetric matrix, EV – eigenvalues and eigendirections, X – Extended version) is selected to compute the eigenvalues and eigenvectors, which correspond to the principal strains and principal directions, respectively. To utilise DSYEVX, the strain vector $\boldsymbol{\varepsilon}_{xyz-\varepsilon}^{t+\Delta t} = [\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{xy}, \varepsilon_{yz}, \varepsilon_{xz}]^T$ must be written in the tensor format described by the following matrix:

$$\boldsymbol{\varepsilon}_{xyz[3 \times 3]-\varepsilon}^{t+\Delta t} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \quad (3.91)$$

The superscript t represents the variable at the beginning of the step, and $t + \Delta t$ represents the variable at the end of the step. If a variable does not present the superscript t or $t + \Delta t$, it is implicit that the variable remains constant throughout the current step. The strain tensor includes the tensorial shear strain components, ε_{ij} , instead of the engineering shear strain γ_{ij} [243]. This ensures that the principal directions of the strain tensor are equal to the principal directions of the stress tensor. To clearly distinguish the strain vector or tensor nomenclature limited to this chapter, the subscript “ $-\varepsilon$ ” is appended to the coordinate indices to indicate that the strain vector or tensor is constituted by the tensorial shear strain components ε_{ij} instead of the engineering shear strain γ_{ij} .

The principal strains are stored in a vector, $\boldsymbol{\varepsilon}_{nst-\varepsilon}^{t+\Delta t} = [\varepsilon_{nn}, \varepsilon_{ss}, \varepsilon_{tt}, \varepsilon_{ns}, \varepsilon_{st}, \varepsilon_{nt}]^T$, while the principal directions are stored in the columns of the rotation vector, which is given by:

$$\mathbf{R} = [\mathbf{n} \ \mathbf{s} \ \mathbf{t}] = \begin{bmatrix} c_{xn} & c_{xs} & c_{xt} \\ c_{yn} & c_{ys} & c_{yt} \\ c_{zn} & c_{zs} & c_{zt} \end{bmatrix} \quad (3.92)$$

where c_{ij} is the cosine of the angle between the j vector and the i vector.

The principal strains can be obtained through the rotation of the strain vector, as described by the following equation:

$$\boldsymbol{\varepsilon}_{nst[3 \times 3]-\varepsilon} = \mathbf{R}^T \times \boldsymbol{\varepsilon}_{xyz[3 \times 3]-\varepsilon} \times \mathbf{R} \quad (3.93)$$

where $\boldsymbol{\varepsilon}_{\text{nst},[3 \times 3],t}$ is the strain tensor representation for the principal strains, characterised by the principal strain values in the diagonal elements, while the off-diagonal elements are zeros.

The principal strains are stored in a single vector $\boldsymbol{\varepsilon}_{\text{nst}-\varepsilon}^{t+\Delta t}$ and the principal directions are stored in the matrix $\mathbf{R}^{t+\Delta t}$. Notice that the shear strain components in the principal directions of the vector $\boldsymbol{\varepsilon}_{\text{nst}-\varepsilon}^{t+\Delta t}$ are obviously null, $\varepsilon_{ns} = \varepsilon_{st} = \varepsilon_{nt} = 0$.

In DIANA FEA, as in other typical finite element software, the stress and strain tensors are generally written in a vectorial form. Therefore, the strain vector $\boldsymbol{\varepsilon}_{\text{nst}-\varepsilon}^{t+\Delta t} = [\varepsilon_n, \varepsilon_s, \varepsilon_t, \varepsilon_{ns}, \varepsilon_{st}, \varepsilon_{tn}]^T$ can be obtained by a rotation of the strain vector in the global coordinate system $\boldsymbol{\varepsilon}_{xyz-\varepsilon}^{t+\Delta t} = [\varepsilon_x, \varepsilon_y, \varepsilon_z, \varepsilon_{xy}, \varepsilon_{yz}, \varepsilon_{zx}]^T$, according to the following equation:

$$\boldsymbol{\varepsilon}_{\text{nst}-\varepsilon}^{t+\Delta t} = \mathbf{T} \boldsymbol{\varepsilon}_{xyz-\varepsilon}^{t+\Delta t} \quad (3.94)$$

where $\mathbf{T}$ is the transformation matrix, which is given by:

$$\mathbf{T} = \begin{bmatrix} c_{xn}^2 & c_{yn}^2 & c_{zn}^2 & 2 \cdot c_{xn}c_{yn} & 2 \cdot c_{yn}c_{zn} & 2 \cdot c_{xn}c_{zn} \\ c_{xs}^2 & c_{ys}^2 & c_{zs}^2 & 2 \cdot c_{xs}c_{ys} & 2 \cdot c_{ys}c_{zs} & 2 \cdot c_{xs}c_{zs} \\ c_{xt}^2 & c_{yt}^2 & c_{zt}^2 & 2 \cdot c_{xt}c_{yt} & 2 \cdot c_{yt}c_{zt} & 2 \cdot c_{xt}c_{zt} \\ c_{xn}c_{xs} & c_{yn}c_{ys} & c_{zn}c_{zs} & c_{xn}c_{ys} + c_{xs}c_{yn} & c_{yn}c_{zs} + c_{ys}c_{zn} & c_{xn}c_{zs} + c_{xs}c_{zn} \\ c_{xs}c_{xt} & c_{ys}c_{yt} & c_{zs}c_{zt} & c_{xs}c_{yt} + c_{xt}c_{ys} & c_{ys}c_{zt} + c_{yt}c_{zs} & c_{xs}c_{zt} + c_{xt}c_{zs} \\ c_{xn}c_{xt} & c_{yn}c_{yt} & c_{zn}c_{zt} & c_{xn}c_{yt} + c_{xt}c_{yn} & c_{yn}c_{zt} + c_{yt}c_{zn} & c_{xn}c_{zt} + c_{xt}c_{zn} \end{bmatrix} \quad (3.95)$$

where c_{ij} is the cosine of the angle between the j vector and the i vector.

The reverse operation is performed according to the following equation:

$$\boldsymbol{\varepsilon}_{xyz-\varepsilon}^{t+\Delta t} = \mathbf{T}^{-1} \boldsymbol{\varepsilon}_{\text{nst}-\varepsilon}^{t+\Delta t} \quad (3.96)$$

where $\mathbf{T}^{-1}$ is the inverse of the transformation matrix $\mathbf{T}$, given by:

$$\mathbf{T}^{-1} = \begin{bmatrix} c_{xn}^2 & c_{xs}^2 & c_{xt}^2 & 2 \cdot c_{xn}c_{xs} & 2 \cdot c_{xs}c_{xt} & 2 \cdot c_{xn}c_{xt} \\ c_{yn}^2 & c_{ys}^2 & c_{yt}^2 & 2 \cdot c_{yn}c_{ys} & 2 \cdot c_{ys}c_{yt} & 2 \cdot c_{yn}c_{yt} \\ c_{zn}^2 & c_{zs}^2 & c_{zt}^2 & 2 \cdot c_{zn}c_{zs} & 2 \cdot c_{zs}c_{zt} & 2 \cdot c_{zn}c_{zt} \\ c_{xn}c_{yn} & c_{xs}c_{ys} & c_{xt}c_{yt} & c_{xn}c_{ys} + c_{xs}c_{yn} & c_{xs}c_{yt} + c_{xt}c_{ys} & c_{xn}c_{yt} + c_{xt}c_{yn} \\ c_{yn}c_{zn} & c_{ys}c_{zs} & c_{yt}c_{zt} & c_{yn}c_{zs} + c_{ys}c_{zn} & c_{ys}c_{zt} + c_{yt}c_{zs} & c_{yn}c_{zt} + c_{yt}c_{zn} \\ c_{xn}c_{zn} & c_{xs}c_{zs} & c_{xt}c_{zt} & c_{xn}c_{zs} + c_{xs}c_{zn} & c_{xs}c_{zt} + c_{xt}c_{zs} & c_{xn}c_{zt} + c_{xt}c_{zn} \end{bmatrix} \quad (3.97)$$

Note that although the rotation matrix $\mathbf{R}$ is orthogonal ($\mathbf{R}^{-1} = \mathbf{R}^T$), this characteristic does not extend to the transformation matrix $\mathbf{T}$. This distinction can be validated by comparing the transpose of the transformation matrix in Equation (3.95) with its inverse presented in Equation (3.97), where it is evident that the off-diagonal terms do not match ($\mathbf{T}^{-1} \neq \mathbf{T}^T$).

3.8.2.3.1 Discussion of the formulation of total strain models for linear behaviour simulation

In the total strain model formulation, constitutive laws are defined directly in the principal-strain directions, in contrast with the linear model in Chapter 3.8.2.1 that computes stresses in the global coordinate system xyz . This chapter compares stress calculations in the global coordinate system xyz with those performed on the principal coordinate system or other rotated systems nst . As shown in Chapter 3.8.2.3, the transformation matrix is not orthogonal ($\mathbf{T}^T \neq \mathbf{T}^{-1}$). To decide which form of the transformation matrix, the inverse $\mathbf{T}^{-1}$ or the transposed $\mathbf{T}^T$, should be used in the total strain models, let's consider the linear-elastic simulation of concrete governed by the following equation:

$$\Delta \sigma_{xyz} = \mathbf{D}^{co} \Delta \epsilon_{xyz} \quad (3.98)$$

Rotating equation (3.98) to the principal directions, one obtains:

$$\Delta \sigma_{nst} = \mathbf{T} \mathbf{D}^{co} \mathbf{T}^{-1} \Delta \epsilon_{nst} \rightarrow \Delta \sigma_{nst} = \mathbf{T} \mathbf{D}^{co} \mathbf{T}^{-1} \mathbf{T} \Delta \epsilon_{xyz} \quad (3.99)$$

Since the $\mathbf{T}^{-1} \mathbf{T} = \mathbf{I}$ (where $\mathbf{I}$ is the identity matrix), substitution into equation (3.99) results in:

$$\Delta \sigma_{nst} = \mathbf{T} \mathbf{D}^{co} \Delta \epsilon_{xyz} \quad (3.100)$$

Combining with equation (3.98) recovers the rotation of the stress vector from the global coordinate system to the principal coordinate system:

$$\Delta \sigma_{nst} = \mathbf{T} \Delta \sigma_{xyz} \quad (3.101)$$

By contrast, if one were to use the transpose $\mathbf{T}^T$ matrix, then $\mathbf{T}^T \mathbf{T} \neq \mathbf{I}$, and Equation (3.99) would not be satisfied.

In the total strain models, a linear constitutive behaviour would result in the following equation:

$$\sigma_{nst} = \mathbf{D}_{lin} \epsilon_{nst-\epsilon} \quad (3.102)$$

where $\mathbf{D}_{lin}$ is the multiplication of the isotropic version of Poisson's ratio matrix $\mathcal{P}^{-1}$ by the modulus of elasticity.

In the total strain model with rotating cracks, the stress and strain vectors are formulated in the principal coordinate system, so all shear components vanish. Consequently, the stiffness matrix $\mathbf{D}_{lin}$ presents similarities with the matrix $\mathbf{D}^{co}$, without the shear components. However, $\mathbf{D}_{lin} \neq \mathbf{T} \mathbf{D}^{co} \mathbf{T}^{-1}$, which is the matrix used in equation (3.99). Despite these differences, both approaches yield the same stress because they employ different strain vectors. In the total strain model with rotating cracks, the strain vector in the principal directions, $\epsilon_{nst-\epsilon}$, does not have shear components, whereas in equation (3.99) the strain vector, $\Delta \epsilon_{nst}$, contains engineering shear strains that are not zero in the principal coordinate system. The distinctions in the formulation of the strain vector guarantee mathematical equivalence despite the differences in the stiffness matrix.

When cracks are assumed to be fixed, the principal axes generally do not coincide with the crack directions. Denoting the fixed-crack transformation matrix $\mathbf{T}_{\text{fixed}} \neq \mathbf{T}$, the strain vector in the fixed coordinate system, is given by the following equation.

$$\Delta \boldsymbol{\varepsilon}_{\text{fixed}-\varepsilon} = \mathbf{T}_{\text{fixed}} \Delta \boldsymbol{\varepsilon}_{xyz-\varepsilon} \quad (3.103)$$

The shear strain components ε_{xy} , ε_{yz} and ε_{xz} have, in general, nonzero values. Consequently, the constitutive law in Equation (3.102) must be written in full $[6 \times 6]$ form. The linear behaviour equality provided by Equation (3.98) is granted by considering the new shear terms $D_{\text{lin},ii} = 2 \times D_{ii}^{\text{co}}$ for $i > 3$. An alternative is to convert the tensorial shear strains into engineering shear strains $\Delta \boldsymbol{\varepsilon}_{\text{fixed}-\varepsilon} \rightarrow \Delta \boldsymbol{\varepsilon}_{\text{fixed}}$ and then simply use the $\mathbf{D}^{\text{co}}$. This is mathematically equivalent to defining a new global coordinate system xyz' defined by the $\mathbf{T}_{\text{fixed}}$. Both derivations prove that the total strain model exactly reproduces linear-elastic behaviour. However, caution is required whenever the crack orientation does not coincide with the principal-stress axes since tensorial and engineering shear strains are no longer equivalent under general rotations.

3.8.2.3.2 Stress-total strain relationship

In the total strain models, the principal stresses are computed based on a prescribed stress-strain relationship defined by the uniaxial behaviour of concrete for the three principal directions nst according to the following equation:

$$\boldsymbol{\sigma}_{nst}^{t+\Delta t} = f(\tilde{\boldsymbol{\varepsilon}}_{nst}^{t+\Delta t}, \boldsymbol{\kappa}) \quad (3.104)$$

where $\boldsymbol{\kappa}$ are internal state variables that keep track of damage and other parameters that may influence the stress calculation.

The function $f(\tilde{\boldsymbol{\varepsilon}}_{nst}^{t+\Delta t}, \boldsymbol{\kappa})$ is normally given by the uniaxial behaviour of concrete, i.e., the tension softening model. In total strain models, the function $f(\tilde{\boldsymbol{\varepsilon}}_{nst}^{t+\Delta t}, \boldsymbol{\kappa})$ can be formulated accounting for the sum of the viscoelastic and cracking components of the total strain [229] ($\varepsilon = \varepsilon_{ve} + \varepsilon_{cr}$). Therefore, the stress-strain relationship is given by the following equation:

$$\sigma(\varepsilon) = \int_0^\varepsilon \frac{1}{E_t(\varepsilon')} d\varepsilon' = \int_0^\varepsilon \left[\frac{1}{\tilde{E}} + \frac{1}{D_{cr}(\varepsilon_{cr})} \right] d\varepsilon' \quad (3.105)$$

where ε_{ve} is the viscoelastic part of the total strain, ε_{cr} is the cracking part of the total strain (crack strain in the present example), D_{cr} is the cracking modulus in tension softening and E_t is the total strain modulus.

Fig. 49 shows the tension and shear relationship between elastic and inelastic components given by Equation (3.105).

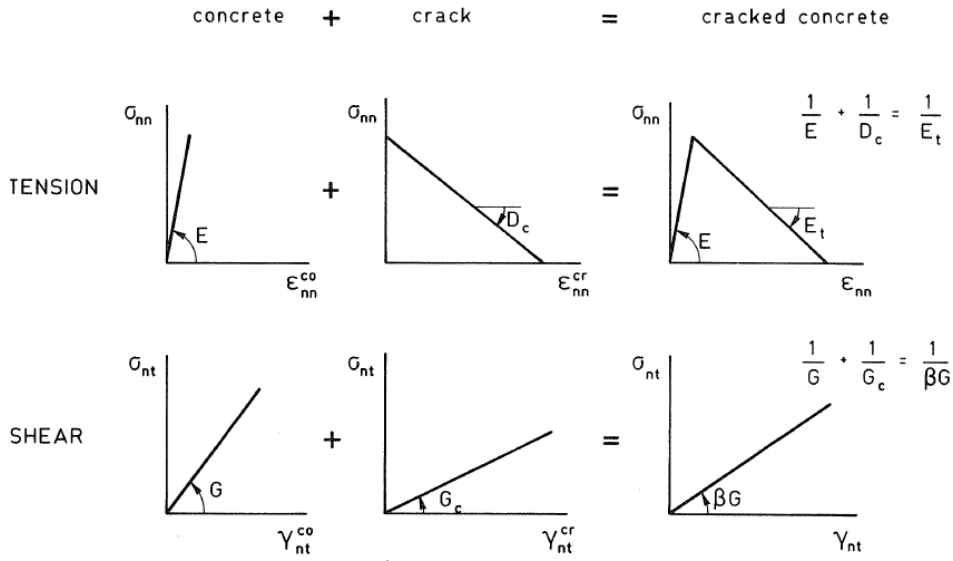


Fig. 49 – Illustration of a series arrangement of concrete and crack [229].

In the smeared crack approach in finite element analysis, the crack band theory is assumed for the fracture simulation [208]. The user specifies the crack bandwidth in the pointwise model, typically using either the finite element size orthogonal to the direction of crack propagation or the cube root of the finite element's volume. Therefore, $D_{cr}(\epsilon_{cr})$ is dependent on the crack bandwidth, and by analogy, Equation (3.105) becomes also dependent on the FE mesh size.

Fig. 50 shows the computation of the stress in one principal direction, according to the total strain model.

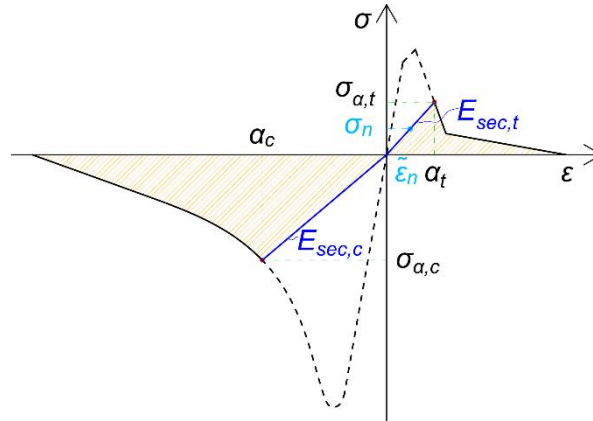


Fig. 50 - Schematic representation of the stress calculation in the total strain model.

The current stress-strain relationship in Fig. 50 is presented for a hypothetical scenario where loading and unloading have occurred in both the tensile and compressive states. The combination of the external dashed line with the continuous line represents the initial stress-strain relationship for monotonically increasing strains. For each principal direction, nst , the internal damage variable is used to monitor deterioration due to cracking α_t or crushing α_c are used in the stress-strain model to determine the auxiliary stress $\sigma_{\alpha,t}$ in tension and $\sigma_{\alpha,c}$ in compression. The elastic secant modulus $E_{sec,nst}$, can be determined according to the following equation:

$$E_{sec,nst} = \frac{\sigma_\alpha}{\alpha} \quad (3.106)$$

The vector α stores the internal damage variables α_t and α_c for each of the principal directions nst . This vector can be updated according to the following equation [230]:

$$\alpha^{t+\Delta t} = \alpha^t + \mathbf{W} \Delta \tilde{\epsilon}_{nst,\alpha} \quad (3.107)$$

where $\Delta \tilde{\epsilon}_{nst,\alpha}$ represents the increment of equivalent strain relative to the previous vector α^t and $\mathbf{W}$ represents a binary matrix that indicates whether loading is occurring at the current step [230]. In the rotating model, the principal directions nst may change over time affecting the storing position of the internal damage variables in the vector α . The model assumes that the principal directions rotate minimally from the previous rotation vector, adhering to the hypothesis that loading is consistently applied in a smooth manner. The methodology for unloading and reloading follows the secant-to-origin path as long as the equivalent uniaxial strain $\tilde{\epsilon}_{nst}$ remains within the strain limits stored in vector α . If these limits are exceeded, the vector α is updated using equation (3.107) and a new elastic secant modulus is computed using equation (3.106).

3.8.2.3.3 Loading and unloading auxiliary parameters

The methodology for handling loading and unloading processes follows a secant-to-origin path adopted in the total strain models described by DIANA FEA [230]. The implemented numerical algorithm can also be used for nonlinear compression behaviour. However, in the pointwise THM model, the compressive behaviour is assumed to be linear, since for the case studies considered in this PhD work, the compressive stresses are expected to be far from the compressive strength. Further investigation on the nonlinear behaviour under compression is considered for future work. The computation of loading and unloading parameters requires the definition of three distinct variables: the vector α , the vector $\mathbf{r}$ and the matrix $\mathbf{W}$. The vector $\mathbf{r}$ contains integer indicators that represent whether each component of the equivalent uniaxial strain vector $\tilde{\epsilon}_{nst}$ is increasing or decreasing, i.e., loading or unloading, respectively and is only used in the computation of matrix $\mathbf{W}$. The indicators for tension are stored in the first three indices of the vector $\mathbf{r}$. The formulation of the vector $\mathbf{r}$ and matrix $\mathbf{W}$ for the compression indices can be found in [230]. The vector $\mathbf{r}$ (for tension indices) is computed according to the following equation:

$$r_i = \begin{cases} 0 & \text{if } \tilde{\epsilon}_{nst,i}^{t+\Delta t} > \alpha_i^t \\ 1 & \text{if } \tilde{\epsilon}_{nst,i}^{t+\Delta t} \leq \alpha_i^t \end{cases} \quad \text{for } i = 1, \dots, \text{length}(nst) \quad (3.108)$$

where $\tilde{\epsilon}_{nst,i}$ is the component i of the equivalent uniaxial strain vector $\tilde{\epsilon}_{nst}$ and α_i^t is a parameter representing the maximum equivalent uniaxial strain for all the previous steps.

The matrix $\mathbf{W}$ is constituted only of 0 or 1 values, indicating whether there is loading or unloading. The matrix $\mathbf{W}$ according to the following Equation:

$$W_{ij} = (1 - r_i) \cdot \delta_{ij} \quad (3.109)$$

where δ_{ij} is the Kronecker delta function that is 1 for $i = j$ and 0 for $i \neq j$.

The computation of matrix $\mathbf{W}$ is only used to update vector $\boldsymbol{\alpha}^{t+\Delta t}$ through Equation (3.107).

3.8.2.3.4 Poisson's ratio matrix and equivalent uniaxial strains

In the total strain models, using a uniaxial stress-strain relationship (as established by Equation (3.104)) requires the consideration of the lateral expansion effects due to Poisson's ratio. Selby [244] modelled this effect by employing a pre-strain concept, in which lateral expansion is accounted for with an additional external loading on the structure. As shown in Chapter 3.8.2.3.1, the concrete behaviour in the principal directions is given by Equation (3.102). For the isotropic behaviour, considering $\mathbf{D}_{lin} = \mathbf{E} \cdot \mathcal{P}^{-1}$ the stresses can be computed according to the following equation:

$$\boldsymbol{\sigma}_{nst} = \begin{bmatrix} E_{sec,n} & 0 & 0 \\ 0 & E_{sec,s} & 0 \\ 0 & 0 & E_{sec,t} \end{bmatrix} \cdot \mathcal{P}^{-1} \boldsymbol{\epsilon}_{nst} \quad (3.110)$$

where $\mathbf{E} = \text{diag}(\mathbf{E}_{sec})$ is the matrix that includes the secant elastic modulus for the principal directions nst , $\mathcal{P}^{-1}$ is the inverse of the Poisson's ratio matrix.

Equation (3.110) can be written in a short form as:

$$\boldsymbol{\sigma}_{nst} = \mathbf{E} \cdot \tilde{\boldsymbol{\epsilon}}_{nst} \quad (3.111)$$

where $\tilde{\boldsymbol{\epsilon}}_{nst} = [\tilde{\epsilon}_n, \tilde{\epsilon}_s, \tilde{\epsilon}_t]$ are the equivalent uniaxial strains for the principal directions nst that account for the lateral effects on concrete as [230]:

$$\tilde{\boldsymbol{\epsilon}}_{nst} = \mathcal{P}^{-1} \boldsymbol{\epsilon}_{nst}^{(1)} \quad (3.112)$$

where $\boldsymbol{\epsilon}_{nst}^{(1)} = [\epsilon_n, \epsilon_s, \epsilon_t]$ are the principal strain values for the directions nst .

In a 3D analysis, the orthotropic matrix for Poisson's ratio is computed as proposed by Lempriere [245]:

$$\mathcal{P} = \begin{bmatrix} 1 & -\nu_{ns} & -\nu_{nt} \\ -\nu_{sn} & 1 & -\nu_{st} \\ -\nu_{tn} & -\nu_{ts} & 1 \end{bmatrix} \quad (3.113)$$

where ν_{ij} presents the Poisson ratio for ij directions.

For simplicity, Poisson's matrix in Equation (3.113) is assumed to be symmetric, resulting in $\nu_{st} = \nu_{ts}$, $\nu_{nt} = \nu_{tn}$ and $\nu_{ns} = \nu_{sn}$ [230]. In the linear state, the Poisson's ratio is equal in all directions, and Equation (3.113) yields the isotropic Poisson's matrix. The inverse of the orthotropic matrix of Poisson's ratio is given by:

$$\mathbf{P}^{-1} = \begin{bmatrix} \frac{1 - \nu_{st}^2}{\Delta'} & \frac{\nu_{ns} + \nu_{nt}\nu_{st}}{\Delta'} & \frac{\nu_{nt} + \nu_{ns}\nu_{st}}{\Delta'} \\ \frac{\nu_{ns} + \nu_{nt}\nu_{st}}{\Delta'} & \frac{1 - \nu_{nt}^2}{\Delta'} & \frac{\nu_{st} + \nu_{nt}\nu_{ns}}{\Delta'} \\ \frac{\nu_{nt} + \nu_{ns}\nu_{st}}{\Delta'} & \frac{\nu_{st} + \nu_{nt}\nu_{ns}}{\Delta'} & \frac{1 - \nu_{ns}^2}{\Delta'} \end{bmatrix} \quad (3.114)$$

where $\Delta' = 1 - \nu_{ns}^2 - \nu_{st}^2 - \nu_{nt}^2 - 2 \nu_{ns} \nu_{st} \nu_{nt}$.

In the nonlinear state, a damage function must be applied to the Poisson's ratios in the matrix to reduce their values according to the extent of the damage. The following damage function is proposed:

$$\mathbf{d}_{v,nst} = \frac{\mathbf{E}_{sec,nst}}{\tilde{E}} \quad (3.115)$$

where $\mathbf{d}_{v,nst} = [d_{v,n}, d_{v,s}, d_{v,t}]$ is a vector that accounts for damage in Poisson's ratio in each of the principal directions and $\mathbf{E}_{sec,nst} = [E_{sec,n}, E_{sec,s}, E_{sec,t}]$ is a vector that contains the elastic secant modulus under the principal directions nst .

The Poisson's ratio ν_{ij} for the ij directions is evaluated according to the following equation:

$$\nu_{ij} = \nu \cdot d_{v,i} \cdot d_{v,j} \quad (3.116)$$

where ν is the initial Poisson's ratio of concrete and $d_{v,i}$ and $d_{v,j}$ are the damage parameters for the directions i and j .

In loading states ($\tilde{\epsilon}_{nst} > \alpha_t$ or $\tilde{\epsilon}_{nst} < \alpha_c$) the elastic secant modulus $\mathbf{E}_{sec,nst}$ is dependent on the equivalent uniaxial strain $\tilde{\epsilon}_{nst}$, introducing nonlinearity into the calculation process. A fixed-point iteration method is employed ($\tilde{\epsilon}_{nst,k+1} = G(\tilde{\epsilon}_{nst,k})$), combining the computation of the elastic secant modulus $\mathbf{E}_{sec,nst}(\tilde{\epsilon}_{nst})$ (Equation (3.106) and Equation (3.107)) and the equivalent uniaxial strains $\tilde{\epsilon}_{nst}$ (Equation (3.113) to Equation (3.112)) [237].

3.8.2.3.5 Global stress calculations

The calculation of the principal stresses is performed according to the equation below.

$$\boldsymbol{\sigma}_{nst}^{(1)} = \mathbf{E}_{sec,nst} \cdot \tilde{\epsilon}_{nst} \quad (3.117)$$

where $\boldsymbol{\sigma}_{nst}^{(1)} = [\sigma_n, \sigma_s, \sigma_t]^T$ is the normal part of the principal stress vector $\boldsymbol{\sigma}_{nst} = [\boldsymbol{\sigma}_{nst}^{(1)}, \boldsymbol{\sigma}_{nst}^{(2)}]^T = [\sigma_n, \sigma_s, \sigma_t, \tau_{ns}, \tau_{st}, \tau_{tn}]^T$ and $\mathbf{E}_{sec,nst}$ represents the corresponding secant modulus for tension or compression, according to the sign of the equivalent uniaxial strains, $\tilde{\epsilon}_{nst}$.

In the total strain model with rotating cracks, the shear stresses $\sigma_{nst}^{(2)} = [\tau_{ns}, \tau_{st}, \tau_{tn}]^T$ in the principal directions are obviously null. The total strain model is completed once the principal stress vector is computed into the global coordinate system, xyz :

$$\sigma_{xyz} = \mathbf{T}^{-1} \sigma_{nst} \quad (3.118)$$

where $\sigma_{xyz} = [\sigma_x, \sigma_y, \sigma_z, \tau_{xy}, \tau_{yz}, \tau_{xz}]^T$ is the stress vector in the global coordinates and $\mathbf{T}^{-1}$ is the inverse of the transformation matrix given by Equation (3.97).

3.8.2.4 Total strain model with fixed crack

The fixed crack concept is a modelling approach in which crack orientations are assumed to remain constant throughout the analysis. In contrast to rotating crack models, where crack orientations realign with the principal stress directions as loading evolves, the fixed crack concept is implemented in total strain models by constraining these orientations to remain fixed. The previously established principal directions coordinate system, nst , is now referred to as the crack coordination system, $nst, fixed$. The total strains in the crack coordinate system are then computed according to the following equation:

$$\epsilon_{nst, fixed}^{t+\Delta t} = \mathbf{T}_{fixed} \epsilon_{xyz}^{t+\Delta t} \quad (3.119)$$

where $\epsilon_{nst, fixed} = [\epsilon_n, \epsilon_s, \epsilon_t, \epsilon_{ns}, \epsilon_{st}, \epsilon_{nt}]^T$ is the strain vector in the $nst, fixed$ coordinates and $\mathbf{T}_{fixed}$ is the transformation matrix for the fixed directions.

In the total strain model with fixed cracks, the principal directions of the strain vector may differ from the fixed cracking directions. In that case, at least one of the shear strain components ϵ_{ns} , ϵ_{st} and ϵ_{nt} in the fixed crack directions, it is no longer equal to zero. Consequently, an additional algorithm is required to evaluate shear stresses at the cracking location. The stress vector in the crack coordinate system is decomposed into the normal components, $\sigma_{nst, fixed}^{(1)} = [\sigma_n, \sigma_s, \sigma_t]^T$, and the tangential components, $\sigma_{nst, fixed}^{(2)} = [\tau_{ns}, \tau_{st}, \tau_{nt}]^T$. The computation of normal stress within the crack coordinate system $\sigma_{nst, fixed}^{(1)}$ follows the procedure already described for the total strain model with rotating cracks. The shear stresses $\sigma_{nst, fixed}^{(2)}$ can be computed according to the following equation.

$$\sigma_{nst, fixed}^{(2)} = \begin{bmatrix} \tau_{ns} \\ \tau_{st} \\ \tau_{nt} \end{bmatrix} = \mathbf{D}_{\theta\theta, nst} \begin{bmatrix} \gamma_{ns} \\ \gamma_{st} \\ \gamma_{nt} \end{bmatrix} \quad (3.120)$$

where τ_{ij} are the tangential stress values at the $nst, fixed$ coordinate system ij , and $\gamma_{ij} = 2 \cdot \epsilon_{ij}$ are the engineering shear strains in the $nst, fixed$ coordinate system ij .

The tangent stiffness submatrix $\mathbf{D}_{\theta\theta, nst}$ is evaluated according to [230, 231]:

$$\mathbf{D}_{\theta\theta,nst} = \begin{bmatrix} \beta G_{ns} & 0 & 0 \\ 0 & \beta G_{st} & 0 \\ 0 & 0 & \beta G_{nt} \end{bmatrix} \quad (3.121)$$

where G_{ij} is the shear modulus and β is the shear retention factor.

The shear retention factor β is used to simulate the cracking effect on the shear stress continuum model. The current implementation of the pointwise THM model adopts a constant shear retention factor β , which is provided as input by the user. The shear retention factor should vary between 0 and 1, with 1 equal to the continuum model and 0 indicating that no shear stress retention after cracking.

Determining the shear modulus for orthotropic materials is challenging due to its relationship with elasticity and Poisson's ratio. SolidWorks [246] proposes to evaluate the shear modulus for orthotropic materials according to the following equation.

$$G_{ij} = \frac{E_{sec,nst,i}^{t+\Delta t} E_{sec,nst,j}^{t+\Delta t}}{E_{sec,nst,i}^{t+\Delta t} (1 + \nu_{ij}) + E_{sec,nst,j}^{t+\Delta t} (1 + \nu_{ij})} \quad (3.122)$$

where $E_{sec,nst,i}^{t+\Delta t}$ is the secant modulus of component i and ν_{ij} is the Poisson's ratio for the ij direction.

Equation (3.122) requires further investigation. Therefore, the pointwise THM model considers the same shear modulus for all directions, as suggested by DIANA FEA [230]. The shear modulus is calculated according to the following equation.

$$G = \frac{E}{2(1 + \nu)} \quad (3.123)$$

The total strain model with fixed cracks is completed once the stress vector in the crack coordinate system is converted into global directions, combining the normal and tangential parts into a single vector, $\boldsymbol{\sigma}_{nst, fixed} = [\boldsymbol{\sigma}_{nst, fixed}^{(1)}; \boldsymbol{\sigma}_{nst, fixed}^{(2)}]$. The global stress vector can be calculated according to the following equation.

$$\boldsymbol{\sigma}_{xyz} = \mathbf{T}_{fixed}^{-1} \boldsymbol{\sigma}_{nst, fixed} \quad (3.124)$$

where $\boldsymbol{\sigma}_{xyz}^{t+\Delta t} = [\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \tau_{xy}, \tau_{yz}, \tau_{xz}]^T$ is the stress vector in the global coordinates, $\mathbf{T}_{fixed}^{-1}$ is the transformation matrix.

3.8.2.4.1 Uniaxial tension softening model in the total strain formulation

Different tension softening models can be used for the numerical simulation of cracking [50, 125, 247-249]. In the pointwise THM model, two tension-softening models were implemented:

- the bilinear tension softening model, according to MC2010;
- the Hordijk tension softening model.

These two models were selected due to their widely spread performance in the cracking simulation of concrete elements. Further work may include the implementation of more tension-softening models. The following chapters present details on implementing these tension softening models in the total strain cracking model.

3.8.2.4.1.1 The bilinear tension softening model

The bilinear tension softening model proposed by the MC2010 [50] is illustrated in the following figure.

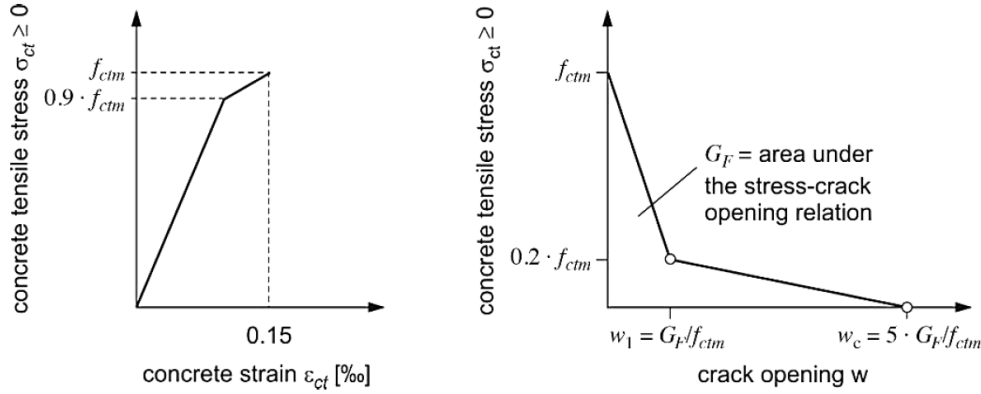


Fig. 51 – Bilinear tension softening model according to MC2010 [50].

The computation of the stress-strain law using the bilinear tension softening of MC2010 starts with calculating an auxiliary strain vector, which accommodates the variations in the bilinear behaviour. The auxiliary strain vector components are evaluated through Equation (3.105) resulting in the following transition strains $\varepsilon_{\alpha i}$ for the bilinear tension softening model:

$$\left\{ \begin{array}{l} \varepsilon_{\alpha 1} = 0.9 \frac{f_{ct}^{t+\Delta t}}{\tilde{E}} \\ \varepsilon_{\alpha 2} = \varepsilon_{\alpha 1} + \left(1.5 \times 10^{-4} - 0.9 \frac{f_{ct}^{t+\Delta t}}{\tilde{E}} \right) + \frac{f_{ct}^{t+\Delta t} - 0.9 f_{ct}^{t+\Delta t}}{\tilde{E}} \\ \varepsilon_{\alpha 3} = \varepsilon_{\alpha 2} + \frac{G_f}{h \cdot f_{ct}^{t+\Delta t}} + \frac{0.2 f_{ct}^{t+\Delta t} - f_{ct}^{t+\Delta t}}{\tilde{E}} \\ \varepsilon_{\alpha 4} = \varepsilon_{\alpha 3} + \left(5 \frac{G_f}{h \cdot f_{ct}^{t+\Delta t}} - \frac{G_f}{h \cdot f_{ct}^{t+\Delta t}} \right) + \frac{-0.2 f_{ct}^{t+\Delta t}}{\tilde{E}} \end{array} \right. \quad (3.125)$$

where $f_{ct}^{t+\Delta t}$ is the tensile strength at the current step, G_f is the fracture energy, which is an input in the data file and h is the crackband width, which is an input in the data file and can be considered equal to the lateral dimension of the finite element.

The parameter $\varepsilon_{\alpha 2}$ is calculated based on the MC2010 tension softening bilinear behaviour before cracking, which assumes a constant strain value of 1.5×10^{-4} . The assumption of a constant value reveals constraints regarding the cracking behaviour of different concrete mixtures and delayed effects on the modulus of elasticity. Therefore, in the pointwise THM model, the computation of the parameter $\varepsilon_{\alpha 2}$ is performed according to the following equation:

$$\varepsilon_{\alpha 2} = \varepsilon_{\alpha 1} + \left(1.5 \times 10^{-4} \frac{E_{static}}{\tilde{E}} - 0.9 \frac{f_{ct}^{t+\Delta t}}{\tilde{E}} \right) + \frac{f_{ct}^{t+\Delta t} - 0.9 f_{ct}^{t+\Delta t}}{\tilde{E}} \quad (3.126)$$

where E_{static} is a calibration parameter introduced to account for strength and creep deformation in the ascending bilinear part of the MC2010 tension softening model. Considering $E_{static} = \tilde{E}$ returns the MC2010 tension softening model. In the pointwise THM model, $E_{static} = 33.6$ GPa is considered, which results in the tension softening model at 28 days for the C30/37 concrete. Further investigations are required to provide a more realistic relationship for the bilinear ascending part simulated in the MC2010 tension softening model. Fig. 52 shows the MC2010 tension softening model for the total strain model.

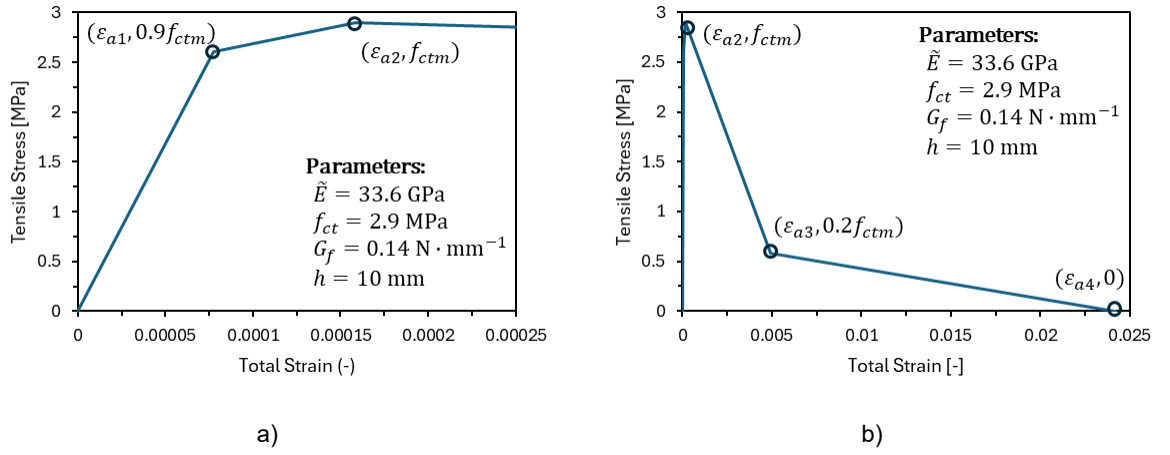


Fig. 52 – MC2010 bilinear tension softening model for total strain models: a) ascending part; b) softening part.

The auxiliary stress vector σ_{α} is computed to store the stress state for the corresponding maximum strains in vector α . The calculation is performed according to the following equation.

$$\sigma_{\alpha,k} = \begin{cases} \tilde{E} \cdot \alpha_k^{t+\Delta t}, & \text{if } \alpha_k \leq \varepsilon_{\alpha 1} \\ 0.9 f_{ct}^{t+\Delta t} + 0.1 f_{ct}^{t+\Delta t} \frac{(\alpha_k^{t+\Delta t} - \varepsilon_{\alpha 1})}{(\varepsilon_{\alpha 2} - \varepsilon_{\alpha 1})}, & \text{if } \varepsilon_{\alpha 1} < \alpha_k < \varepsilon_{\alpha 2} \\ f_{ct}^{t+\Delta t} - 0.8 f_{ct}^{t+\Delta t} \frac{(\alpha_k^{t+\Delta t} - \varepsilon_{\alpha 2})}{(\varepsilon_{\alpha 3} - \varepsilon_{\alpha 2})}, & \text{if } \varepsilon_{\alpha 2} \leq \alpha_k < \varepsilon_{\alpha 3} \\ 0.2 f_{ct}^{t+\Delta t} - 0.2 f_{ct}^{t+\Delta t} \frac{(\alpha_k^{t+\Delta t} - \varepsilon_{\alpha 3})}{(\varepsilon_{\alpha 4} - \varepsilon_{\alpha 3})}, & \text{if } \varepsilon_{\alpha 3} \leq \alpha_k < \varepsilon_{\alpha 4} \\ 0, & \text{if } \alpha_k \geq \varepsilon_{\alpha 4} \end{cases} \quad (3.127)$$

where $\sigma_{\alpha,k}$ is the component k of the temporary stress vector σ_{α} and $\tilde{E}$ is the incremental modulus.

3.8.2.4.1.2 The Hordijk tension softening model

The tension softening model proposed by Hordijk [247] is implemented in the pointwise THM model for the numerical simulation of cracking. The exact computation of the Hordijk tension softening following Equation (3.105) would result in the numerical integration of a nonlinear function that can not be done analytically. The trapezoidal integration method was used to investigate the integration of

this nonlinear function. However, for huge total strain values, the numerical integration process loses accuracy or becomes highly computationally demanding. For those reasons, an alternative approach was considered. Instead of integrating the entire Hordijk function within Equation (3.105), only the strain limits in the Hordijk tension softening model are updated according to the total strain formulation. This numerical strategy provides accurate and stable results for modelling the Hordijk tension softening behaviour while requiring lower computational resources. The following equation gives the auxiliary strain parameters.

$$\begin{cases} \varepsilon_{\alpha 1} = \frac{f_{ct}^{t+\Delta t}}{\tilde{E}} \\ \varepsilon_{\alpha 2} = \varepsilon_{\alpha 1} + 5.136 \frac{G_f}{h \cdot f_{ct}^{t+\Delta t}} \end{cases} \quad (3.128)$$

where f_{ct} is the tensile strength at the current step, G_f is the fracture energy and h is the crackband width.

The Hordijk tension softening equation is used in the total strain model with the new limits introduced by equation (3.128). Fig. 53 shows the Hordijk tension softening model for the total strain model.

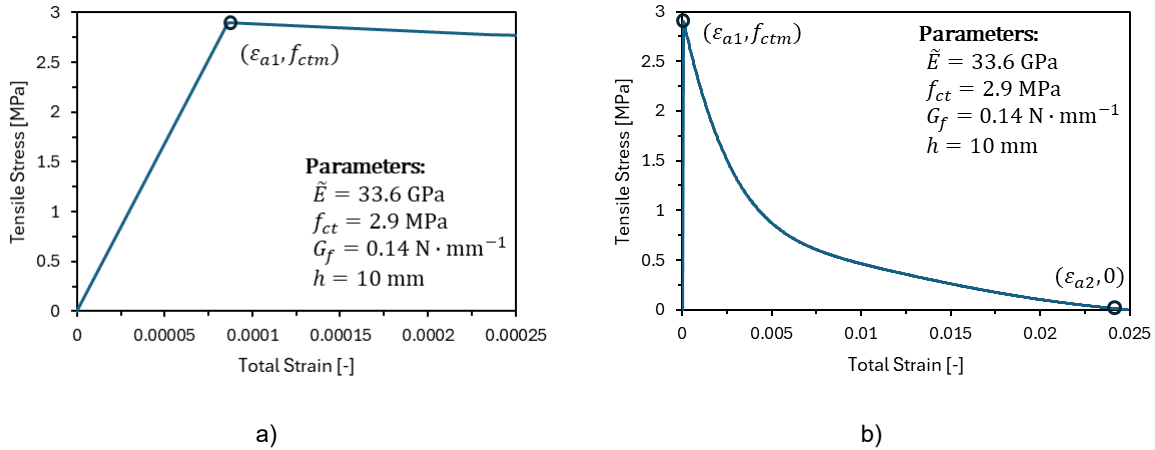


Fig. 53 – Hordijk tension softening model for total strain models: a) ascending part; b) softening part.

The auxiliary stress vector σ_{α} is utilised to store the limit stress state corresponding to the maximum strains in the vector α . The calculation of these temporary stresses is performed according to the following formulation.

$$\sigma_{\alpha,k} = \begin{cases} \tilde{E} \cdot \alpha_k^{t+\Delta t}, & \text{if } \alpha_k^{t+\Delta t} \leq \varepsilon_{\alpha 1} \\ f_{ct}^{t+\Delta t} \left[\left(1 + \left(c_1 \cdot \frac{\alpha_k^{t+\Delta t} - \varepsilon_{\alpha 1}}{\varepsilon_{\alpha 2} - \varepsilon_{\alpha 1}} \right)^3 \right) \exp \left[-c_2 \cdot \frac{\alpha_k^{t+\Delta t} - \varepsilon_{\alpha 1}}{\varepsilon_{\alpha 2} - \varepsilon_{\alpha 1}} \right] - \frac{\alpha_k^{t+\Delta t} - \varepsilon_{\alpha 1}}{\varepsilon_{\alpha 2} - \varepsilon_{\alpha 1}} (1 + c_1^3) \cdot \exp[-c_2] \right], & \text{if } \varepsilon_{\alpha 1} < \alpha_k^{t+\Delta t} \leq \varepsilon_{\alpha 2} \\ 0, & \text{if } \alpha_k^{t+\Delta t} > \varepsilon_{\alpha 2} \end{cases} \quad (3.129)$$

where $\sigma_{\alpha,k}$ is the component k of the temporary stress vector σ_{α} and $\tilde{E}$ is the incremental modulus and c_1 and c_2 are empirical parameters, for which Hordijk [247] suggests considering $c_1 = 3$ and $c_2 = 6.93$.

3.8.2.5 Time dependencies on the total strain model

The stress-strain relationship provided by Equation (3.105) is formulated based on the current step incremental modulus, $\tilde{E}_i$, which accounts for creep due to the stress increment resulting from the current step stress calculation in the modulus of elasticity. The incremental modulus varies with the time increment and material maturity, as given by equation (3.78). The subscript i denotes the step. The conceptualization of the stress-strain relationship in the total strain model suggests that a change in the incremental modulus between steps, that is $\tilde{E}_{i+1} \neq \tilde{E}_i$, inherently results in alterations to the stress-strain relationship obtained through Equation (3.105). Consequently, the same total strain would result in different stresses between the end of step i and the beginning of step $i+1$ ($\tilde{E}_{nst,i} \tilde{\epsilon}_{nst,i} \neq \tilde{E}_{nst,i+1} \tilde{\epsilon}_{nst,i}$). The model must ensure that the stress state at the beginning of a given step, $\sigma_{nst,i+1}^t = \tilde{E}_{nst,i+1} \tilde{\epsilon}_{nst,i}^t$, aligns with the stress state at the end of the previous step, $\sigma_{nst,i}^{t+\Delta t} = \tilde{E}_{nst,i} \tilde{\epsilon}_{nst,i}^{t+\Delta t}$. The proposed algorithm is designed to preserve this continuity by updating the vector $\alpha_i^{t+\Delta t}$ to the new vector α_{i+1}^t , compatible with the current step stress-strain relationship. Fig. 54 schematizes the algorithm implemented for the tensile behaviour, considering a bilinear tension softening model similar to the one proposed by fib [50].

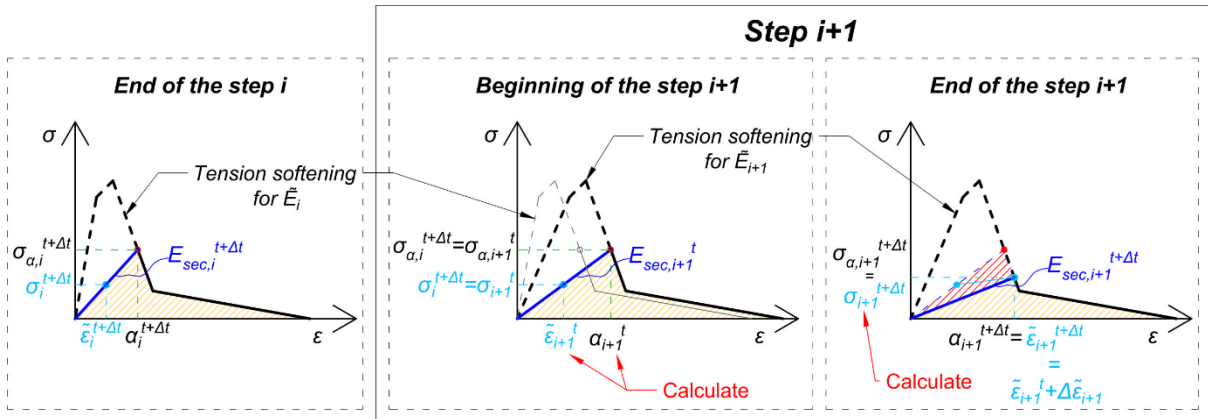


Fig. 54 - Scheme of the algorithm for computation of time dependencies in the total strain model.

Fig. 54 presents a hypothetical scenario where the stress-strain relationship evaluated by Equation (3.105) changes drastically during two steps, obtained, for example, for $\Delta t_{i+1} \gg \Delta t_i$ which results in an incremental modulus $\tilde{E}_{i+1} \ll \tilde{E}_i$. The purpose of such variations is to allow for an easy identification in the illustration of the stress-strain relationship changes between two steps. However, in FE analysis, it is recommended that such strong stress-strain variations between two steps should be avoided due to the non-linearity typical of fracture simulations. Gradual changes in time increments are preferable and recommended.

The crack strain threshold for switching between the rotating and fixed crack is also converted into the respective total strain threshold. This process is made by employing Equation (3.105) to determine which total strain corresponds to the crack strain threshold specified by the user. The total strain threshold may vary over the steps due to the adaptive stress-strain relationship associated with Equation (3.105), but the crack strain threshold remains constant over the entire analysis since D_{cr} is not

dependent on creep or other delayed effects. The switching is performed according to the numerical procedure specified in Chapter 3.1.

The algorithm in Box 3.3 describes the procedure of Fig. 54 to compute the total strains while accounting for the time dependencies between two subsequent steps.

Box 3.3 - Algorithm for considering time dependencies in the total strain model.

1. Calculate the principal stresses $\sigma_{nst,i+1}^t$ for the initial stress state $\sigma_{xyz,i+1}^t$ using the transformation matrix $\mathbf{T}_i$ obtained from the previous principal crack directions:

$$\sigma_{nst,i+1}^t = \mathbf{T}_i \sigma_{xyz,i+1}^t$$

2. Calculate the tensile stress limits $\sigma_{\alpha,i}^{t+\Delta t}$ in the stress-strain relationship defined for the previous incremental modulus $\tilde{E}_i$ for the three principal directions nst , and update these stress limits for the current step $\sigma_{\alpha,i}^{t+\Delta t} = \sigma_{\alpha,i+1}^t$.

3. Using the stress-strain relationship formulated for the current step incremental modulus $\tilde{E}_{i+1}$, calculate the new strain limits α_{i+1}^t corresponding to the tensile stress limits $\sigma_{\alpha,i+1}^t$.

4. Compute the updated secant modulus $E_{sec,i+1}^t$ and evaluate the equivalent total strains:

$$\tilde{\epsilon}_{i+1}^t = [E_{sec,i+1}^t]^{-1} \sigma_{nst,i+1}^t$$

5. Determine the orthotropic Poisson's matrix $\mathcal{P}$ and evaluate the principal strains:

$$\epsilon_{i+1}^t = \mathcal{P} \tilde{\epsilon}_{i+1}^t$$

6. In the fixed concept, compute the lateral strains in the crack direction system:

$$[\gamma_{ns}|\gamma_{st}|\gamma_{nt}] = \mathbf{D}_{\theta\theta}^{-1} [\tau_{ns}|\tau_{st}|\tau_{nt}]$$

7. Rotate the principal strains ϵ_{nst} to the global coordinate system xyz to obtain the total strains at the beginning of the current step:

$$\epsilon_{xyz,i+1}^t = \mathbf{T}_i^{-1} \cdot \epsilon_{nst,i+1}^t$$

8. Update the total strain vector in the global coordinate system:

$$\epsilon_{xyz}^{t+\Delta t} = \epsilon_{xyz}^t + (\Delta \epsilon - \Delta \epsilon_T - \Delta \epsilon_{sh} - \Delta \epsilon_{cs})$$

Use the total strain model presented in subchapter 3.8.2.3 or 3.8.2.4 to calculate the stress vector $\sigma_{xyz}^{t+\Delta t}$.

For the particular case where the tension softening is exhausted, the value of $E_{sec} \cong 0$ may lead to numerical problems in the total strain models. A practical approach that controls the damage development upon tension softening exhaustion can be achieved by incorporating a residual behaviour with very low stiffness into the tension-softening model presented in Chapter 3.8.2.4.1. The approach assumes a linear variation between the user-defined residual stress $RES \geq 0.001$ MPa and the total strain for which the tension softening is exhausted ε_u , multiplied by a large parameter. In the pointwise THM model, the secant modulus after RES is exceeded is given by the following equation:

$$E_{sec} = \frac{RES}{\varepsilon_u \times 10^3} \quad (3.130)$$

where ε_{ult} is the ultimate total strain in the tension softening model.

This approach is valid as long as the total strain does not exceed $\varepsilon_{ult} \times 10^3$. Otherwise, the analysis will stop with a numerical error “*ULTIMATE TOTAL STRAIN EXCEEDED*” printed in the console and output file. It is important to note that such a violation conservatively corresponds to crack widths exceeding 200 mm, which are beyond the expected simulation limits of the present pointwise THM model.

3.8.2.6 Single-crack model with strain decomposition

The smeared cracking models with strain decomposition explicitly separate the crack strains from the concrete strains [211-213]. The single-crack model with strain decomposition implemented in the pointwise THM model is based on the numerical framework employed by Sena-Cruz [214]. The single-crack fixed model can be formulated into the multi-directional fixed model, which allows the generation of multiple cracks in an integration point once several conditions are satisfied. In the pointwise THM model, the crack generation is limited to a single crack. This option is justified by the number of state variables allocated to the material subroutine, which may drastically increase if multiple cracks are formed at each integration point. Implementing multi-directional cracks is out of the scope of the current PhD work and is considered future work. The stress-strain relationship for the smeared cracking models should concern the fixed principal n, s, t axes of orthotropy. Where n refers to the direction normal to the crack, which represents mode I, and s, t refer to the directions tangential to the crack in 3D (mode II and mode III). Fig. 55 shows the local coordinate system and tractions across a crack.

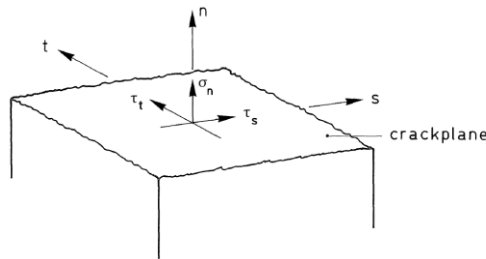


Fig. 55 – Local coordinate system and tractions across a crack (adopted from [231]).

The global stress increment $\Delta\sigma_{xyz}$ in the Voigt notation is given by:

$$\Delta\sigma_{xyz} = [\Delta\sigma_x \quad \Delta\sigma_y \quad \Delta\sigma_z \quad \Delta\tau_{xy} \quad \Delta\tau_{yz} \quad \Delta\tau_{xz}]^T \quad (3.131)$$

The local stress increment at the crack plane $\Delta\sigma_{nst}$ is given by:

$$\Delta\sigma_{nst} = [\Delta\sigma_{nn} \quad \Delta\tau_{ns} \quad \Delta\tau_{nt}]^T \quad (3.132)$$

A relationship between the global stress increment, Equation (3.131), and the local stress increment at the crack plane, Equation (3.132), is given by:

$$\Delta\sigma_{nst} = \mathbf{T}_{s-cr} \Delta\sigma_{xyz} \quad \text{or} \quad \Delta\sigma_{xyz} = \mathbf{T}_{s-cr}^T \Delta\sigma_{nst} \quad (3.133)$$

where $\mathbf{T}_{s-cr}$ is the transformation matrix for the single crack model given by:

$$\mathbf{T}_{s-cr} = \begin{bmatrix} C_{xn}^2 & C_{yn}^2 & C_{zn}^2 & 2 \cdot C_{xn}C_{yn} & 2 \cdot C_{yn}C_{zn} & 2 \cdot C_{xn}C_{zn} \\ C_{xn}C_{xs} & C_{yn}C_{ys} & C_{zn}C_{zs} & C_{xn}C_{ys} + C_{xs}C_{yn} & C_{yn}C_{zs} + C_{ys}C_{zn} & C_{xn}C_{zs} + C_{xs}C_{zn} \\ C_{xn}C_{xt} & C_{yn}C_{yt} & C_{zn}C_{zt} & C_{xn}C_{yt} + C_{xt}C_{yn} & C_{yn}C_{zt} + C_{yt}C_{zn} & C_{xn}C_{zt} + C_{xt}C_{zn} \end{bmatrix} \quad (3.134)$$

where c_{ij} is the cosine of the angle between the j vector and the i vector.

In the decomposed strain crack models, the total strain increment, $\Delta\epsilon_{xyz}$, is split into a strain component of the crack $\Delta\epsilon_{cr,xyz}$ and the strain component of the solid material between cracks, $\Delta\epsilon_{co,xyz}$:

$$\Delta\epsilon_{xyz} = \Delta\epsilon_{cr,xyz} + \Delta\epsilon_{co,xyz} \quad (3.135)$$

The global crack strain increment $\Delta\epsilon_{cr,xyz}$ is given by:

$$\Delta\epsilon_{cr,xyz} = [\Delta\epsilon_{cr,x} \quad \Delta\epsilon_{cr,y} \quad \Delta\epsilon_{cr,z} \quad \Delta\gamma_{cr,zy} \quad \Delta\gamma_{cr,yz} \quad \Delta\gamma_{cr,xt}]^T \quad (3.136)$$

The local crack strain increment $\Delta\epsilon_{cr,nst}$ is given by:

$$\Delta\epsilon_{cr,nst} = [\Delta\epsilon_{cr,n} \quad \Delta\gamma_{cr,s} \quad \Delta\gamma_{cr,t}]^T \quad (3.137)$$

By analogy with the global and local stress relationship in Equation (3.133), the relationship between global and local crack strains is given by:

$$\Delta\epsilon_{cr,nst} = \mathbf{T}_{s-cr} \Delta\epsilon_{cr,xyz} \quad \text{or} \quad \Delta\epsilon_{cr,xyz} = \mathbf{T}_{s-cr}^T \Delta\epsilon_{cr,nst} \quad (3.138)$$

The constitutive model becomes complete by prescribing the stress-strain relationship. For the concrete between the cracks, the Hooke's law relationship is assumed as:

$$\Delta\sigma_{xyz} = \mathbf{D}^{co} \Delta\epsilon_{co,xyz} \quad (3.139)$$

where $\mathbf{D}^{co} = \tilde{\mathbf{E}} \cdot \mathbf{D}$ is the elastic stiffness tensor.

In the same way, a relation must be prescribed for the cracking stresses and cracking strains:

$$\Delta \sigma_{cr,nst} = \mathbf{D}^{cr} \Delta \epsilon_{cr,nst} \quad (3.140)$$

where $\mathbf{D}^{cr}$ is a 3×3 matrix that accounts for the mode I, mode II, mode III and mixed-mode properties of the crack:

$$\mathbf{D}^{cr} = \begin{bmatrix} D^I & 0 & 0 \\ 0 & D^{II} & 0 \\ 0 & 0 & D^{III} \end{bmatrix} \quad (3.141)$$

Recalling Equation (3.139) and considering the relationships in Equation (3.135) and Equation (3.138), one obtains the stress increment as:

$$\Delta \sigma_{xyz} = \mathbf{D}^{co} [\Delta \epsilon_{xyz} - \mathbf{T}_{s-cr}^T \Delta \epsilon_{cr,nst}] \quad (3.142)$$

Equation (3.142) specifies how the stress increment is computed in the single fixed crack model. The crack strain increment $\Delta \epsilon_{cr,nst}$ is unknown. The determination of the crack strains can be obtained by the equality between the crack stress and the global stress increment in the crack referential ($\sigma_{nst} = \sigma_{cr,nst}$). Multiplying Equation (3.142) by the transformation matrix $\mathbf{T}_{s-cr}$, and accounting for the relationship in Equation (3.133) and Equation (3.140), one obtains the following equation:

$$\sigma_{cr,nst} + \Delta \sigma_{cr,nst}(\Delta \epsilon_{cr,nst}) - \mathbf{T}_{s-cr} \sigma_{xyz} - \mathbf{T}_{s-cr} \mathbf{D}^{co} [\Delta \epsilon_{xyz} - \mathbf{T}_{s-cr}^T \Delta \epsilon_{cr,nst}] = 0 \rightarrow f(\Delta \epsilon_{cr}) = \mathbf{0} \quad (3.143)$$

Depending on the adopted tension softening model, Equation (3.143) may be dependent on the solution ($\Delta \epsilon_{cr,nst}$). Therefore, it is required to implement a numerical method to determine the crack strain in Equation (3.143). In the pointwise THM model, the Newton-Raphson method is implemented to determine the crack strains that lead to $f(\Delta \epsilon_{cr}) \cong \mathbf{0}$. The derivative of the function in Equation (3.143) is given by:

$$\frac{\partial f(\Delta \epsilon_{cr})}{\partial \Delta \epsilon_{cr}} = [\mathbf{D}^{cr} + \mathbf{T}_{s-cr} \mathbf{D}^{co} \mathbf{T}_{s-cr}^T] \quad (3.144)$$

If the norm of the vector $f(\Delta \epsilon_{cr})$ in Equation (3.143) is bigger than the tolerance $\|f(\Delta \epsilon_{cr})\| > Toler$, the change in the increment of strain can be computed according to the following equation:

$$\delta \Delta \epsilon_{cr,nst} = f(\Delta \epsilon_{cr}) \cdot \left[\frac{\partial f(\Delta \epsilon_{cr})}{\partial \Delta \epsilon_{cr}} \right]^{-1} \quad (3.145)$$

For the current algorithm, the tolerance was considered equal to $Toler = 1.0 \times 10^{-1}$, while the maximum number of iterations is considered equal to 1000. If convergence is not achieved, the solution is assumed to be equal to the iteration that resulted in the minimum value of $\|f(\Delta \epsilon_{cr})\|$. In the implemented model, there is an instruction to plot “N-R not converged” in the DIANA FEA results file

when convergence was not achieved. Sena-Cruz [214] suggested using the fixed-point iterative method if the Newton-Raphson method did not converge.

To manage the phenomena of crack closure and re-opening, the maximum crack strain, denoted as $\varepsilon_{cr,n,max}$, is stored in a state variable. When the current crack strain satisfies $\varepsilon_{cr,n} < \varepsilon_{cr,n,max}$, the numerical model transitions into a loading or reloading regime following a secant-to-origin approach. The numerical framework of the fixed crack model is preserved with changes to the calculation of the parameters in Equation (3.143) to handle unloading and reloading. In cases where the crack strain in the principal direction remains positive yet is lower than the maximum crack strain, the mode I parameter, D^I , is recalculated as the stress for the maximum crack strain divided by the maximum crack strain, and the stress for the current crack strain value is computed by multiplying the current crack strain by the new mode I parameter. The following equation illustrates these modifications:

$$\begin{cases} D^I = \sigma(\varepsilon_{cr,n,max}) / \varepsilon_{cr,n,max} \\ \sigma(\varepsilon_{cr,n}) = D^I \cdot \varepsilon_{cr,n} \end{cases} \quad (3.146)$$

If somehow the Newton-Raphson method returns a negative value for the crack strain, the existing crack has been closed, and the numerical model has turned into compression. To handle this issue, the crack strains and crack stress are equal to zero, returning to Hooke's law.:

$$\begin{cases} \varepsilon_{cr,n} = 0 \\ D^I = \tilde{E} \\ \sigma(\varepsilon_{cr,n}) = 0 \end{cases} \quad (3.147)$$

3.8.2.6.1 Tension softening models

In contrast with the total strain models, the cracking models with the strain decomposition require the description of the tension softening model regarding the crack strains instead of the total strain. Two tension-softening models were considered in the single-crack fixed model:

- the bilinear tension softening model, according to MC2010;
- the Hordijk tension softening model.

3.8.2.6.1.1 The bilinear tension softening model

The bilinear tension softening model proposed by the MC2010 [50] is illustrated in Fig. 51. In the strain decomposition models, it is only possible to simulate the softening part of the MC2010 model. Therefore, the bilinear ascending part in the tension softening model is not considered in the strain decomposition models. The auxiliary strain vector with the transition strains is given by:

$$\begin{cases} \varepsilon_{cr,\alpha1} = 0 \\ \varepsilon_{cr,\alpha2} = \frac{G_f}{f_{ct} \cdot h} \\ \varepsilon_{cr,\alpha3} = \frac{5 \cdot G_f}{f_{ct} \cdot h} \end{cases} \quad (3.148)$$

Fig. 52 shows the MC2010 tension softening model based on the crack strains.

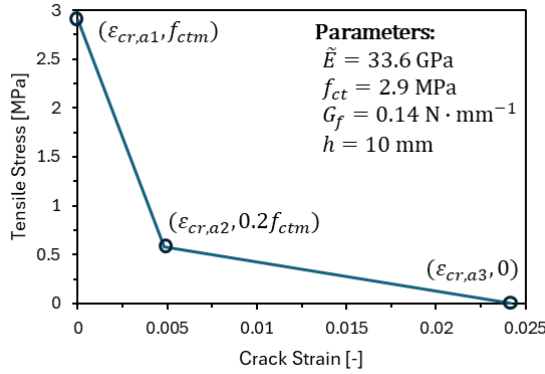


Fig. 56 – MC2010 bilinear tension softening model.

The stress in the tension-softening model, σ_{cr} , is computed regarding the crack strain $\alpha_{cr,k}$. The calculation is performed according to the following equation.

$$\sigma_{cr}(\alpha_{cr,k}) = \begin{cases} f_{ct} - 0.8 \cdot f_{ct} \frac{(\alpha_{cr,k} - \varepsilon_{cr,\alpha1})}{(\varepsilon_{cr,\alpha2} - \varepsilon_{cr,\alpha1})}, & \text{if } \varepsilon_{cr,\alpha1} \leq \alpha_{cr,k} < \varepsilon_{cr,\alpha2} \\ 0.2 \cdot f_{ct} - 0.2 \cdot f_{ct} \frac{(\alpha_{cr,k} - \varepsilon_{cr,\alpha2})}{(\varepsilon_{cr,\alpha3} - \varepsilon_{cr,\alpha2})}, & \text{if } \varepsilon_{cr,\alpha2} \leq \alpha_{cr,k} < \varepsilon_{cr,\alpha3} \\ RES, & \text{if } \alpha_{cr,k} \geq \varepsilon_{cr,\alpha3} \end{cases} \quad (3.149)$$

When the crack strains exceed the crack strain $\varepsilon_{cr,\alpha3}$ the tension softening model would return the stress equal to zero, which can give rise to numerical problems regarding the loading and unloading schemes. Instead of setting up the crack stress to zero, a residual value of $RES = 0.001$ MPa is used. The user may specify any other residual stress for the tension softening through the data file input.

In the single-crack fixed model, the mode I stiffness is required for computing the $\mathbf{D}^{cr}$ matrix. For the bilinear tension softening model, the mode I stiffness is given by the following equation:

$$D^I(\alpha_{cr,k}) = \begin{cases} \frac{-0.8 \cdot f_{ct}}{(\varepsilon_{cr,\alpha2} - \varepsilon_{cr,\alpha1})}, & \text{if } \varepsilon_{cr,\alpha1} \leq \alpha_{cr,k} < \varepsilon_{cr,\alpha2} \\ \frac{-0.2 \cdot f_{ct}}{(\varepsilon_{cr,\alpha3} - \varepsilon_{cr,\alpha2})}, & \text{if } \varepsilon_{cr,\alpha2} \leq \alpha_{cr,k} < \varepsilon_{cr,\alpha3} \\ 0, & \text{if } \alpha_{cr,k} \geq \varepsilon_{cr,\alpha3} \end{cases} \quad (3.150)$$

3.8.2.6.1.2 The Hordijk tension softening model

The Hordijk tension softening model is implemented in the single-crack fixed model. The following equation gives the auxiliary strain parameters:

$$\begin{cases} \varepsilon_{cr,\alpha1} = 0 \\ \varepsilon_{cr,\alpha2} = 5.136 \frac{G_f}{h \cdot f_{ct}^{t+\Delta t}} \end{cases} \quad (3.151)$$

Fig. 53 shows the Hordijk tension softening model for the single-crack fixed model.

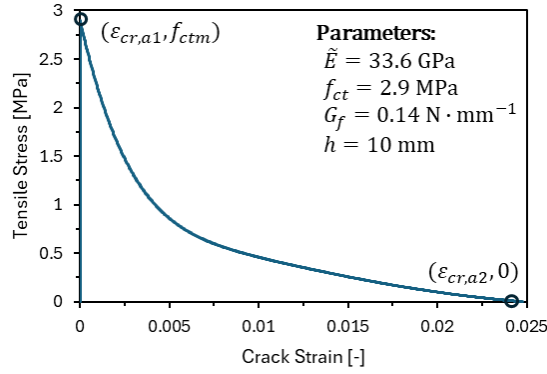


Fig. 57 – Hordijk tension softening model.

The stress in the tension-softening model, σ_{cr} , is computed regarding the crack strain $\alpha_{cr,k}$. The calculation is performed according to the following equation:

$$\sigma_{cr}(\alpha_{cr,k}) = \begin{cases} f_{ct}^{t+\Delta t} \left[\left(1 + \left(c_1 \cdot \frac{\alpha_{cr,k}}{\varepsilon_{cr,\alpha2}} \right)^3 \right) \exp \left[-c_2 \cdot \frac{\alpha_{cr,k}}{\varepsilon_{cr,\alpha2}} \right] - \frac{\alpha_{cr,k}}{\varepsilon_{cr,\alpha2}} (1 + c_1^3) \cdot \exp[-c_2] \right], & \text{if } \varepsilon_{cr,\alpha1} < \alpha_{cr,k} \leq \varepsilon_{cr,\alpha2} \\ \text{RES}, & \text{if } \alpha_{cr,k} > \varepsilon_{cr,\alpha2} \end{cases} \quad (3.152)$$

where c_1 and c_2 are empirical parameters, which Hordijk [247] suggests considering as $c_1 = 3$ and $c_2 = 6.93$.

In the single-crack fixed model, the mode I stiffness is required for computing the $\mathbf{D}^{cr}$ matrix. For the Hordijk tension softening model, the mode I stiffness can be obtained using the derivative of Equation (3.152). The mode I stiffness is given by the following equation:

$$D^I(\alpha_{cr,k}) = \begin{cases} f_{ct} \left[\frac{3 \cdot (c_1)^3 \cdot (\alpha_{cr,k})^2 \cdot \exp\left[-\frac{c_2 \cdot \alpha_{cr,k}}{\varepsilon_{cr,\alpha 2}}\right]}{(\varepsilon_{cr,\alpha 2})^3} - \frac{c_2 \cdot \exp\left[-c_2 \cdot \frac{\alpha_{cr,k}}{\varepsilon_{cr,\alpha 2}}\right] \cdot \left(\frac{(c_1)^3 \cdot (\alpha_{cr,k})^3}{(\varepsilon_{cr,\alpha 2})^3} + 1\right)}{\varepsilon_{cr,\alpha 2}} \right], & \text{if } \varepsilon_{cr,\alpha 1} \leq \alpha_{cr,k} < \varepsilon_{cr,\alpha 2} \\ \frac{\exp[-c_2] \cdot ((c_1)^3 + 1)}{\varepsilon_{cr,\alpha 2}}, & \text{if } \alpha_k \geq \varepsilon_{\alpha 3} \end{cases} \quad (3.153)$$

3.8.2.6.1.3 Mode II and mode III parameters

The mode II and III parameters consider the shear effect in the cracked state [211]. The shear stresses are zero when the principal stresses are orthogonal to the crack plane. For the fixed crack models, where the crack orientation is kept locked upon crack initiation, it is necessary to consider stress retention due to the roughness of the interlock between the crack surfaces. This effect can be accounted for by introducing the shear retention factor β . The mode II and III stiffnesses are given by:

$$D^{II} = D^{III} = \frac{\beta}{1 - \beta} G \quad (3.154)$$

where G is the shear modulus and β is the shear retention factor.

A constant shear retention factor approach is assumed in the single-crack fixed model implemented in the pointwise THM model. The value for β is specified by the user in the input data file.

3.9 CONSIDERATIONS AND LIMITATIONS IN THE IMPLEMENTATION OF THE USER-SUPPLIED ROUTINE

The integration of a user-supplied routine within external software presents both advantages and limitations. This subchapter presents some considerations and limitations associated with such routines, particularly focusing on the DIANA FEA software.

DIANA FEA is a software designed for multipurpose advanced analysis in multiple areas of engineering. The software supports the application of very flexible and interactive pre-processing tools, including modelling approaches that comprise a vast number of finite element types, geometries, loadings, connections, and meshing options. The software also includes numerous post-processing tools for evaluating the finite element results. DIANA FEA enables the performance of nonlinear analyses, providing a comprehensive set of numerical methods and convergence criteria. It is equipped with algorithms to handle geometrical nonlinearities and can conduct nonlinear analyses over time, accounting for load, temperature, and other time-dependent factors. The available material libraries enable the specification of concrete, steel, and other construction materials in accordance with code approaches. DIANA FEA includes many implemented material models, such as total strain cracking

models and multifixed crack models, as well as models for creep simulation, including the Kelvin Chain, Maxwell Chain, and Taylor series. Furthermore, DIANA FEA allows users to define material models, interface behaviour, and ambient influences through user-supplied routines, which is the case in the present work. Using a user-supplied material routine requires the complete numerical implementation of the material's behaviour, regardless of the material models available in DIANA FEA.

3.9.1 ITERATIVE METHOD FOR NONLINEAR ANALYSIS

In nonlinear finite element analysis, the nonlinear system of equations must be iteratively solved until equilibrium is achieved. DIANA offers well-known iteration schemes, including the Constant and Linear Stiffness approaches, Regular and Modified Newton-Raphson methods and Quasi-Newton methods [230]. These iterative methods intend to adapt the incremental displacement vector $\Delta \mathbf{u}$ by iterative increments $\delta \mathbf{u}_{i+1}$, until equilibrium is reached. A direct approach to determine the iterative increment vector $\delta \mathbf{u}_{i+1}$ is provided by the following equation:

$$\delta \mathbf{u}_{i+1} = \mathbf{K}_i^{-1} \mathbf{g}_i \quad (3.155)$$

where $\mathbf{K}_i^{-1}$ is the inverse of the stiffness matrix and $\mathbf{g}_i$ is the out-of-balance force vector, or residual, given by $\mathbf{g}_i = \mathbf{f}_{ext}^{t+\Delta t} - \mathbf{f}_{int,i}$, where $\mathbf{f}_{ext}^{t+\Delta t}$ is the external force vector and $\mathbf{f}_{int,i}$ is the internal force vector at the iteration i .

The Newton-Raphson method computes the inverse of the stiffness matrix utilising the tangent stiffness matrix, whereas the Quasi-Newton method derives the inverse stiffness matrix based on previously determined positions along the equilibrium path. Due to its advantages and specific applicability in the context of this research, the ensuing discussion will concentrate exclusively on the Quasi-Newton method, while other methods and their applications to nonlinear finite element analysis are comprehensively detailed in the literature [173, 230, 250]. From the obtained incremental displacement vector, $\delta \mathbf{u}_{i+1}$, a new internal force vector $\mathbf{f}_{int,i+1}$ can be computed. Following the Quasi-Newton approach, the secant-like approximation to the tangential stiffness matrix can be obtained using the following equation [173]:

$$\mathbf{K}_{i+1} \delta \mathbf{u}_{i+1} = \delta \mathbf{f}_{int,i+1} \quad (3.156)$$

where $\delta \mathbf{f}_{int,i+1} = \mathbf{f}_{int,i+1} - \mathbf{f}_{int,i}$.

The Quasi-Newton method applied to a one-dimensional problem can be obtained by combining Equation (3.156) and Equation (3.155). Fig. 58 shows a one-dimensional representation of the Quasi-Newton iterative problem.

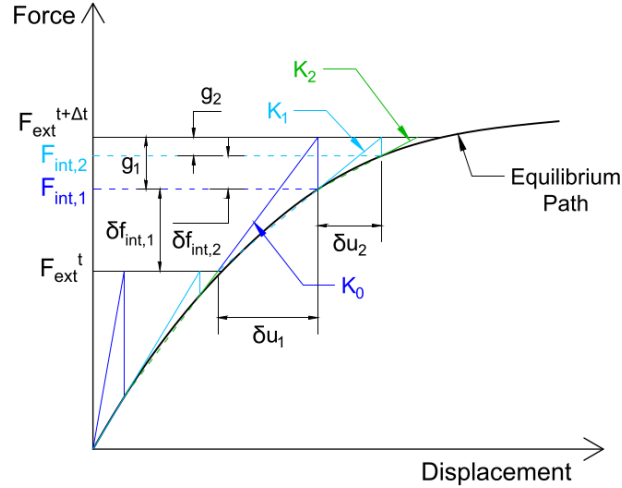


Fig. 58 – One-dimensional representation of the Quasi-Newton iterative problem.

The iterative process begins by setting up the initial stiffness, K_0 , and out-of-balance force, g_0 , and evaluating the first estimate of the incremental displacement value δu_1 by using Equation (3.155). The second stage involves calculating the internal force $f_{int,1}$ based on the prescribed material law and the updated displacement $u_1 = u_0 + \delta u_1$. Subsequently, the new secant stiffness value K_1 can be obtained by substituting δu_1 and $\delta f_{int,1} = f_{int,1} - f_{int,0}$ in Equation (3.156). In case the system has not yet converged to the required criteria, the iterative cycle is repeated, employing Equation (3.155) to determine the new incremental displacement δu_2 . This iterative mechanism continues until the convergence criteria is satisfied.

For the multi-dimensional case, the computation of the secant-like approximation of the tangent stiffness matrix described in Equation (3.156) is not straightforward. Different numerical approaches have been proposed to extend the model to a multi-dimensional case [173]. One of the most recurrently used in structural nonlinear finite element analysis is the one proposed by Broyden-Fletcher-Goldfarb-Shanno, also known as the BFGS method. The BFGS method updates the inverse secant stiffness matrix, $\mathbf{K}_{i+1}^{-1}$, based on the displacement increment $\delta \mathbf{u}_{i+1}$, and the change in the internal forces $\delta \mathbf{f}_{int,i+1} = \mathbf{f}_{int,i+1} - \mathbf{f}_{int,i}$. This process is performed according to the following Equation:

$$\mathbf{K}_{i+1}^{-1} = \left(\mathbf{I} + \frac{\delta \mathbf{u}_{i+1} \delta \mathbf{f}_{int,i+1}^T}{\delta \mathbf{u}_{i+1}^T \delta \mathbf{f}_{int,i+1}} \right) \mathbf{K}_i^{-1} \left(\mathbf{I} - \frac{\delta \mathbf{f}_{int,i+1} \delta \mathbf{u}_{i+1}^T}{\delta \mathbf{u}_{i+1}^T \delta \mathbf{f}_{int,i+1}} \right) + \frac{\delta \mathbf{u}_{i+1} \delta \mathbf{u}_{i+1}^T}{\delta \mathbf{u}_{i+1}^T \delta \mathbf{f}_{int,i+1}} \quad (3.157)$$

where $\mathbf{K}_i^{-1}$ is the inverse of the secant stiffness matrix in the previous iteration and $\mathbf{I}$ is the identity matrix with the same size as the inverse of the secant stiffness matrix.

The iterative method is completed by combining Equation (3.157) into Equation (3.155) [173, 230]. Despite the additional storage requirement, this numerical scheme is computationally fast since it is limited to algebraic multiplications and does not require the explicit inversion of the stiffness matrix. The BFGS method does not require the stiffness matrix output of the user-supplied routine and can achieve convergence within a few steps, with a rough estimate of the initial stiffness matrix, $\mathbf{K}_0^{-1}$. DIANA FEA provides different approaches for the initial setup of the inverse of the stiffness matrix

$\mathbf{K}_0^{-1}$. In the pointwise THM model, at the beginning of the analysis, the inverse of the stiffness matrix, $\mathbf{K}_0^{-1}$, is determined based on the linear stiffness matrix. For the first iteration of the subsequent steps, the inverse of the stiffness matrix of the last iteration of the previous step is used. The BFGS method presents a superlinear convergence behaviour which deteriorates with the number of iterations, in contrast with the quadratic convergence of the Newton-Raphson [173]. Nevertheless, the method is very stable in handling nonlinear behaviours like cracking progression.

3.9.2 CONVERGENCE CRITERIA

The convergence criteria ensure that the numerical solution approaches the proper solution, which is a fundamental issue for the accuracy and reliability of the numerical simulations. DIANA FEA offers four different convergence criteria to the users:

$$\text{Force norm ratio} = \frac{\sqrt{\mathbf{g}_i^T \cdot \mathbf{g}_i}}{\sqrt{\mathbf{g}_1^T \cdot \mathbf{g}_1}} \quad (3.158)$$

$$\text{Displacement norm ratio} = \frac{\sqrt{\delta \mathbf{u}_i^T \cdot \delta \mathbf{u}_i}}{\sqrt{\delta \mathbf{u}_1^T \cdot \delta \mathbf{u}_1}} \quad (3.159)$$

$$\text{Energy norm ratio} = \frac{|\delta \mathbf{u}_i^T (\mathbf{f}_{int,i+1} + \mathbf{f}_{int,i})|}{|\delta \mathbf{u}_1^T (\mathbf{f}_{int,2} + \mathbf{f}_{int,1})|} \quad (3.160)$$

$$\text{Residual norm ratio} = \frac{|\sqrt{\mathbf{g}_i^T \cdot \mathbf{g}_i} - \sqrt{\mathbf{g}_{i-1}^T \cdot \mathbf{g}_{i-1}}|}{|\sqrt{\mathbf{g}_1^T \cdot \mathbf{g}_1} - \sqrt{\mathbf{g}_n^T \cdot \mathbf{g}_n}|} \quad (3.161)$$

where $\delta \mathbf{u}_i$ refers to the additional increment, $\mathbf{g}_i$ refers to the out-of-balance force, or residual, and $\mathbf{f}_{int,i}$ refers to the internal force vector for the iteration i .

In the numerical analysis of delayed effects, including thermal, shrinkage, and creep strains, challenges arise in selecting appropriate convergence criteria, particularly when using user-supplied routines. For instance, in time-controlled analyses where creep strains are considered in the material routine, the first prediction of the displacement vector $\delta \mathbf{u}_1$ is typically a near-zero vector. Therefore, for numerical simulations of creep and relaxation, the displacement and energy norm ratios can result in errors, as noted by Borst et al. [173]. Consequently, the force norm or residual norm ratio are more suitable in such cases. In this case, the creep strains are simulated through the change in the internal force, $\mathbf{f}_{int,1}$, and, consequently, a change in the residual. Convergence is achieved when the strain deformation in the iterative process aligns with the strains modelled in the material routine, resulting in a negligible difference in internal forces between the previous and the current time step $|\mathbf{f}_{int,i}^{t+\Delta t} - \mathbf{f}_{int,m}^t| \approx [\mathbf{0}]$.

Borst et al. [173] suggested considering a tolerance criterion of 1×10^{-3} for the force norm ratio, ensuring accuracy and computational efficiency. In this PhD work, the suggested tolerance criterion was applied within the force norm ratio.

3.10 EXAMPLE OF DATA INPUT IN THE POINTWISE MECHANICAL MODEL

The user specifies the inputs of the pointwise mechanical routine through the material table in the data file. The pointwise mechanical routine utilises different variable types, each serving a distinct purpose:

- **material parameters:** these variables, once set, remain constant within the user-supplied routine and cannot be changed during the numerical analysis. Examples include the water-cement ratio, equation parameters, the specific number of Kelvin-Voigt elements in the Kelvin chain, etc;
- **integer indicators:** these integer variables are both modifiable and usable within the routine, typically serving to select the appropriate material model when multiple options are available. Examples include the cement hydration model indicator and the continuum or fracture model indicator;
- **state variables:** these variables are essential to the subroutine's operations, changing based on the simulation's progress. Examples include the degree of hydration, equivalent age, microprestress, creep strains, etc.

The data file must follow the precise input format specified by the latest version of the user-supplied routine. Any discrepancies in inputting material variables, temperature, or concentration tables could lead to incorrect outcomes or complete analysis failure. Box 3.4 shows an example of the material routine input in the material table.

Box 3.4 - Material input for the mechanical analysis in DIANA FEA using the Pointwise THM model.

```
'MATERI '
  1 NAME      MACONC
    YOUNG      3.30000E+04
    POISON     2.00000E-01
    THERMX     1.00000E-05
    CONCEX     1.00000E-03
    POIRED DAMAGE
:    POIRED NONE
    TENCRV     HORDYK
    CRKVAL     2.9
    GF         0.14
    CRACKB     10
:CRACK WIDTH FOR SWITCHING FROM ROTATING TO FIXED CRACKS (IN MM)
    EPSFIX     0.01
```

```

RESTST    0.01
BETA      0.1
USRMAT    USRMOD

:===== INTEGER INDICATORS =====
:NUMBER OF KELVIN CHAIN ELEMENTS
    USRIND    10
:CRACK MODEL SELECTOR (-1 - Crack model Disabled; 0 - Standard;
:  1 - Tot. Rotating Model; 2 - Tot. Fixed Model;
:  4 - Single Crack Fixed Model W/Strain Decomposition )
    4
:SINGLE PARTICLE CEMENT HYDRATION MODEL (1 - ACTIVE)
    0
:SHRINKAGE MODEL ( 0-Linear Sh.; 1 - BN EQ; 2 - KWAQ EQUATION )
    0

:===== MATERIAL PARAMETERS =====
:CREEP MODEL PARAMETERS: Q1 Q2 Q3 Q4
    USRVAL    22.55E-06 120.58E-06 4.65E-06 5.57E-06
:MICROPRESTRESS PARAMETERS: COMPS / K1 / BMPS / PBMPs
    0.005     1.10     5.0E-4  1.4
:REDUCED TIME ACTIVATION ENERGY: QE / QR / QS
    2.2478E+04 4.157E+04 2.4942E+04
:REDUCED TIME HYGRAL PARAMETERS: HE / HR / HS
    1.0E1 1.0E-1 1.0E-1
:PARAMETERS FOR CEMENT HYDRATION: FBL / A/C / W/C
    350. 6.6667E+00 4.8333E-01
:RETARDATION TIMES
    5.0E+00 5.0E+01 5.0E+02 5.0E+03 5.0E+04 5.0E+05
    5.0E+06 5.0E+07 5.0E+08 5.0E+09
: TENSILE STRENGTH EVOLUTION PARAMETER: S / NTFCT/ NFCT
    0.25 0.75 0
:SHRINKAGE COEFFICIENT MODEL
    1.0 0.2 2.0

:===== STATE VARIABLES =====
:CONCRETE EQUIVALENT AGE (SETTING TIME OF ANALYSIS IN SECONDS)
    USRSTA    1296
:TENSILE STRENGTH / CRACK STATUS
    0.0 0.0
:ACCUMULATIVE THERMAL STRAIN AND SHRINKAGE STRAIN
    0.0 0.0
:MICROPRESTRESS AND VISCOSITY MODULUS (FOR SETTING TIME)
    13333.33 2693.0

```



```
:CRACK STRAIN AT THE INTEGRATION POINT
      0.0 0.0 0.0 0.0 0.0 0.0
: VARIABLES FOR THE SINGLE PARTICLE CEMENT HYDRATION MODEL
: 1- Degree of Hydration; 2- Vol. Cem; 3- Vol. Gel;
: 4- Vol. CH; 5- Porosity; 6- Saturation;
: 7- Self-Desiccation; 8 - Internal Radius;
: 9- External radius
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
:DAMAGE FUNCTION ALFA
      0.0 0.0 0.0 0.0 0.0 0.0
:PRINCIPAL OR CRACK DIRECTIONS
      1.0 0.0 0.0
      0.0 1.0 0.0
      0.0 0.0 1.0
:VISCOELASTIC STRESS STATE VARIABLES
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
:INCREMENTAL MODULUS
      0.0
```

The data input of the pointwise THM model is summarized as follows:

1. Primary material constants:
 - a. YOUNG: Initial guess for Young's modulus in the BFGS stiffness update (Chapter 3.9.1). A recommended value of 33.6 GPa is considered the default. The precision is not relevant.
 - b. POISON: Isotropic Poisson's ratio
 - c. THERMX: Coefficient of thermal expansion (for thermal-strain simulation).
 - d. CONCEX: Shrinkage coefficient for shrinkage simulation; choose according to the selected shrinkage model.
2. Damage model parameters:
 - a. POIRED DAMAGE for Poisson's ratio evolves via the orthotropic damage law; POIRED NONE for constant isotropic Poisson's ratio (only in total strain models).
 - b. TENCrv HORDYK for Hordijk tension softening model; TENCrv MC2010 for bilinear MC2010 tension softening model (any other value defaults to Hordijk)
 - c. CRKVAL: the 28-day tensile strength value.
 - d. GF: the 28-day fracture energy value.

- e. CRACKB: the crack bandwidth.
 - f. EPSFIX: the crack width at which the rotating-crack model switches to a fixed crack if the cracking model “0” is selected.
 - g. RESTST: the residual stress at the end of softening.
 - h. BETA: the shear-retention coefficient.
3. Pointwise THM model variables:
- a. Four Integer switches:
 - i. Number of Kelvin-Voigt elements in the solidifying Kelvin Chain creep model.
 - ii. Crack model selector
 - iii. Single-particle cement-hydration model activation (1 to active).
 - iv. Shrinkage model: 0 – linear shrinkage coefficient; 1 – BN shrinkage coefficient model; 2- Kwak rate shrinkage coefficient model.
 - b. Material parameters:
 - i. Four parameters to the creep model: q_1, q_2, q_3, q_4
 - ii. Microprestress solidification parameters: $c_0, k_1, b_{XMPs}, p_{XMPs}$
 - iii. Transformed-time parameters: $Q_e, Q_r, Q_s, \alpha_e, \alpha_r, \alpha_s$.
 - iv. Single-particle cement hydration parameters.
 - v. Retardation times, according to the number of Kelvin-Voigt elements: $\tau_\mu, \dots, \tau_i$
 - vi. Tensile strength evolution: three parameters (Equation (3.86)).
 - vii. Shrinkage coefficient model: three parameters (Equation (3.47) or (3.48)).
 - c. State variables:
 - i. Concrete age (in seconds): Use at least 1296 s (0.015 days) rather than 0 s for realistic initial conditions.
 - ii. Tensile strength evolution (computed internally).
 - iii. Active crack model at each integration point.
 - iv. Accumulated thermal strain.
 - v. Accumulated shrinkage.
 - vi. Initial microprestress: set by Equation (2.123) using the age from state variable 1.
 - vii. Initial dashpot viscosity modulus, from Equation (2.122).
 - viii. Principal direction crack strains: six state variables.
 - ix. Single-particle cement hydration outputs: nine state variables.
 - x. Rotation tensor for the crack model: nine state variables
 - xi. Viscoelastic creep variables: number of Kelvin-Voigt elements times six.
 - xii. Previous step incremental modulus for the time dependencies in the total strain model.

The pointwise THM model requires the input of the temperatures and relative humidity values. Box 3.5 shows the example of temperature and relative humidity input in the data file.

Box 3.5 - Temperature and relative humidity input for using the Pointwise THM model.

```
'TEMPER'
NODES
    0.00000E+00    1.80000E+96
/ 1-8 /
    2.00000E+01    2.00000E+01
'CONCEN'
NODES
    0.00000E+00    1.80000E+96
/ 1-8 /
    1.00000E+00    1.00000E+00
```

The inputs for temperature and relative humidity share an identical structure. The keyword **NODES** denotes that the data will be supplied for all nodes. Next, the vector of time points at which the temperature or relative humidity is supplied must be defined. DIANA will perform linear interpolation between the analysis time and these supplied time points. Subsequently, the target node or group of nodes should be indicated using the notation “/ n-n /”. Finally, a vector of temperature and relative humidity values is provided, with each entry corresponding to the previously defined time points.

Some specifications are required in the numerical analysis file to use the pointwise THM model. Box 3.6 shows an example of the specifications for the numerical analysis for using the pointwise THM model.

Box 3.6 - Analysis specifications in the “dcf” file for using the Pointwise THM model.

```
*FILOS
INITIA
*INPUT
*FORTRAN
USE "PTHMV0.dll"
*NONLIN
(...)
BEGIN OUTPUT
    FILE "Results"
    STATUS USER
END OUTPUT
(...)
```

The keyword FORTRAN indicates that an external material model, written in Fortran, will be employed in the numerical analysis as a Dynamic Link Library (DLL). The specified model file is PTHMV0.dll, corresponding to version V0 of the pointwise THM model. The STATUS USER option in the output command directs the solver to include the state variable in the analysis results. Enabling this option can substantially increase the output file size since that state variable will be provided for every integration point at each analysis step, in addition to any other user-requested output.

3.11 VALIDATION OF THE NUMERICAL IMPLEMENTATION OF THE POINTWISE MECHANICAL MODEL

This chapter presents the validation and quality assurance of the implemented submodels of the pointwise THM mechanical model. The comparison is performed using two sets of simulations in multiple stress scenarios: one based on the pointwise THM model and the other on DIANA's built-in models. In the absence of hygrothermal variations, the pointwise THM model can be reproduced by equivalent models available in DIANA FEA. Therefore, agreement between the results of the pointwise THM model and similar models available in DIANA FEA provides confidence in the correctness and reliability of the implemented formulations. The validation is performed by a series of benchmark tests using a single finite element. Some of the benchmark tests are purely numerical and developed to explore different properties of the implemented numerical models. Therefore, the set of loads, loading times, and other modelling properties presented in the present chapter may not be representative of real structural behaviour. The use of the pointwise THM model to simulate the real structural behaviour is reserved for Chapter 4. The same material parameters are used in both analyses. The material parameters used are presented in Box 3.4 and summarised in the following table:

Table 9 – Parameters used in the pointwise THM model validation.

Model	Parameter	Value
Fracture	f_{ctm}	2.9 MPa
	G_f	0.140 N · mm
	h	10 mm
Creep parameters	q_1	$22.55 \times 10^{-6} \text{ MPa}^{-1}$
	q_2	$120.58 \times 10^{-6} \text{ MPa}^{-1}$
	q_3	$4.65 \times 10^{-6} \text{ MPa}^{-1}$
	q_4	$5.57 \times 10^{-6} \text{ MPa}^{-1}$

In these benchmark simulations, the maturity effects on the fracture properties are disabled. Temperature and relative humidity are considered constant (20 °C, RH = 1.0), so the transformed times equal the concrete age.

All analyses use the Hordijk tension-softening law. In DIANA FEA, creep is represented by an ageing Kelvin chain calibrated against the target creep-compliance curve: a least-squares fit determines the spring moduli of each Kelvin–Voigt element to match compliance data at prescribed loading times.

Fig. 59 compares the creep compliance at different loading times using the direct input through an ageing Kelvin chain available in DIANA FEA material models (DIANA-KC), with the results obtained through the present pointwise THM model (PTHM).

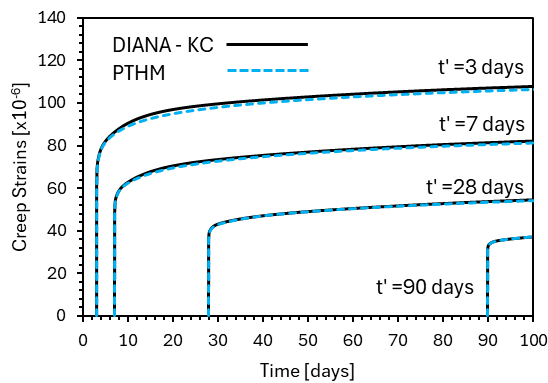


Fig. 59 – Comparison between the ageing Kelvin Chain in DIANA FEA (DIANA-KC) and the creep model in the Pointwise THM model (PTHM).

The comparison between the obtained creep compliances yields consistent results between the two approaches, thereby validating the numerical implementation of the pointwise THM model for simulating the ageing part of the concrete creep.

The benchmark for the mechanical models is tested using a single finite element with the application of an imposed deformation in one direction. Fig. 60 presents the single finite element used in the pointwise THM model validation.

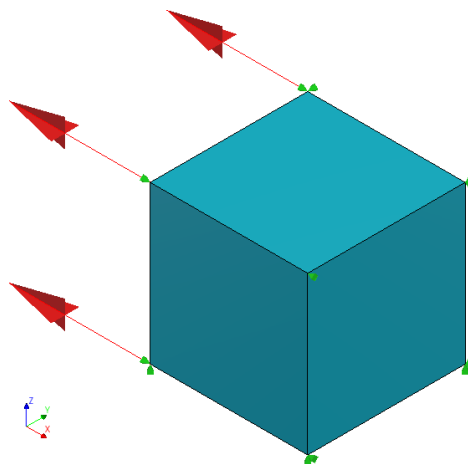


Fig. 60 – Single finite element for the pointwise THM model validation.

In most tests, deformations are imposed along the X-direction; all other degrees of freedom remain free, although some scenarios include lateral supports to assess their effect on stress responses.

The finite element in the numerical simulations is an eight-node isoparametric solid brick element (HX24L in DIANA FEA V10.6). A $2 \times 2 \times 2$ integration scheme is used in the numerical analysis. The

analysis is run through time steps discretised to capture the transition behaviour in the tensile softening models implemented and in loading and unloading regimes. All the analysis uses more than 100 steps. Such high time-step discretisations are not strictly required, and the analysis could be done with fewer steps. However, the time spent preparing detailed step discretisations for each test is higher than assuming more steps than required. The run time of all tests considered in this chapter is generally in the range of one minute. The imposed deformation is applied in a time-load table.

Each analysis in this chapter is labelled “TnXX,” where “n” is the test number and “XX” identifies the numerical model. For example, T1DA denotes Test 1 using DIANA’s multi-directional fixed-crack model. The notation used throughout is:

- DA – DIANA FEA’s multi-directional fixed crack model;
- DR – DIANA FEA’s total strain model with rotating cracks;
- DF – DIANA FEA’s total strain model with fixed cracks;
- SF – Pointwise THM model with a single-crack fixed model (Chapter 3.8.2.6);
- TR – Pointwise THM model with total strain, rotating crack formulation;
- TF – Pointwise THM model with total strain, fixed crack formulation.

Not all tests are performed for every model. Omitted cases produce identical results.

3.11.1 TEST 1 - TENSION SOFTENING MODEL WITH IMPOSED DEFORMATION

The first series of tests for validating the pointwise THM model is based on numerical simulations of the tension softening test. Three tests were carried out:

- Test 1.1 – Tension softening model;
- Test 1.2 and Test 1.3 – Creep effects on tension softening model.

3.11.1.1 Test 1.1 - Tension softening model

In the first test, an imposed deformation large enough to fully describe the Hordijk tension-softening curve was applied at 28 days through a total of 145 days until reaching a strain of 0.03. Fig. 61 shows the stress over the strain evolution for the test T11, considering three different numerical models (DA – DIANA FEA’s multi-directional fixed crack model; SF – Pointwise THM model with a single-crack fixed model; TR – Pointwise THM model with total strain, rotating crack formulation).

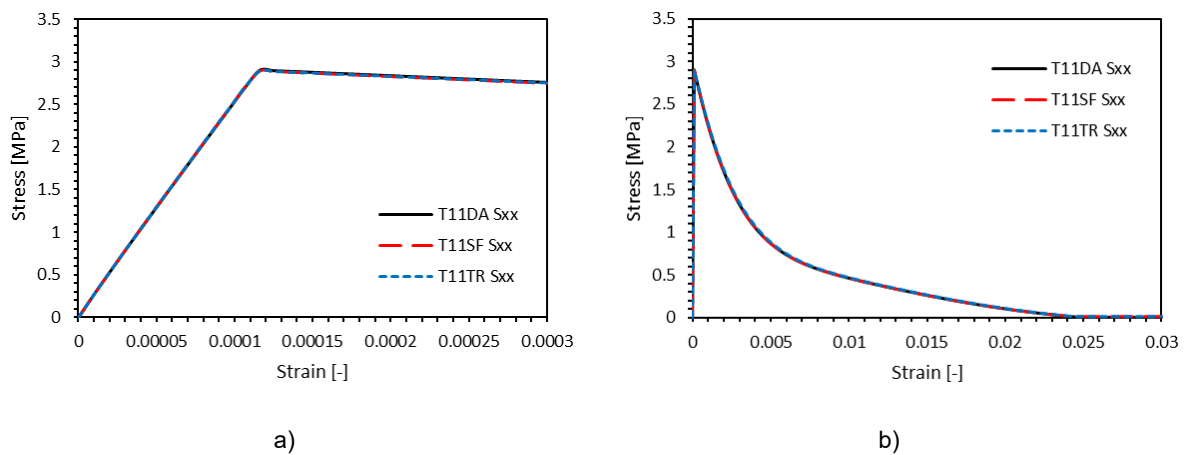


Fig. 61 – Test 1 - Validation of the Hordijk tension softening model: a) at cracking limits; b) at the softening part.

The numerical test validates the capabilities of the total strain model and the single-crack fixed model to simulate the tensile softening behaviour. Stress-strain curves obtained with the pointwise THM model (T11SF and T11TR) and DIANA FEA (T11DA) exhibit good agreement.

Test 1 also investigates the damage-dependent function affecting the Poisson ratio. Fig. 62 shows the evolution of the strains in the X-direction and the Y-direction, which is equivalent to the Z-direction for the Test 1.1 (T11).

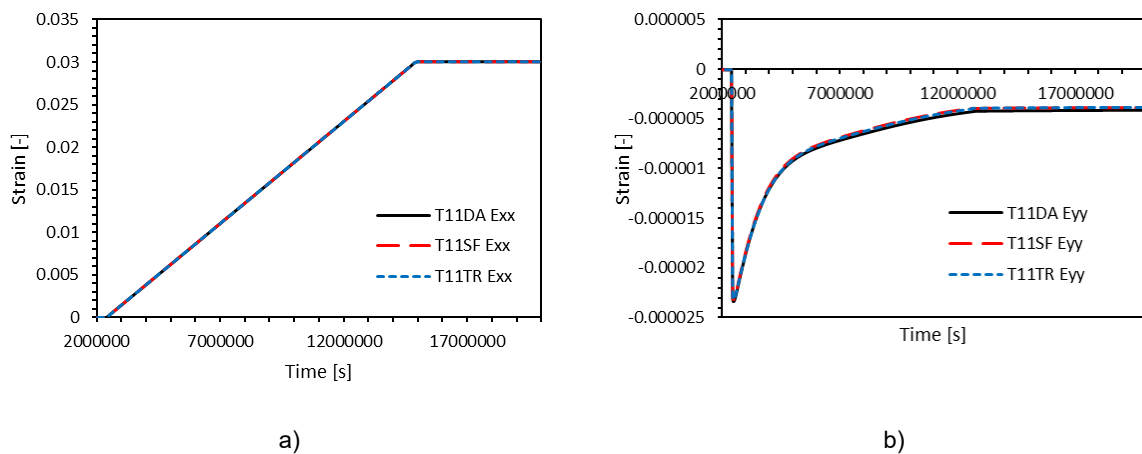


Fig. 62 – Test 1 - Strain evolution over time for: a) the loading X-direction; b) the lateral Y-direction.

The strain in concrete along the X-direction increases over time under the imposed deformation. Strains in the Y and Z directions remain negative. The evolution of the Y-direction strain follows the tension-softening curve, reflecting the damage function that progressively reduces the effective Poisson's ratio. Close agreement among all three analyses confirms the numerical model's validity for tension-softening simulation.

3.11.1.2 Test 1.2 and Test 1.3 – Creep effects on the tension softening model

The second series of tests investigates the creep effects on the tension softening model. The tests assumed the same modelling configuration as Test 1.1, but in this case, the loading is applied at 5 days

instead of 28 days to increase the creep effects on the tension softening test. Two tests are compared to assess the effects of creep on the tensile softening model:

- Test 1.2 - assumes the application of an imposed deformation for 145 days (similar to Test 1);
- Test 1.3 - assumes the application of an imposed deformation for 0.5 days.

Fig. 63 shows the strain evolution in the X-direction due to the application of the imposed deformation for Test 1.2 (T12) and Test 1.3 (T13).

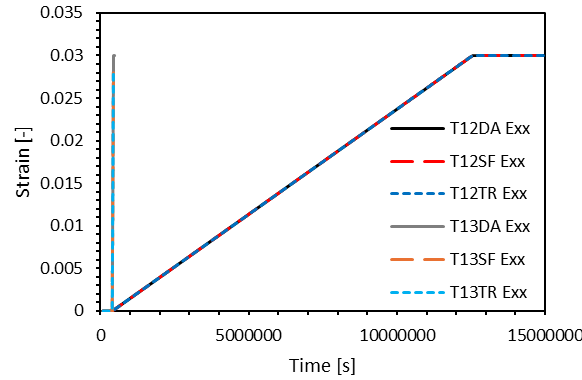


Fig. 63 – Strain evolution over time for Test 1.2 and Test 1.3

In Test 1.2, the strain evolution over time increases smoothly until reaching the value of 0.03 at 150 days. In contrast, the strain in Test 1.3 increases at a much higher rate, reaching the value of 0.03 at 5.5 days. Fig. 64 compares the stress-strain curve for Test 1.2 (T12) and Test 1.3 (T13).

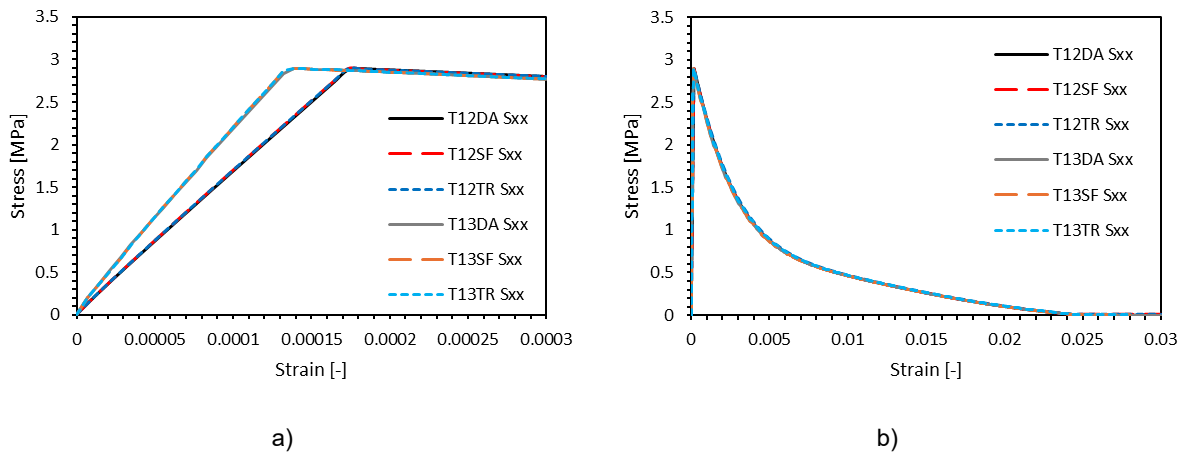


Fig. 64 – Tension softening curve for Test 1.2 and Test 1.3: a) at cracking limits; b) at the softening part.

The results show a different behaviour in the evolution of stresses at the cracking limits. Test 1.3 (T13) series shows a higher stress rate during the elastic part than Test 1.2 (T12) series. These results are expected, since the long application time of the imposed deformation in Test 1.2 (T12) leads to stress relaxation. In Test 1.3 (T13), the application of the imposed deformation is faster. Therefore, the creep effects are not as pronounced as in Test 1.2 (T12), leading to a stiffer behaviour during the elastic part.

Nevertheless, the differences in the softening part evolution are unidentifiable when comparing the results of Test 1.2 and Test 1.3. This occurs because the crack strains are much higher than creep or

elastic strains in the smeared crack concrete. Therefore, the results between all tests in the series Test 1.2 and Test 1.3 present similar softening evolution. For all the tests, good agreement was achieved between the pointwise THM model (SF and TR) and the models implemented in DIANA FEA (DA). The observed results also validate the approach adopted for the simulation of the Hordijk model in the total strain models detailed in Chapter 3.8.2.4.1.2.

3.11.2 TEST 2 – RELOADING AND UNLOADING TESTS

The second validation of the pointwise THM model is based on numerical simulations of reloading and unloading tests. Three tests were carried out:

- Test 2.1 – Unloading under tension, followed by reloading;
- Test 2.2 – Unloading into compression, followed by reloading;
- Test 2.3 – Unloading into compression after full exhaustion of the tension softening model, followed by reloading.

3.11.2.1 Test 2.1 – Unloading under tension, followed by reloading

Test 2.1 objective is to analyse the reloading and unloading schemes in the pointwise THM model under tension. Fig. 65 shows the results for Test 2.1 (T21).

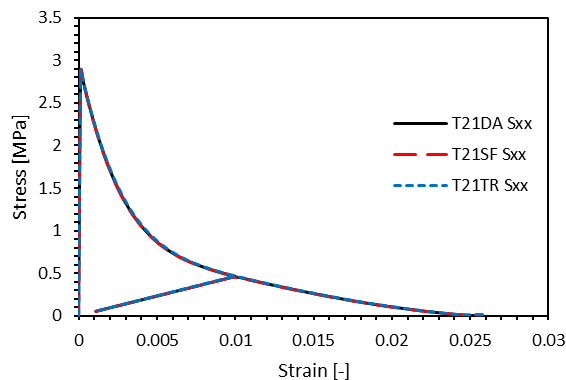


Fig. 65 – Test 2.1 – Stress evolution for the normal X-direction.

The results show good agreement in the unloading and reloading tests under tension. The secant-to-origin path approach is assumed and seems well simulated through the cracking models implemented in the pointwise THM model. Fig. 66 shows the strain evolution for Test 2.1 (T21).

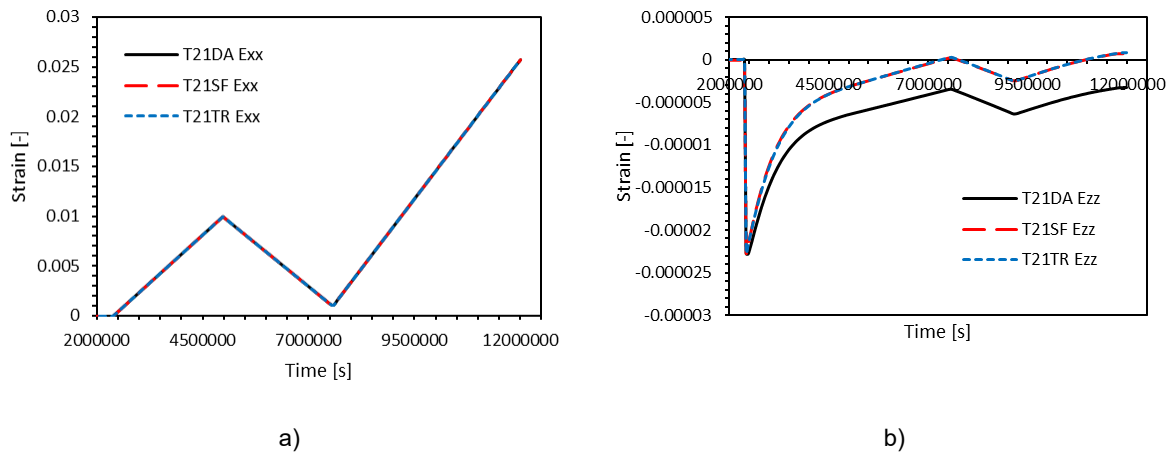


Fig. 66 – Test 2.1 - Strain evolution over time for: a) the normal X-direction; b) the lateral Y-direction.

All three analyses exhibit a similar normal strain evolution governed by the imposed deformation. In contrast, the lateral strains diverge between the pointwise THM model (T21SF and T21TR) and the multi-direction fixed-crack formulation in DIANA FEA (T21DA). Throughout the loading phase, the pointwise THM model (T21SF and T21TR) replicates the lateral strain curve shown in Fig. 62 b), whereas the T21DA simulation predicts substantially lower lateral strains. These discrepancies are unexpected since Tests T1 and T21 share an identical loading history until the first unloading event in T21 at approximately 5 000 000 s. However, by that stage, T21DA had already deviated significantly from the T21SF and T21TR results.

To identify the cause of such deviations, Test 2.1 (T21) was repeated under fully restrained boundary conditions. With lateral displacement prevented, transverse strains remain zero, and tensile stresses develop in the lateral directions. Fig. 67 shows the evolution of both normal and lateral stresses for Test 21r (full restraint, T21r).

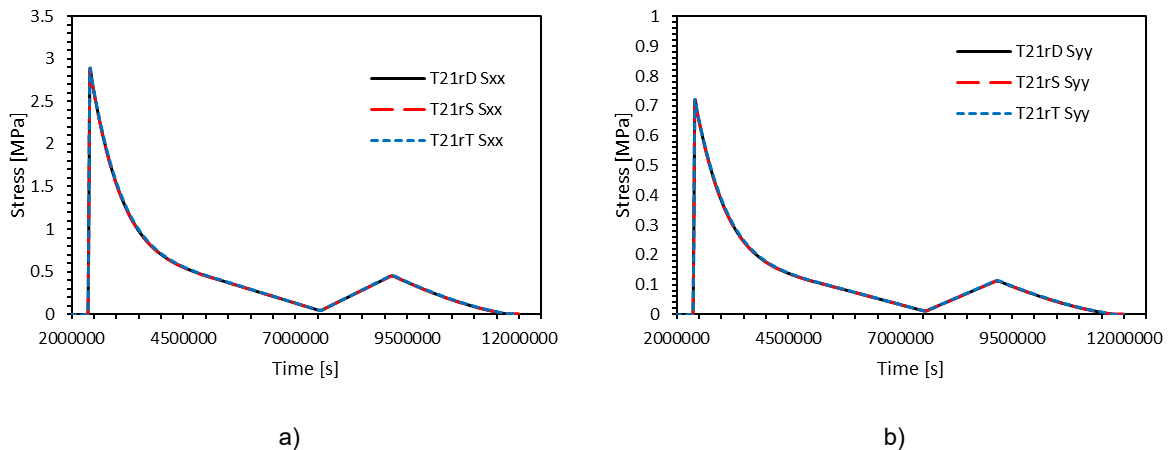


Fig. 67 – Test 2.1r - Stress evolution over time for: a) the normal X-direction; b) the lateral Y-direction.

The results demonstrate good agreement in the lateral (Y-direction) stress simulation. Although the anomalous lateral-strain behaviour observed in the T21DA simulations remains unexplained, it appears to exert negligible influence on the stress response once those strains are restrained. A possible

justification for the differences may be associated with regularised continuum models implemented in DIANA FEA.

3.11.2.2 Test 2.2 – Unloading into compression, followed by reloading.

Test 2.2 investigates the transition from tension to compression. The analysis is conducted by imposing a deformation in the X-direction, which induces crack formation, followed by unloading into compression. Fig. 68 shows the stress-strain evolution for the normal direction for Test 2.2 (T22).

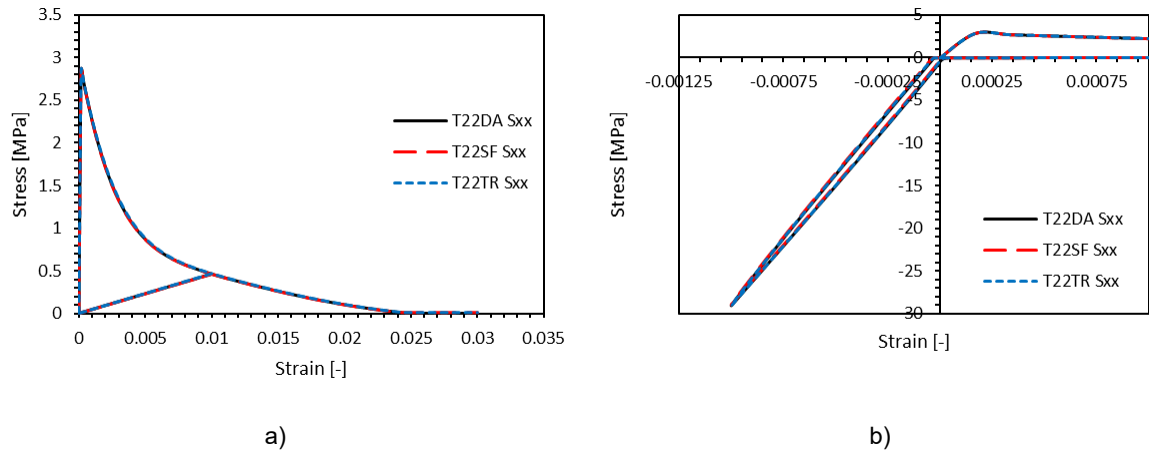


Fig. 68 – Test 2.2 – Stress-strain evolution for the normal directions: a) in tension; b) in compression.

The results indicate good agreement between the cracking models in the pointwise THM model (T22SF and T22TR) and the multi-directional fixed crack model available in DIANA FEA (T22DA). Another key behaviour to examine is the Poisson effect during the transition between compression and tension. To this end, the evolution of both normal and lateral strains are analysed. Fig. 69 shows the evolution of the normal strain E_{xx} and lateral strain E_{yy} .

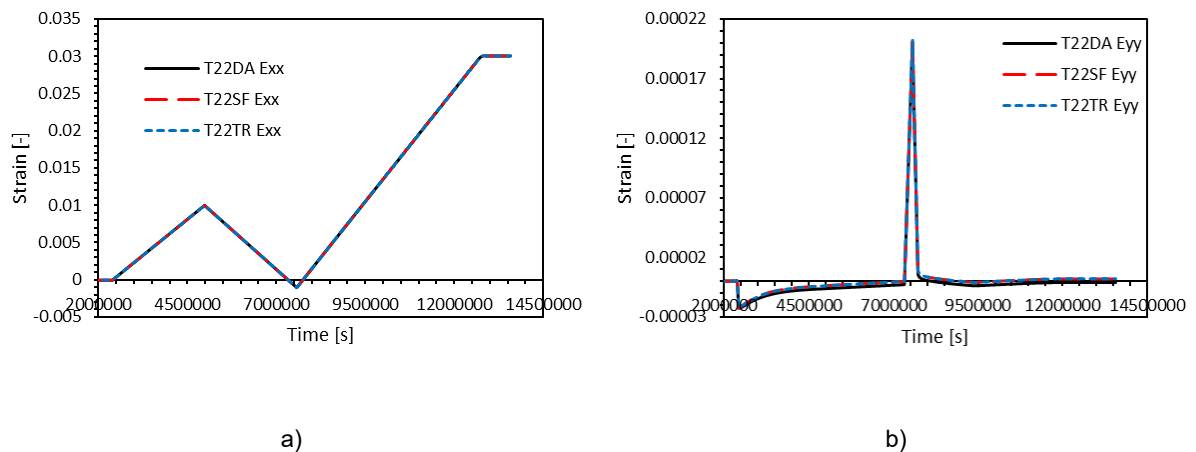


Fig. 69 – Test 2.2 - Strain evolution over time for: a) the loading X-direction; b) the lateral Y-direction.

The results demonstrate close agreement for the normal strain E_{xx} , with only minor discrepancies in the lateral strain E_{yy} , as previously observed in Test 2.1. Upon reversal of loading, DIANA FEA (T22DA) fully recovers the original Poisson's ratio, and the single-crack fixed-crack model (T22SF) behaves

similarly. In contrast, the total-strain formulation (T22TR) can accommodate damage-induced changes in Poisson's ratio by preserving an orthotropic relationship based on the damaged Poisson's ratio. However, to maintain consistency with the DIANA FEA (T22DA) and single-crack fixed-crack approaches (T22SF), the total strain model (T22TR) reverts to an isotropic no-damage Poisson's ratio once compressive stresses are reached. Further investigation into Poisson's ratio recovery upon transition from tension to compression is recommended for future work.

3.11.2.3 Test 2.3 – Unloading into compression after full exhaustion of the tension softening model, followed by reloading

Test 2.3 follows the same procedure as Test 2.2. However, in this instance, the unloading into compression is delayed until the tension-softening model has exceeded the ultimate crack-strain threshold. Fig. 70 shows the strain and stress evolution over time for the normal X-direction for Test 2.3 (T23).

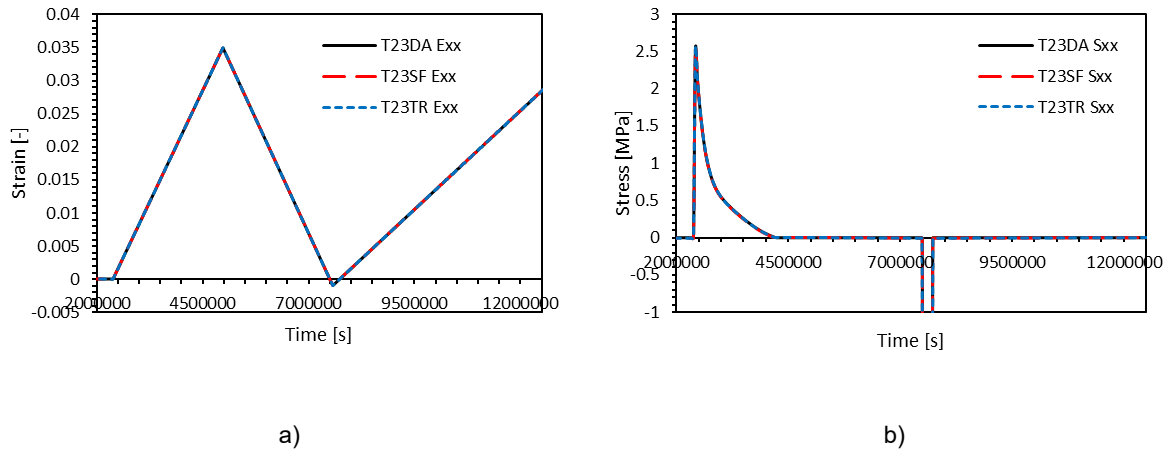


Fig. 70 – Test 2.3 – a) Strain evolution in time; b) Stress evolution in time.

After complete exhaustion of the tension-softening response at approximately 4 500 000 s, the axial stress stabilises at around 0.01 MPa. During unloading, the stress remains near zero until compressive strains develop. Thereafter, the compressive stress rises abruptly, reflecting the greater stiffness of concrete in compression. Upon reloading in tension, the stress returns to roughly 0.01 MPa. These findings exhibit close agreement between the cracking algorithms of the pointwise THM model (T23SF and T23TR) and those available in DIANA FEA (T23DA), thereby validating the unloading–reloading procedure for both the total strain and single-crack fixed formulations.

3.11.3 TEST 3 – ROTATIONAL TESTS FOR THE CRACK DIRECTIONS AND PRINCIPAL DIRECTIONS

In Tests 1 and 2, loading was applied along the X-axis so that the principal directions coincided with the global coordinate axes. By contrast, Test 3 was planned to assess how rotation affects the principal or crack directions, specifically to capture crack formation in orientations that do not align with the global axes. Test 3 imposes loading along three distinct directions at different nodes, divided into two loading

setups. Fig. 71 shows the two load setups applied to one finite element and the node that is going to be used for the pointwise THM model validation.

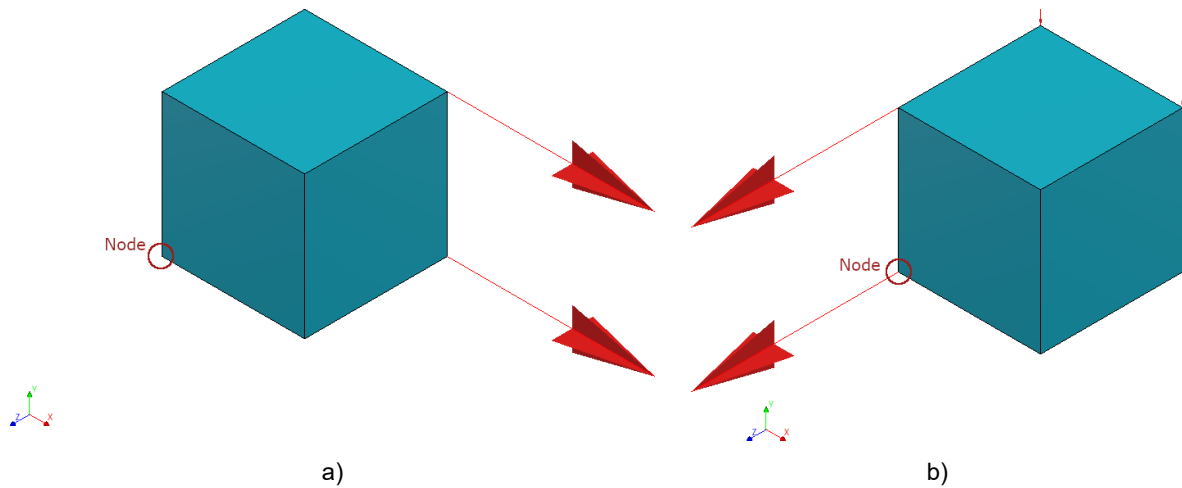


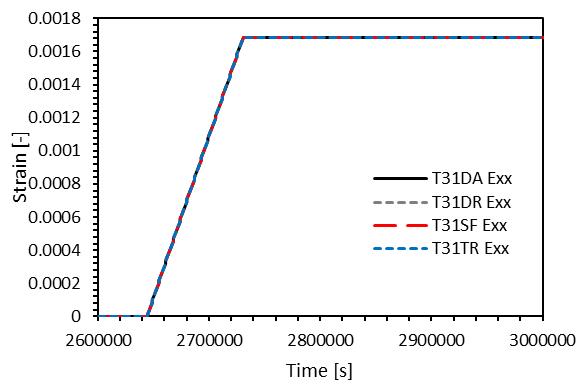
Fig. 71 – Load application: a) load case 1; b) load case 2.

Load case 1 consists of an imposed deformation in the X-direction at two nodes, with a factor of 1.0. Load case 2 comprises an imposed deformation in the Z-direction at two nodes (factor 0.75) combined with a negative deformation in the Y-direction at two other nodes (factor -0.05). All the finite element nodes in Test 3 are restrained in all directions. Two tests were conducted:

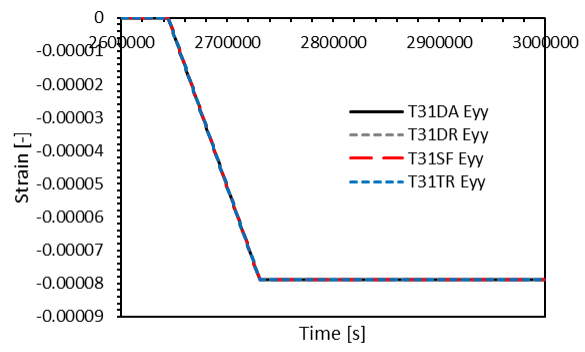
- Test 3.1 – Load cases 1 and 2 applied simultaneously;
- Test 3.2 – Load case 1 is applied first. After crack initiation, load case 2 is imposed to induce crack rotation.

3.11.3.1 Test 3.1 – Load cases 1 and 2 applied simultaneously

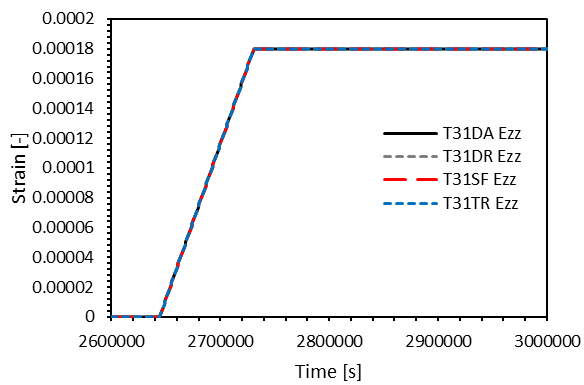
Test 3.1 investigates the computation of the principal or crack directions in the cracking models implemented in the pointwise THM model or those available in DIANA FEA. Fig. 72 shows the strain evolution, while Fig. 73 shows the stress evolution for Test 3.1 (T31), considering the models DIANA FEA's multi-directional fixed crack model (DA), DIANA FEA's total strain model with rotating cracks (DR), Pointwise THM model with a single-crack fixed model (SF) and Pointwise THM model with total strain, rotating crack formulation (TR).



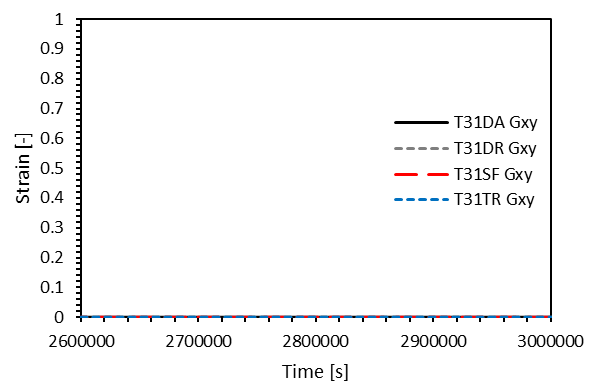
a)



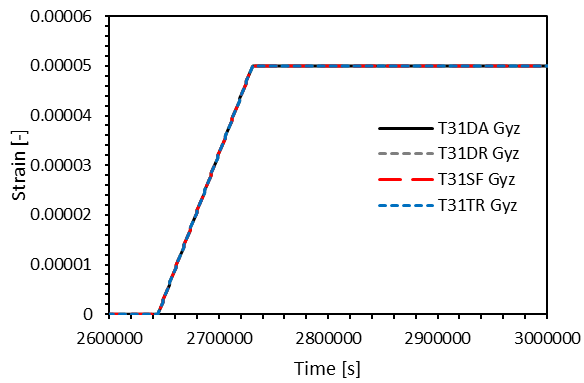
b)



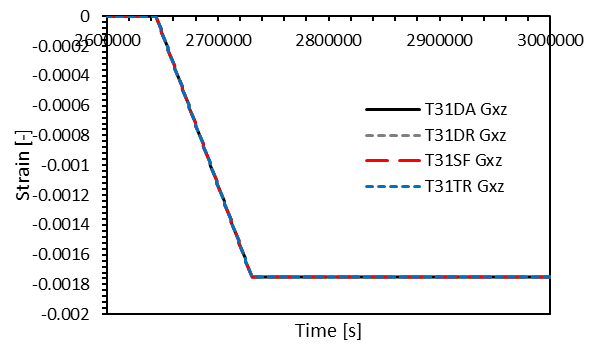
c)



d)



e)



f)

Fig. 72 – Test 3.1 - Strain evolution.

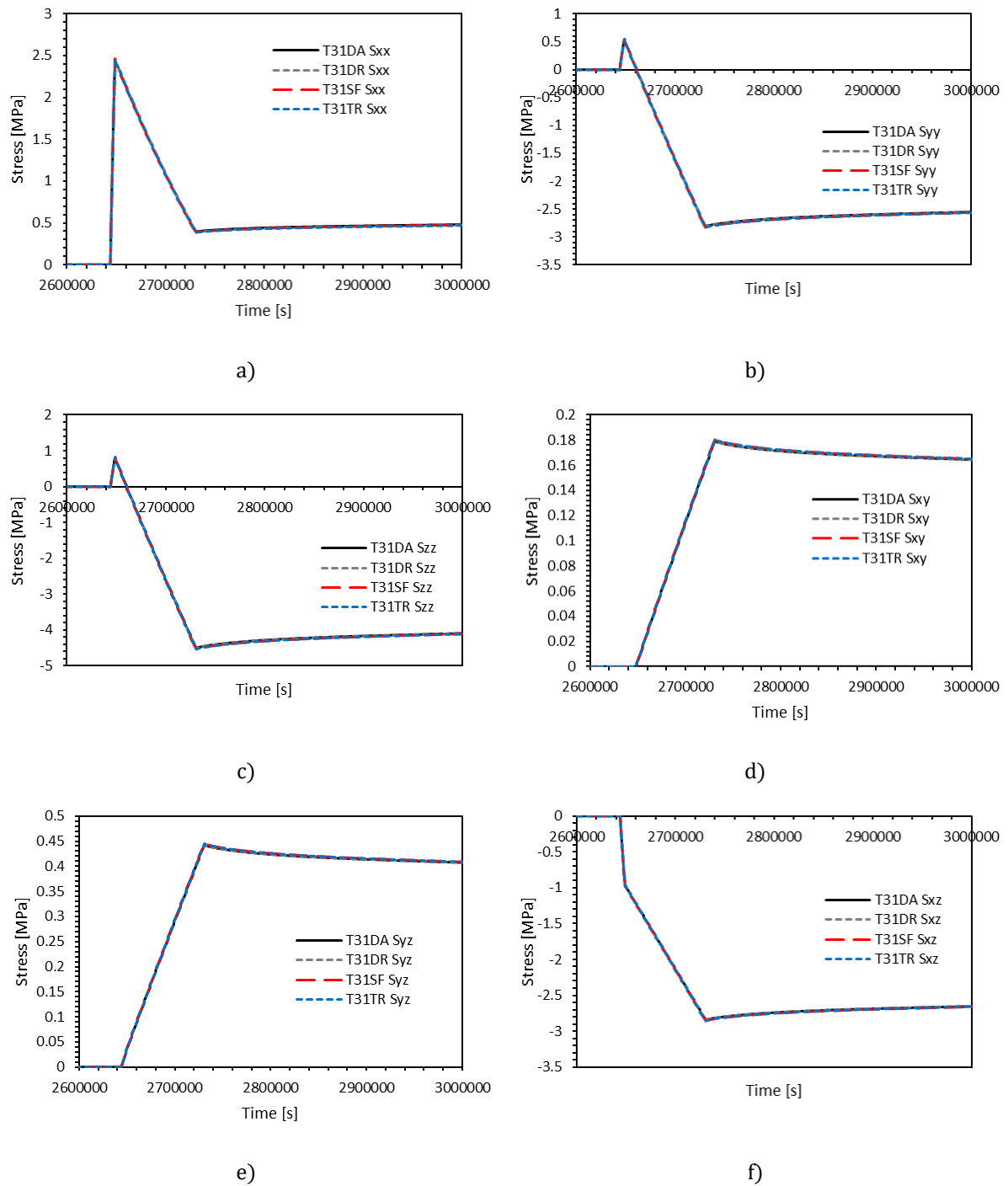


Fig. 73 – Test 3.1 - Stress evolution.

The computed strains and stresses in all orientations exhibit close concordance, demonstrating the models' ability to reproduce stress behaviour under rotating principal axes. This test thus validates the capacity of the cracking and rotating model algorithms to accurately identify principal directions and apply tension-softening constitutive laws even when those directions do not coincide with any global axes.

3.11.3.2 Test 3.2 – Unloading into compression after full exhaustion of the tension softening model

Test 3.2 investigates the rotation of the principal or crack directions in the cracking models implemented in the pointwise THM model (SF, TR and TF) and those available in DIANA FEA (DA and DR). Load Case 1 is applied first, and only after crack initiation is Load Case 2 imposed. Fig. 74 shows the strain evolution, while Fig. 75 shows the stress evolution for all the global directions for test (T32).

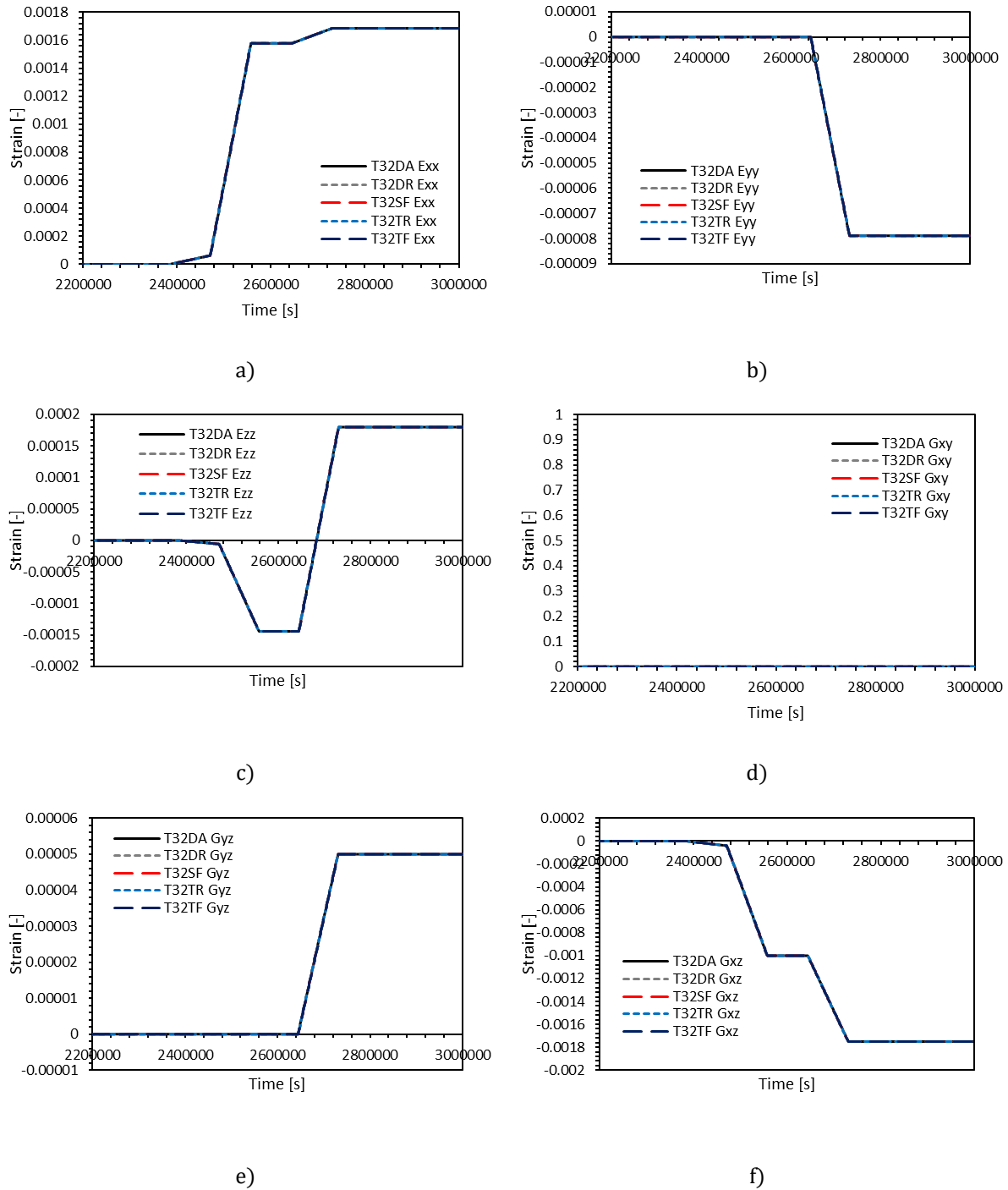


Fig. 74 – Test 3.2 - Strain evolution.

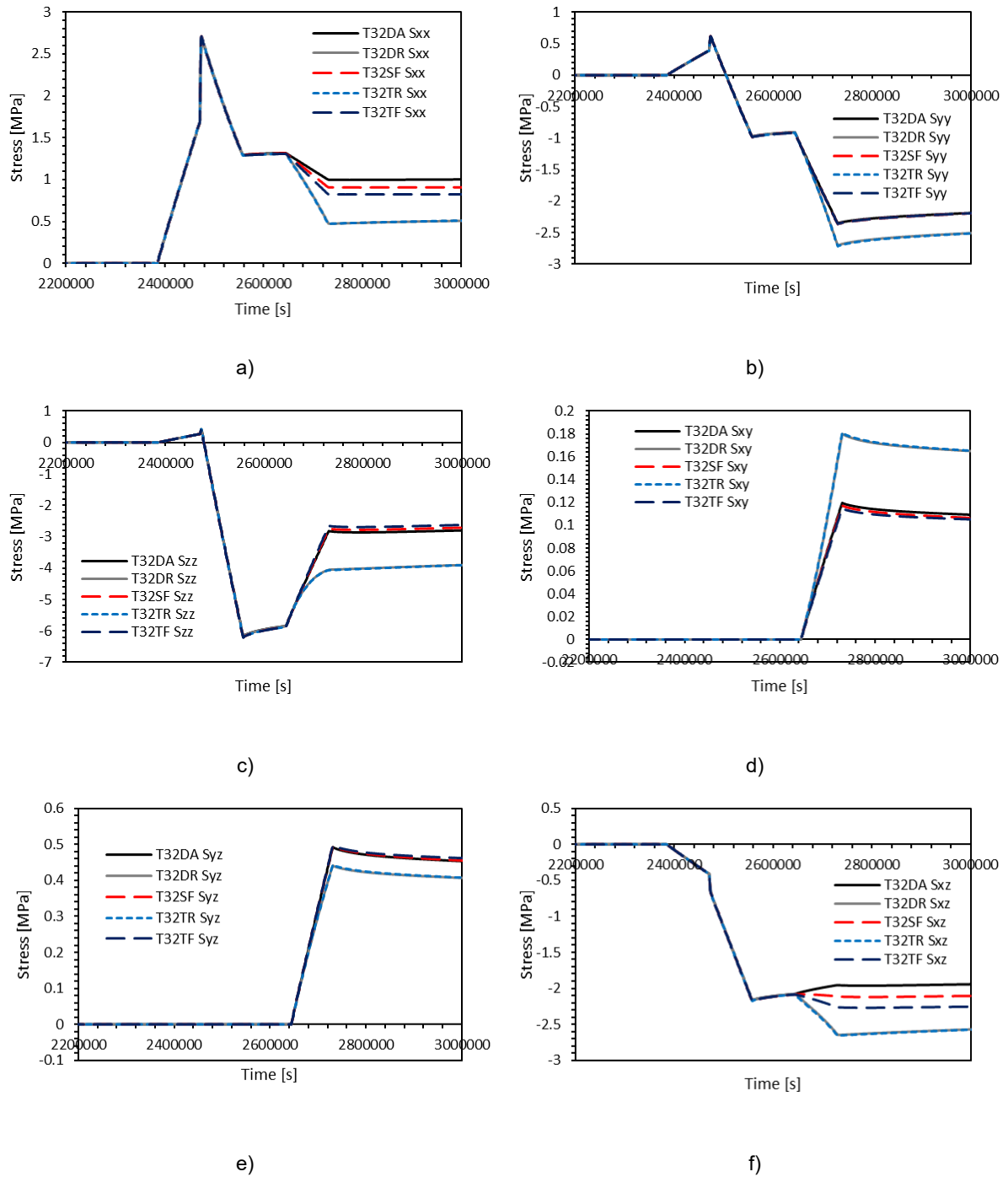


Fig. 75 – Test 3.2 – Stress evolution.

The stress predictions demonstrate good agreement between the total strain model with rotating cracks in the pointwise THM implementation (T32TR) and the equivalent rotating crack formulation in DIANA FEA (T32DR). After approximately 2 640 000 s, the principal stress directions begin to rotate away from the crack orientation, leading to differences in numerical results for the fixed crack schemes. Overall, all fixed crack models yield very similar results for S_{yy} , S_{zz} , S_{xy} and S_{yz} . In contrast, for S_{xx} and S_{xz} , the total-strain model with fixed cracks predicts lower stress magnitudes. For those tests, the single-crack fixed model (T32SF) underpredicts stresses compared to the DIANA FEA's fixed crack

model (T32DA). These discrepancies may arise from slight differences in how each numerical scheme evaluates shear strains. To clarify these effects, the DIANA FEA total strain fixed crack model (T32DF) was also used in the simulation of Test 3.2. Fig. 76 compares the stress evolution for all the fixed crack models.

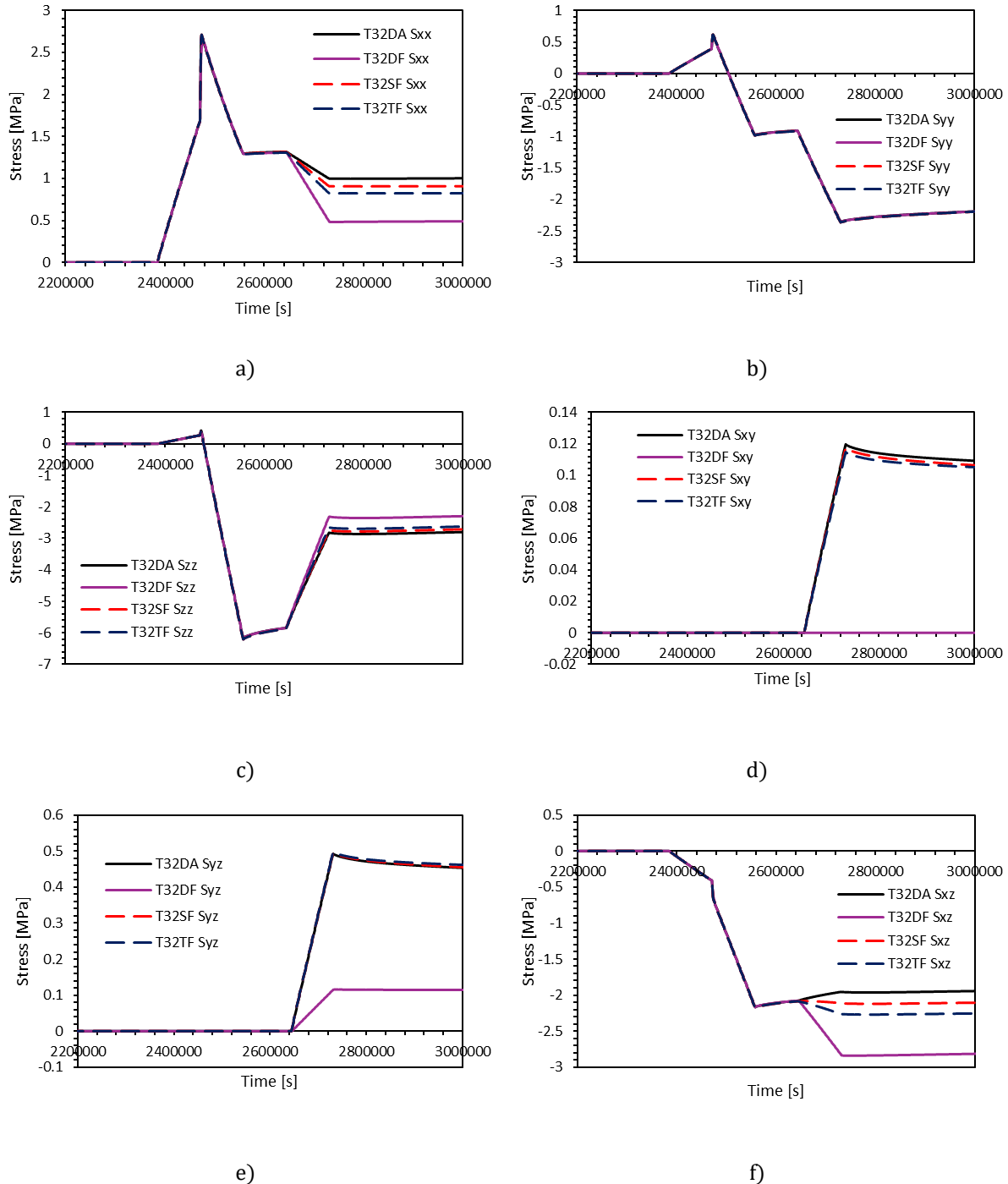


Fig. 76 – Validation of the stress evolution for the crack models.

The evolution of S_{yy} and S_{zz} exhibits good agreement across all models. However, discrepancies emerge in the remaining stress components when using DIANA FEA's total strain fixed crack formulation (T32DF). This finding demonstrates that even in these straightforward tests, the pointwise

THM models (T32SF and T32TF) can produce results slightly different from those obtained using DIANA's fixed crack algorithms (T32DA and T32DF), although the precise origins of these differences remain unclear. Nevertheless, both pointwise THM crack formulations, the single-crack fixed model (SF) and the total strain fixed crack model (TF), closely replicate the multi-directional fixed crack response (DA). Although the same shear retention model is assumed in all analyses, the observed deviations may be attributable to differences in the implementation of the shear model. More investigations would be required to address these differences in the shear behaviour. For the present case, since the fixed crack models implemented in the pointwise THM model (SF and TF) present small deviations from the fixed crack models available in DIANA FEA (DA and DF), the pointwise THM crack models are considered validated for fixed crack analyses.

3.11.4 TEST 4 – EIGENSTRAINS AND STRAIN LOCALISATION

The final benchmark test examines the influence of mesh discretisation and the restraint of eigenstrains. The model comprises five cubic elements (edge length 10 mm) arranged in series over a total length of 50 mm, with axial restraint applied in the X-direction. Fig. 77 shows the finite element mesh.

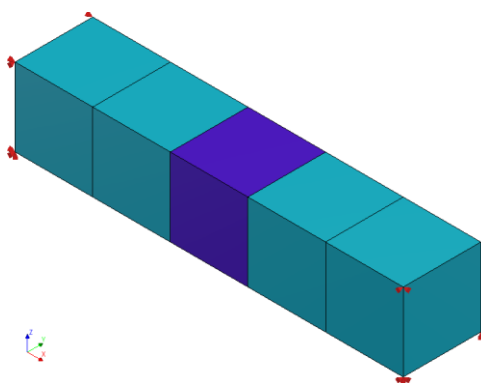


Fig. 77 – Test 4 – Finite element mesh

A temperature drop is imposed to induce cracking, which is permitted in only one of the elements (dark blue in Fig. 77). The temperature history is defined hypothetically to generate crack strains that fully exhaust the tension-softening response. Fig. 78 shows the temperature history applied in Test 4 (T41).

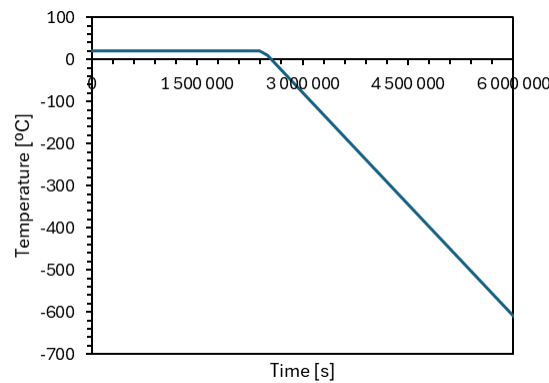


Fig. 78 – Test 4 – Temperature history.

In the pointwise THM models, the temperature history affects the mechanical properties of concrete through the concept of transformed times. To avoid these effects, which would lead to differences in the mechanical response between DIANA FEA models and the pointwise THM models, the activation energy is set to zero ($Q_e = Q_r = Q_s = 0$). Fig. 79 shows the stress evolution for Test 4 (T41) in the cracked finite element.

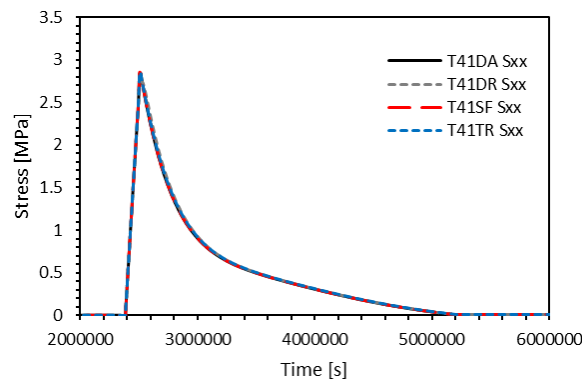


Fig. 79 – Test 4 – Stress evolution in the cracked finite element.

The results show a good agreement between all the numerical analyses. The same stress evolution is observed in the uncracked elements. Fig. 80 shows the normalised mesh deformation at the end of the analysis for the analysis T41SF.

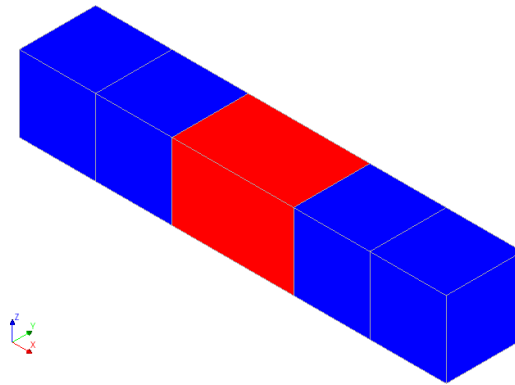


Fig. 80 – Test 4 – Stress evolution in the cracked finite element.

The deformed mesh shows the strain concentration in the cracked finite element. All the numerical analyses provide similar mesh deformation at the end of the analysis, showing good performance of the pointwise THM model (SF) in dealing with strain localisation.

3.11.5 FINAL REMARKS ON THE BENCHMARK TESTS FOR VALIDATING THE POINTWISE THM MODEL

The preceding benchmark comparisons demonstrate that the pointwise THM implementation reproduces DIANA FEA's crack model response with high fidelity under carefully controlled loading paths and time step discretisation. This confirms the model's capability to simulate cracking under different loading conditions in the mechanical analyses. In the present benchmark tests, the analysis performed using DIANA FEA models and the pointwise THM model shows numerical convergence obtained after two iterations (by step) for tests performed in a single finite element and up to five iterations (by step) for multiple finite elements (Test 4). Regularised damage techniques can be implemented in the pointwise THM model to improve the applicability and convergence of the numerical crack models and ensure smoother strain localisation in densely meshed regions [173]. Implementing regularised damage may improve numerical convergence and yield more robust results in highly refined meshes where the crack path is unknown a priori. On the other hand, the models may also induce small deviations in the softening behaviour, as shown in the comparison of the present benchmark tests. Therefore, investigating regularised damage strategies within the pointwise THM framework is recommended for future work.

These benchmark comparisons confirm the robustness of the cracking formulations in the pointwise THM model across both single-element and multi-element simulations, demonstrated its accuracy under diverse controlled loading and boundary conditions. The pointwise THM model is now be applied to more complex structural concrete simulations in Chapter 4.

3.12 REINFORCEMENT AND BOND-SLIP

In reinforced concrete structures, when a crack occurs, the distribution of forces and displacements depends on the bond between reinforcement and concrete. This bond action may vary depending on multiple criteria, such as casting conditions or the type of reinforcement. The FE analysis in this thesis

will simulate the bond-slip behaviour using an interface FE element that connects the reinforcement and concrete elements. The reinforcement will be simulated using truss elements with an uniaxial constant elastic behaviour without plasticity criteria. Such an approach is valid in the numerical simulation of the service life of RC structures, where the stress level of reinforcement is below the yield strength. For the interface element, it is essential to prescribe a bond-slip law. In this work, the bond-slip relationship endorsed by MC2010 is considered:

$$\tau_b = \tau_{bmax}(s/s_1)^\alpha \quad \text{for } s \leq s_1 \quad (3.162a)$$

$$\tau_b = \tau_{bmax} \quad \text{for } s_1 \leq s \leq s_2 \quad (3.162b)$$

$$\tau_b = \tau_{bmax} - (\tau_{bmax} - \tau_{bf}) \frac{(s - s_2)}{(s_3 - s_2)} \quad \text{for } s_2 \leq s \leq s_3 \quad (3.162c)$$

$$\tau_b = \tau_{bf} \quad \text{for } s_3 < s \quad (3.162d)$$

where τ_b is the bond stresses between the concrete and the reinforcement bar, and s is the slip value. Fig. 81 presents the bond-slip relationship provided by MC2010.

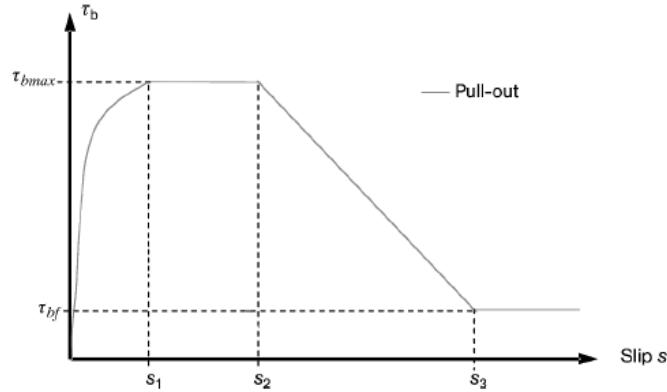


Fig. 81 – Analytical bond stress-slip relationship for monotonic loading (adopted from [50]).

Table 10 gives the parameters of Equation (3.162).

Table 10 – Parameters defining the mean bond stress-slip relationship of ribbed bars [50]

Pull-out		
$\varepsilon_s < \varepsilon_{s,y}$		
	Good bond conditions	All other bond conditions
τ_{bmax}	$2.5 \sqrt{f_{cm}}$	$1.25 \sqrt{f_{cm}}$
s_1	1.0 mm	1.8 mm
s_2	2.0 mm	3.6 mm
s_3	c_{clear}	c_{clear}
a	0.4	0.4
τ_{bf}	$0.40 \tau_{bmax}$	$0.40 \tau_{bmax}$

where c_{clear} is the clear distance between ribs.

The unloading and reloading follow a constant elastic stiffness determined for a full recovery of bond slips until 0.01 mm. The relationship between normal traction and normal relative displacement is kept linear.

4

APPLICATIONS OF THE POINTWISE THERMO-HYGRO-MECHANICAL MODEL

4.1 HYGROMECHANICAL BEHAVIOUR OF CONCRETE

Moisture transport significantly influences the mechanical behaviour of concrete. In this chapter, the pointwise THM model is employed to investigate the hygromechanical response of concrete. The studies presented cover five cases:

- the first section explores the relationship between the hygral model and shrinkage behaviour by performing numerical simulations and comparing the results with experimental data. The discussion focuses on the adaptability of different shrinkage models in simulating shrinkage based on relative humidity profiles;
- the second section examines the size effect on shrinkage and creep by numerically simulating slabs and prisms of different dimensions. Strategies for calibrating the hygral and shrinkage models without relative humidity experimental data are discussed. The performance of the creep model implemented within the pointwise THM framework is investigated, resulting in modifications to the MPS theory to enhance the prediction of creep compliance across specimens of different sizes. Additionally, the influence of notional size is investigated by comparing the shrinkage and creep results of slabs and prisms with different dimensions;
- the shrinkage behaviour of prisms and unrestrained ring tests is simulated in the third section. The results highlight the differences in shrinkage development between different drying geometries. The influence of the insulation permeability in the ring tests is also analysed;
- the fourth section presents the numerical simulation of ring tests considering top and bottom and radial drying. The results include an analysis of the stress distribution across the specimen cross-section and a comparison of axial and radial drying conditions;
- the final section involves the numerical simulation of various ring test geometries. Four ring test setups currently used in the literature are analysed and compared, assuming the same concrete mixture for all the numerical tests. The analyses consider both drying under top and bottom drying and radial drying. The discussion centres on the advantages and disadvantages of each ring test geometry concerning the degree of restraint, steel strains, concrete stresses and cracking occurrence.

4.1.1 NUMERICAL SIMULATION OF THE RELATIVE HUMIDITY AND SHRINKAGE TESTS OF THE INTEGRACRETE EXPERIMENTAL CAMPAIGN

The IntegraCrete project involved experimental research on the effects of loads and restrained shrinkage in slabs [204]. The concrete underwent extensive material characterisation, including mechanical strength tests and the preparation of dummy specimens for relative humidity and shrinkage monitoring. The experimental data provide a basis for calibrating the hygral and shrinkage model used in the pointwise THM model. Relative humidity was monitored in specimens with thicknesses of 10 cm × 10 cm × 40 cm (H10) and 15 cm × 15 cm × 60 cm (H15), corresponding to a slab-like drying, i.e. drying in one direction through two exposed surfaces, 10 cm for H10 and 15 cm for H15. The relative humidity in the H10 specimen was monitored at depths of 2, 4, and 5 cm, while in the H15 specimen, it was monitored at depths of 2, 4, and 7.5 cm. The experimental measurements of the relative humidity started after exposure to drying at the concrete age of 7 days. Shrinkage was measured in cylindrical specimens ($\phi 15 \times 30 \text{ cm}^3$) and in a dummy specimen (50 cm × 50 cm × 10 cm), with a slab-like drying corresponding to the thickness direction of 10 cm. The concrete mixture used in the IntegraCrete project was of strength class C20/25, with exposure class X0(P), a maximum aggregate size of 12.5 mm, and consistency class S3. Table 11 presents the composition of the concrete mixture.

Table 11 – IntegraCrete Concrete mixture composition.

Component	Specification	
Aggregates	Fine sand 0/2.36	547 kg/m ³
	Coarse sand 0/4.75	432 kg/m ³
	Gravel 2/8	220 kg/m ³
	Gravel 6/14	763 kg/m ³
Cement	CEM II A/L 42,5 R	291 kg/m ³
Additives	Plasticiser Chrysoplast 775	2.32 kg/m ³
Water	[-]	171 kg/m ³

4.1.1.1 Hygrometric simulation of the relative humidity tests

The hygral model is calibrated to reproduce the moisture distribution in specimens H10 and H15. Table 12 presents the parameters used for the shrinkage and hygral model employed in the numerical simulation of the IntegraCrete experimental campaign.

Table 12 – Parameters used in the shrinkage and hygral model for the IntegraCrete experimental campaign.

Parameter	Value
α_0	0.05
D_1	$3.00 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
h_c	0.8
n_h	5
η_e^*	$3.00 \times 10^{-8} \text{ m s}^{-1}$
h_{env}	0.60
k_{sh}^* (dKwak)	4.6122×10^{-3}
ε_{bs0}	40.00×10^{-6}
α_h	10

The numerical simulation of moisture distribution is performed on a slice of the cross-section of the experimental specimen. Only one-quarter of the cross-section is simulated due to symmetry conditions. This corresponds to a $5 \text{ cm} \times 5 \text{ cm} \times 2 \text{ cm}$ for H10 and $7.5 \text{ cm} \times 7.5 \text{ cm} \times 2 \text{ cm}$ for H15. Fig. 82 shows the FE meshes utilised in the hygrothermic simulations of specimens H10 and H15.

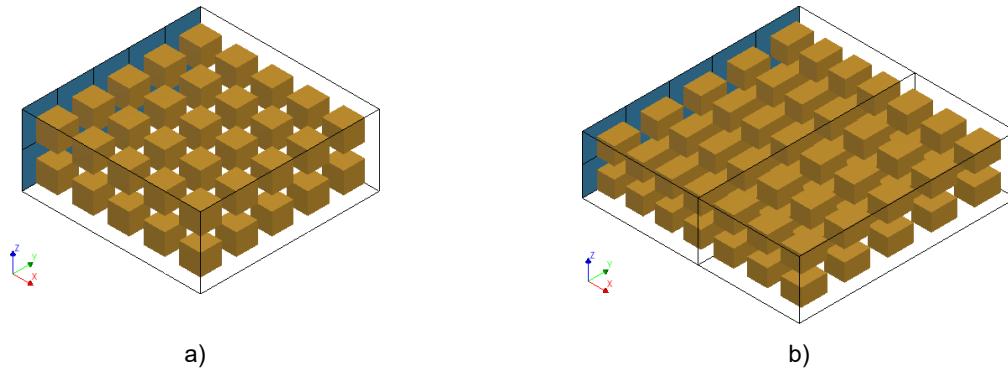


Fig. 82 – Finite element mesh for the hygrothermal analysis: a) for H10; b) for H15

The boundary elements are represented by dark blue sheets, indicating that moisture transport is restricted to one-dimensional flow occurring only in the X-direction. The finite element sizes are determined to allow for a direct comparison between the numerical results for the relative humidity at the nodes and the depths for which experimental results are available. For the drying X-direction:

- in the H10 specimen, all finite elements have a length of 10 mm;
- in the H15 specimens, the first four finite elements have a length of 10 mm, and the remaining three have a length of 15 mm.

Moisture transport in the Y and Z directions is prevented. Therefore, in practice, only a column of finite elements in the X direction is strictly necessary for the numerical simulation of the present case study. Nevertheless, simulating the entire cross-section (with the symmetry conditions) facilitates interoperability between the results of the hygral model and the relative humidity tables required as input for the mechanical model. The current simulation uses a small number of finite elements, resulting in a

relatively low analysis time in the hygral model. Therefore, a more concise mesh design is not required. The second layer of finite elements in the Z-direction is included to check for potential symmetry errors in moisture transport, a standard practice in the hygral simulations conducted in the present PhD work.

Fig. 83 shows the comparison between the experimental and numerical relative humidity distribution for the specimens H10 and H15.

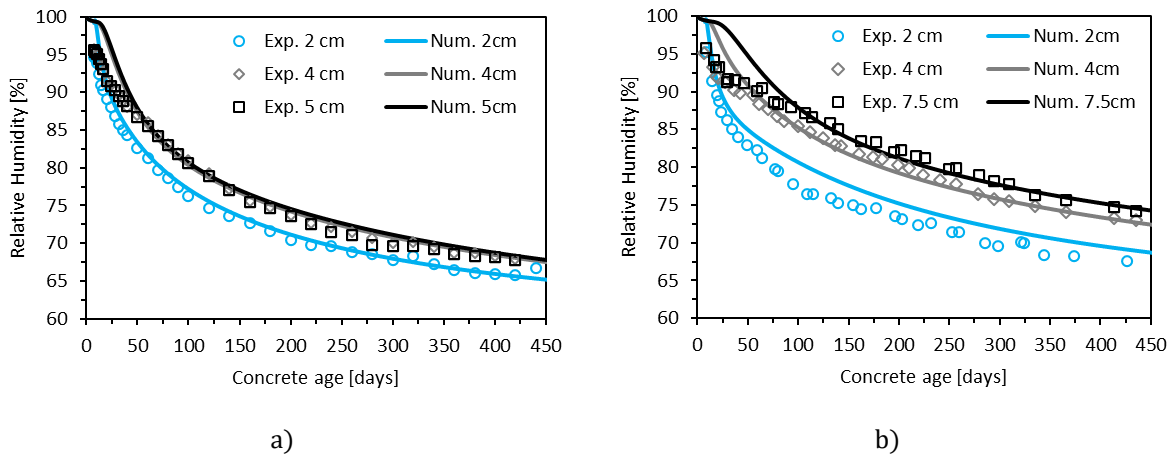


Fig. 83 – Comparison between numerical and experimental results of the relative humidity at different depths: a) for H10; b) for H15.

Experimental measurements began prior to slab stripping at seven days and indicated a drop in relative humidity to approximately 98%, primarily due to self-desiccation. A comparison between the numerical and experimental results shows good agreement in the long-term evolution of relative humidity. However, Fig. 83 b) shows discrepancies in the numerical simulation of specimen H15 during the days immediately following stripping. These deviations may be partially attributed to the accuracy of the experimental measurement. The measurements were taken using the Vaisala® HMP40S sensor to measure the relative humidity in impermeable sleeves. The sleeves are embedded in the concrete specimen at different depths with an extremity in contact with concrete pores containing GORE-TEX, a waterproof yet breathable fabric that allows water vapour to enter the sleeve but avoids liquid water. The sleeve's other extremity is closed and only opened for inserting the Vaisala® HMP40S sensor. It is assumed that the air within the sleeve remains in equilibrium with the air in contact with the concrete pores. However, the measurement process requires the sleeve to be opened momentarily to insert the sensor, allowing ambient air to enter or escape. Although this is intended to be a quick procedure, even minimal air exchange can lead to a measurable reduction in the relative humidity inside the sleeve, especially in the presence of big differences between the relative humidity in the air in the sleeves and the environment's relative humidity. The greater the difference between the environment's relative humidity and the sleeve's internal relative humidity, the more pronounced this effect will likely be. Additionally, repeated use of the sensors in high-humidity conditions may affect their calibration, with pronounced sensitivity when performing relative humidity measurements above 95%. The first recalibration of the device following slab stripping was performed at 54 days.

4.1.1.2 Mechanical simulation of the shrinkage test using different shrinkage models

The IntegraCrete project included free shrinkage tests on cylindrical specimens. However, more representative shrinkage experimental results are obtained in the dummy specimen, which shares the same hygral flux, flow direction and thickness as the H10 specimen. Although the H10 and dummy specimens present the same drying conditions, the dummy specimens have the dimensions of 50 cm × 50 cm × 10 cm. Therefore, two different meshes are used in the numerical simulation of the drying shrinkage tests. Fig. 84 shows the adopted FE mesh for the H10 and dummy specimens.

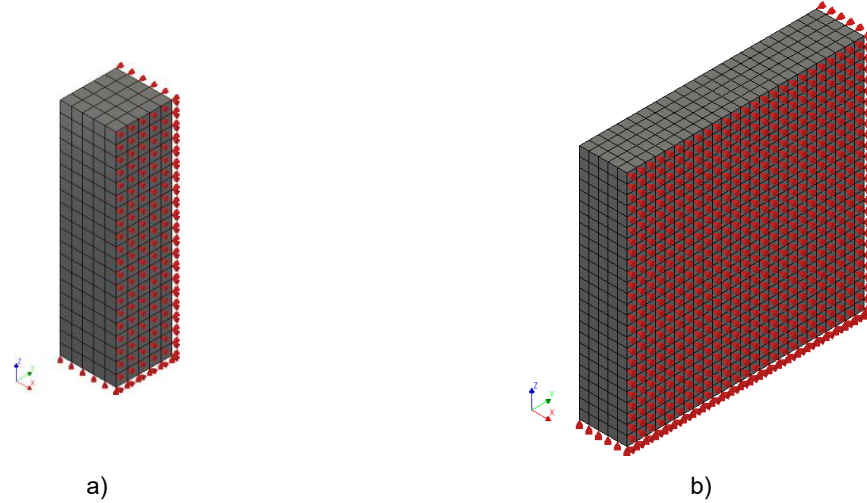


Fig. 84 – Finite element mesh for the mechanical analysis: a) for the H10 specimen; b) for the dummy specimen.

Both meshes represent one-eighth of the experimental specimen geometry by incorporating symmetry in the X, Y and Z directions. This forms a prism with the dimensions 5 cm × 5 cm × 20 cm for H10 and 5 cm × 25 cm × 25 cm for the dummy. All finite elements are of a size of 10 cm × 10 cm × 10 cm for both geometries.

The mechanical simulations use the pointwise mechanical model from Chapter 3. The creep model parameters are determined using model B4 formulations (see Equations (2.98)), considering the cement type RS and the experimental elastic modulus of 29.80 GPa at 28 days. In Model B4 [133], the cement type affects the ageing creep compliance parameter q_2 . Additionally, despite there is no influence of the cement type in the empirical parameters used in the calculation of the non-ageing creep parameter q_3 , the calculation of the non-ageing creep compliance is explicitly dependent on the ageing parameter q_2 (see Equation (2.98c)). Therefore, the non-ageing creep parameter q_3 also becomes dependent on the cement type. In the present PhD work, it is assumed that cement type should only affect the ageing part of the creep compliance. Therefore, Equation (2.98c) is used for the determination of the parameter q_3 is replaced by the following equation:

$$q_3 = 58.6 \times 10^{-3} \cdot p_3 \cdot \left(\frac{a/c}{6} \right)^{p_{3a}} \cdot \left(\frac{w/c}{0.38} \right)^{p_{2w} + p_{3w}} \quad (4.1)$$

This equation calculates the non-ageing creep compliance independently of the cement type used. The resulting value is consistent with what would be obtained when considering a normal (N) cement type.

This approach is justified because the fineness of cement particles is the main factor influencing the type of cement used, and should not represent a fundamental change in the long-term concrete properties. The non-ageing creep compliance should be an intrinsic value dependent on the concrete mixture constituents and independent of ageing parameters.

The present numerical simulations use the total strain model switching from rotating to fixed cracks. The switching crack value is 0.01 mm and the adopted shear retention factor is $\beta = 0.01$. The tensile strength evolution is simulated through Equation (3.86). Table 13 shows the parameters considered in the mechanical analysis for the creep and fracture model.

Table 13 – Creep and fracture model used in the IntegraCrete shrinkage test numerical simulation.

Parameter	Value	Parameter	Value
q_1	$23.49 \mu \text{ MPa}^{-1}$	$f_{ct,28}$	2.2 MPa
q_2	$64.34 \mu \text{ MPa}^{-1}$	$n_{fct,1}$	0.2
q_3	$8.92 \mu \text{ MPa}^{-1}$	$n_{fct,2}$	0.5
q_4	$8.91 \mu \text{ MPa}^{-1}$	$n_{fct,3}$	0.65
k_1	$5.25 \times 10^1 \text{ MPa}$	G_f	0.140

All other material parameters not presented are assumed to have the default values mentioned in Chapters 2 and 3.

The equivalent shrinkage coefficient is now assessed in the numerical simulation of the shrinkage specimen. Four different approaches are considered:

- Approach 1 (Constant 1) - considers a constant equivalent shrinkage coefficient calibrated on long-term shrinkage – Equation (3.45);
- Approach 2 (Constant 2) - considers a constant equivalent shrinkage coefficient calibrated on early-age shrinkage – Equation (3.45);
- Approach 3 (BN eq.) - considers the equivalent shrinkage coefficient based on BN shrinkage model – Equation (3.48);
- Approach 4 (dKwak eq.) - considers the equivalent shrinkage coefficient based on the dKwak shrinkage model – Equation (3.47).

Table 14 presents the shrinkage parameters used in the specified shrinkage models.

Table 14 – Equivalent shrinkage parameters used in the numerical simulation of the shrinkage in the dummy specimen.

	Constant 1	Constant 2	BN eq.	dKwak eq.
k_{sh}	1.66×10^{-3}	2.16×10^{-3}	2.35×10^{-3}	4.61×10^{-3}
c_1	-		0.2	1.0
c_2	-		0.75	0.2
c_3	-		8	2.0

The comparison between the different approaches is performed considering the H10 mesh. The objective of the numerical simulation of the dummy specimen is to investigate any possible geometric effects on the shrinkage simulation. The experimental measurements were performed using embedded vibrating wire strain gauges (VWSG) at the core of the dummy and cylinder specimens. Therefore, for all the numerical analyses, the shrinkage is measured at the core of the specimen. Fig. 85 shows the numerical simulation of the shrinkage in the different shrinkage model approaches and the comparison between the experimental results for the shrinkage in the dummy and cylinders.

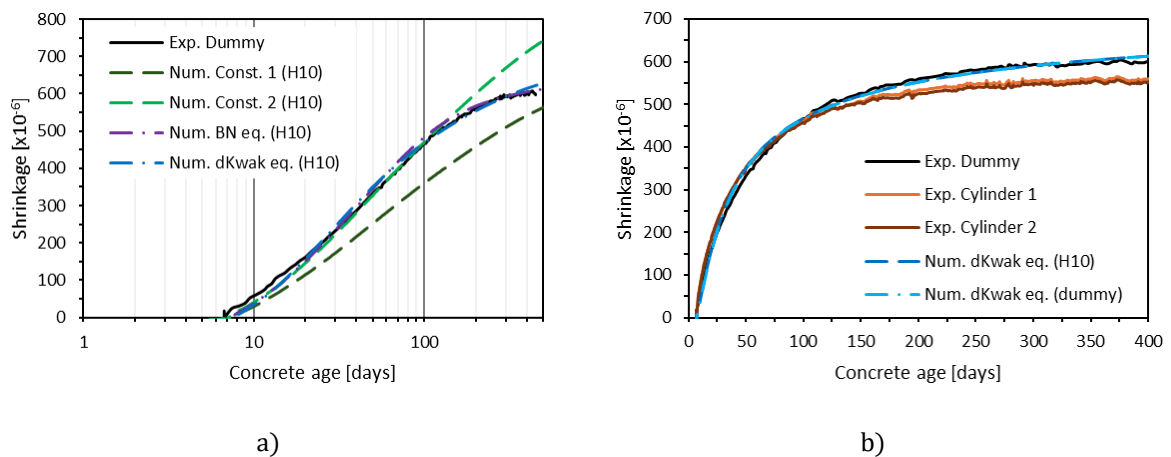


Fig. 85 - a) numerical simulation of shrinkage using different shrinkage models; b) shrinkage in the dummy and cylinders

Fig. 85 a) shows that Approach 1 (Num. Const. 1) deviates significantly from the experimental shrinkage results at the beginning of the analysis. In contrast, Approach 2 (Num. Const. 2) provides good agreement with experimental shrinkage at early ages but overestimates shrinkage beyond 150 days. The numerical Approach 3 (Num. BN eq.) and Approach 4 (Num. dKwak eq.) yield a good fit with the experimental shrinkage data. This study highlights that using a nonlinear equivalent shrinkage coefficient, dKwak equation (Equation (3.47)) or BN equation (Equation (3.48)), is more suitable for simulating the shrinkage behaviour of the present concrete mixture, particularly if the objective is to simulate the early-age to long-term shrinkage behaviour. Fig. 85 b) shows the differences in the shrinkage between the dummy and cylindrical specimens due to geometric differences associated with the surface-to-volume ratio. The cylinders exhibit slightly faster shrinkage at early ages due to their higher surface-to-volume ratio. However, the shrinkage in the cylinders is smaller in the long term than in the dummy specimen. The numerical shrinkage obtained using Approach 3 (Num. dKwak eq.) for the

H10 and dummy mesh shows similar shrinkage evolutions aligned with the experimental results obtained for the dummy specimen, validating the use of H10 for the numerical simulation of the specimens. This is expected since the H10 and dummy specimen present the same relative humidity history provided in Fig. 83 a). Minor differences may be justified by microcracking in the surface layers, resulting from higher internal restraints in the dummy specimen than in the H10 one. Nevertheless, the cracking effects are expected to be minor in the present case study due to the small thickness of the analysed elements, which results in small relative humidity gradients over the element thickness, as observed in Fig. 83 a). Future works should investigate this issue related to the shape effects between specimens that exhibit the same hygral histories but present different geometries, especially in cases where the relative humidity gradients are more pronounced, i.e, in thicker elements. Such approaches may allow for identifying and quantifying the mechanical response of shrinkage elements due to the internal restraint and microcracking effects. The present study shows the importance of implementing different shrinkage models in the pointwise THM model to describe the shrinkage in different concrete mixtures.

4.1.2 SHRINKAGE AND CREEP TESTS FROM BRYANT AND VADHANAVIKKIT

4.1.2.1 Introduction to the experimental campaign

Bryant and Vadhanavikkit [251] performed an experimental campaign on the shrinkage and creep of prismatic and slab specimens of different sizes, sealed and exposed to drying. The concrete used is constituted by 390 kg/cm² of ordinary Portland cement, 1935 kg/m³ of aggregates and 183 kg/m³ of water (no additives). The mixture presents high workability (slump 120 mm). The compressive strength in cylinders at 28 days was 50.1 MPa, and the modulus of elasticity was 29.8 GPa. The specimens were cast in open plywood moulds. The concrete was compacted using a poker vibrator, and the top surfaces were covered with damp burlap and conserved at 20°C for three days. Five different geometries were considered:

- Specimen 100 mm: 100 mm × 100 mm × 400 mm.
- Specimen 150 mm: 150 mm × 150 mm × 600 mm.
- Specimen 200 mm: 200 mm × 200 mm × 800 mm.
- Specimen 300 mm: 300 mm × 300 mm × 1200 mm.
- Specimen 400 mm: 400 mm × 400 mm × 1600 mm.

After three days, all the specimens were demoulded and moved to the controlled environment room held at 20°C and 95% relative humidity. Eight days after casting, the specimens were sealed using aluminium foil. Three different drying conditions were considered:

- Sealed specimens (Sealed).
- Drying from the four prismatic surfaces (Prism).
- Drying from two surfaces (Slab).

The sealed specimens were fully covered by aluminium foil. The two sides and ends of the slab specimens were sealed so that moisture transport occurred only through the top and bottom faces. The two ends of the prism specimens were also sealed, so moisture transport occurs in a 2D flow through the four lateral faces of the prism. Subsequently, the relative humidity of the room was lowered to 60%. The strains were measured using a demountable mechanical gauge with a base length of 200 mm. Initial strain measurements were performed before the humidity was lowered.

Despite the absence of relative humidity measurements, this experimental campaign is a valuable case study for validating the pointwise THM model for shrinkage simulation. The use of the same concrete mixture across various drying scenarios and specimen geometries introduces additional complexity, providing an important validation test for the pointwise THM model. The fundamental principle of the pointwise THM model assumes that the material behaviour is independent of specimen geometry. Therefore, the adopted material model parameters should produce accurate results for all specimens tested in the present experimental campaign.

4.1.2.2 Numerical simulation of the shrinkage specimens

The numerical analysis employs a staggered approach, comprising a thermo-hygral analysis followed by a subsequent mechanical analysis conducted within the THM framework. For the hygrothermal analysis, only one-quarter of the cross-section of the shrinkage specimen is simulated, resulting in a mesh reduced to a single layer of finite elements. Fig. 86 presents the finite element meshes employed in the hygrothermal analyses.

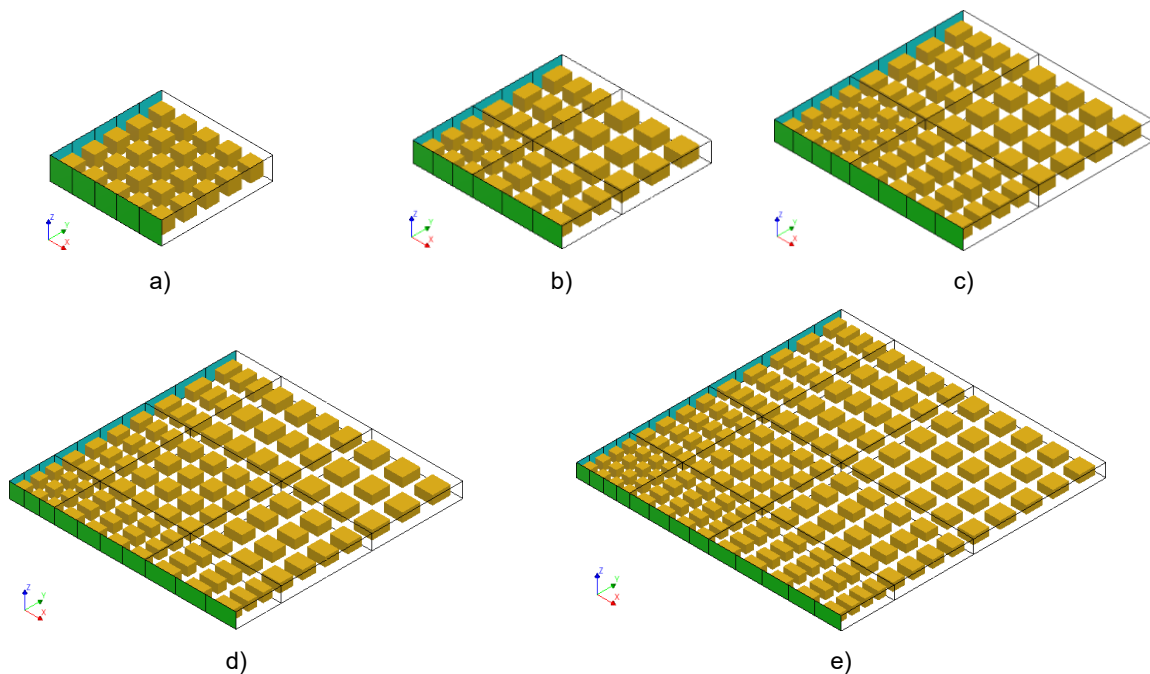


Fig. 86 – Finite element meshes for the hygrothermal analysis: a) for P100 and S100; b) for P150 and S150; c) for P200 and S200; d) for P300 and S300; e) for P400 and S400.

The blue and green polygon sheets model the boundary interfaces, while the rectangular prismatic elements (solid FE) model the concrete. The solid finite elements have been visually shrunk to improve the visual identification of the boundary elements. For the prismatic drying conditions, drying is allowed on both surfaces, blue and green. For slab-like drying conditions, transport through the y-direction interface elements (green sheet) is set to zero, effectively simulating one-dimensional moisture flow.

One-eighth of the shrinkage specimen's geometry is modelled in the mechanical analysis by exploiting symmetry conditions at the centre of the shrinkage specimens. Fig. 87 presents the finite element meshes employed in the mechanical analyses.

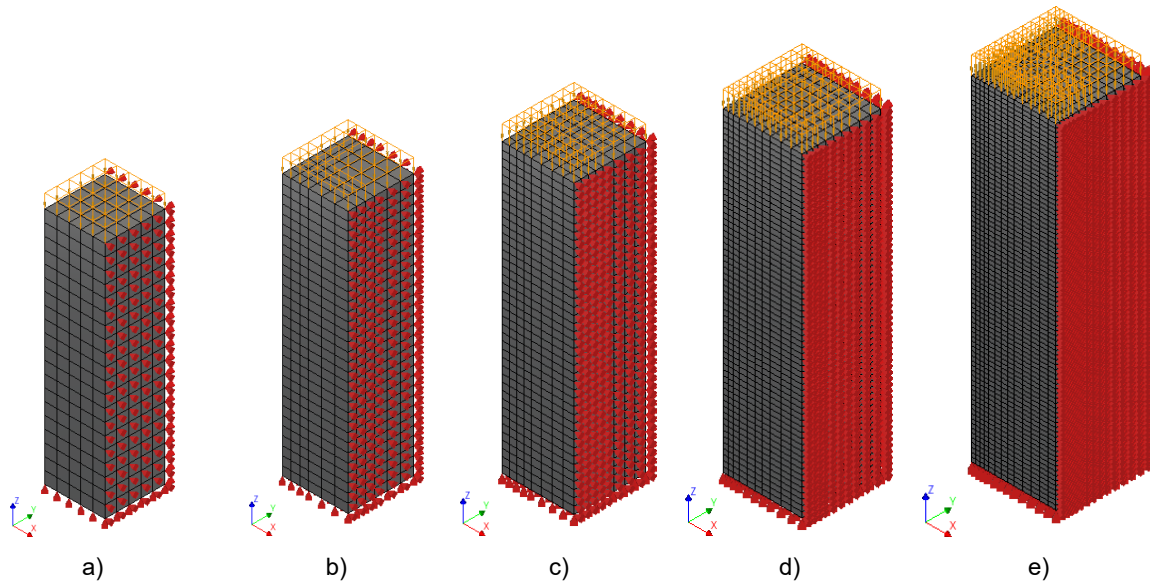


Fig. 87 – Finite element meshes for the mechanical analysis: a) for P100 and S100; b) for P150 and S150; c) for P200 and S200; d) for P300 and S300; e) for P400 and S400.

The mechanical mesh includes symmetry boundary conditions and allows additional loading (yellow arrows at the finite elements at the top surface) for the creep numerical simulations. The hygrothermal and the respective mechanical models share the same cross-section FE discretisation. The model finite element discretisation varies depending on the specimen size, and it is established to optimise computational runtime while ensuring an accurate simulation of the gradients at the boundary surface. The lower bound for the finite element size is considered 10 mm, since smaller sizes may question the assumptions of concrete homogeneity or demand explicit simulations of aggregates and cement paste. For all models, symmetry conditions were applied, resulting in the following discretisations:

- for S100 and P100: the mesh employed a uniform element size of 10 mm × 10 mm × 10 mm;
- for S150 and P150: the mesh was refined into two distinct regions: three layers at the surface with an FE size of 10 mm × 10 mm × 10 mm and three layers at the core with an FE size of 15 mm × 15 mm × 10 mm;
- for S200 and P200: the mesh was refined into two distinct regions: four layers at the surface with an FE size of 10 mm × 10 mm × 10 mm and four layers at the core with an FE size of 15 mm × 15 mm × 10 mm;

- for S300 and P300: the mesh was refined into three distinct regions: three layers at the surface with an FE size of 10 mm × 10 mm × 10 mm, four layers at the transition zone with an FE size of 15 mm × 15 mm × 10 mm and three layers at the core with an FE size of 20 mm × 20 mm × 10 mm;
- for S400 and P400: the mesh was refined into three distinct regions: four layers at the surface with an FE size of 10 mm × 10 mm × 10 mm, four layers at the transition zone with an FE size of 15 mm × 15 mm × 10 mm and five layers at the core with an FE size of 20 mm × 20 mm × 10 mm.

4.1.2.2.1 Calibration procedure for the hygral and shrinkage model based on shrinkage experimental data

The experimental programme of Bryant and Vadhanavikkit [251] did not include measurements of relative humidity profiles or moisture loss. Therefore, the shrinkage and hygral models are calibrated solely based on the experimental shrinkage data. This approach allows for multiple solutions to the combined effects of the hygral and shrinkage models. To minimise the number of possible solutions, several assumptions are required. The present calibration approach for this case study adopts a constant equivalent shrinkage coefficient, consistent with assumptions made by other researchers [240]. This assumption is justified by the composition of the concrete mix, which uses ordinary Portland cement (CEM I), contains no plasticisers, and has a relatively high water-to-cement ratio. These factors support previous findings on the linear nature of desorption and the shrinkage coefficient, as discussed in Chapter 2.2.2.

The initial step involves determining the equivalent shrinkage coefficient, k_{sh}^* , based on the relative humidity drop, Δh , and the corresponding shrinkage variation, $\Delta \varepsilon_{sh}$, as defined by the following equation:

$$k_{sh}^* = \Delta \varepsilon_{sh}(\Delta h) / \Delta h \quad (4.2)$$

The shrinkage variation, $\Delta \varepsilon_{sh}$, for the specimens is assessed based on the long-term shrinkage of thin specimens exposed to drying conditions. For example, in a drying specimen drying at an environmental relative humidity of 0.6, the shrinkage drop would be equal to the shrinkage observed between full saturation and the total shrinkage observed when moisture equilibrium with the environment is achieved, $\Delta \varepsilon_{sh}(h = 1 \rightarrow h = 0.6)$. The basic shrinkage is simulated by determining the basic shrinkage parameter ε_{cb0} in Equation (2.68) that leads to the best curve fit. The basic shrinkage is simulated together with drying shrinkage following the algorithm presented in Box 3.2.

The calibration of the diffusion parameters in Equation (2.53) without experimental relative humidity measurements and based only on shrinkage tests is challenging. Assuming a constant shrinkage coefficient (Equation (3.45)), the diffusion equation governs the development of shrinkage over time. The calibration strategy adopted for the hygral model is based on a predictor-corrector approach. This calibration is performed using two specimens of different drying rates:

- the P100: exhibiting faster drying;
- the S400: characterised by slower drying.

The starting point for the calibration process involves selecting an appropriate initial estimate to validate the hygral model. Table 15 suggests limit values for the parameters commonly used in the numerical simulation of moisture transport (Chapters 2.2 and 3.3).

Table 15 – Suggested limit values for the parameters used in the present hygral model.

Parameter	Min	Mid-range	Max
D_1	$1.5 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$	$3.0 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$	$6.0 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
n_h	2	6 or 8	15
h_c	0.70	0.80	0.90
α_h	0.001	0.05	0.2
η_h^*	$5.00 \times 10^{-9} \text{ m s}^{-1}$	$5.00 \times 10^{-8} \text{ m s}^{-1}$	$1.00 \times 10^{-7} \text{ m s}^{-1}$

By analysing the diffusion equation (Equation (2.53)) illustrated in Fig. 12b), several conclusions can be drawn. The parameter α_h governs the total reduction in the diffusion coefficient between the high and low diffusion regimes, while the parameters n_h and h_c , define the shape of this transition. A value of $n_h = 15$ results in a sharp transition between the high diffusion and the low diffusion states, occurring once the relative humidity h_c is reached. In terms of shrinkage behaviour, this would correspond to a rapid increase in the shrinkage experimental results. Conversely, a value $n_h = 2$ shows that the relative humidity content has a smother influence on the diffusion coefficient.

The calibration procedure initially employs mid-range parameter values. Based on simulations of selected experimental tests, the calibration parameters are subsequently adjusted in accordance with the observed results. Box 4.1 presents guidelines based on the shrinkage simulation outputs, suggesting the hygral model parameter changes to improve the previous uncalibrated shrinkage results.

Box 4.1 Calibration guidelines for the hygral model based on shrinkage results.

- Initial drying or drying in thick elements is not accurately modelled:
 - If drying in the numerical results is too slow, increase the value of D_1 or η_h^* ;
 - If drying in the numerical results is too fast, decrease the value of D_1 or η_h^* .
- Radius of the shrinkage curve transition is not accurately modelled:
 - If there is a high curvature (small radius), decrease the value of n_h ;

- If there is a low curvature (large radius), increase the value of n_h .
- The time occurrence of the shrinkage curve is not accurately modelled:
 - If the transition occurs later than expected, increase the value of h_c ;
 - If the transition occurs earlier than expected, decrease the value of h_c .
- Long-term shrinkage not accurately modelled:
 - If the drying rate in the numerical results is too slow, increase the value of α_h ;
 - If the drying rate in the numerical results is too fast, decrease the value of α_h .

Fig. 88 shows the effect of the parameter n_h in the shrinkage development of prisms P100 and slabs S400 using the mid-range values in Table 15.

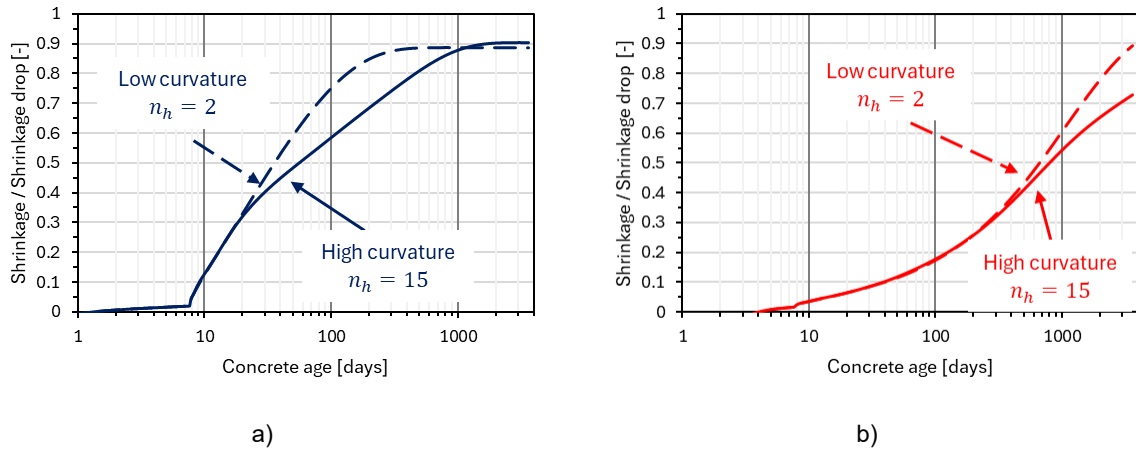


Fig. 88 – Effect of the diffusion parameter n_h in the numerical simulation of shrinkage for: a) P100; b) S400.

The results show that considering a lower value of n_h leads to fast shrinkage evolution, while higher values lead to slower shrinkage development. Assuming $2 < n_h < 15$ would result in average responses between the present limit values. Additionally, the long-term shrinkage does not reach the total shrinkage drop. Instead, shrinkage evolution halts at approximately 0.90 times the shrinkage drop for the specimen P100. This occurs due to microcracking and concrete creep strains resulting from the self-equilibrated stresses generated by non-uniform moisture profiles that decrease the shrinkage value compared to the expected free shrinkage. Therefore, the mechanical properties of the concrete influence the shrinkage simulation; however, its influence can be incorporated into the shrinkage model by increasing the shrinkage drop for the same relative humidity drop used in Equation (4.2).

The guidelines in Box 4.1 highlight the most significant influences of changing a specific diffusion parameter. However, it is important to note that any modification may produce substantial effects on the overall simulation outcomes:

- increasing or decreasing the value of D_1 has a pronounced influence on the numerical results, directly accelerating or decelerating, respectively, the shrinkage development throughout the entire numerical simulation;
- increasing the value of n_h :
 - combined with an increase in h_c results in a sudden increase in shrinkage at early ages, followed by a very slow long-term shrinkage rate. Particularly when $h_c \gg h_{amb}$, the medium to long-term shrinkage rate may be very slow and adjustments to α_h may be necessary to compensate for these changes;
 - combined with a decrease in h_c , leads to a significant increase in the shrinkage rate. Especially when $h_c \leq h_{amb}$, the results would be similar to adopting a constant diffusion coefficient equal to $D(h) = D_1$. In this case, only changes to D_1 or η_h^* would lead to changes in the numerical simulations.
- decreasing the value of n_h results in a low curvature in the shrinkage development, with the influence of parameters h_c and α_h becoming less critical compared to scenarios with high values attributed to n_h . Generally, this adjustment accelerates the overall shrinkage development, although the evolution remains smoother;
- changes in α_h predominantly affect long-term shrinkage behaviour. It may also play an important role in shaping the broader shrinkage curve when n_h is low. Nevertheless, if h_c is low and h_{amb} is high, the parameter α_h has a minor influence on the shrinkage simulations.

Additionally, it should be noted that in some cases, achieving an accurate fit to the experimental shrinkage data is impossible using a constant equivalent shrinkage coefficient, as demonstrated in Chapter 4.1.1. In such cases, alternative approaches involving a non-linear equivalent shrinkage coefficient, such as dKwak equation (Equation (3.47)) or BN equation (Equation (3.48)), should be considered. In the absence of relative humidity measurements, the hygral model parameters can be calibrated following the same procedures outlined in the present chapter, but assuming the new shrinkage models.

4.1.2.2.2 Numerical results of the simulation of the shrinkage specimens

Table 16 presents the parameters calibrated for the hygral and shrinkage model in this PhD, according to Chapter 4.1.2.2.1, and the parameters Havlásek [240] used to simulate the Bryant and Vadhanavikkit experimental campaign.

Table 16 – Parameters used in the hygral and shrinkage model.

Parameter	Value	Values of Havlásek [240]
α_0	0.05	0.18
D_1	$3.50 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$	$4.63 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
h_c	0.75	0.75
n_h	6	10
η_e^*	$5.00 \times 10^{-8} \text{ m s}^{-1}$	-
h_{env}	0.60	0.60
k_{sh}^*	1.9625×10^{-3}	1.95×10^{-3}
ε_{bs0}	35.00×10^{-6}	-
α_h	10	-

The equivalent shrinkage coefficient corresponds to a total shrinkage of $785 \mu\epsilon$ at a relative humidity equilibrium of 0.60, comprising $35 \mu\epsilon$ of basic shrinkage and $750 \mu\epsilon$ of drying shrinkage. The effect of hydration in basic shrinkage is accounted for using the equivalent age, assuming a $\alpha_h = 10$ and a constant temperature of 20°C .

Despite minor differences between the hygral model parameters adopted in this PhD and the parameters used by Havlásek [240], the numerical results for shrinkage evolution remain broadly similar. The primary distinction in calibration lies in the reduction of n_h from 10 to 6. As discussed in Chapter 4.1.2.2.1, this adjustment leads to a broader shrinkage curve and a corresponding increase in overall shrinkage. To compensate, the values of D_1 and α_0 were reduced to decelerate both early-age and long-term shrinkage, yielding results consistent with those obtained by Havlásek [240].

Furthermore, the equivalent shrinkage coefficient adopted in the present numerical simulations is lower than that used by Havlásek [240]. Shrinkage simulations were conducted using both models to compare the two hygral modelling approaches. Notice that the shrinkage results were not extracted directly from Havlásek [240]. Instead, the model parameters used by Havlásek [240] and presented in Table 16 were used within the current THM framework. Any parameters not explicitly provided in Table 16 of Havlásek [240] were assumed to be the same as those used in the present analysis. The mechanical response in both cases was simulated using the same material model within the pointwise THM model developed in this PhD work. The slab specimen S200 and the prism specimen P200 were simulated for the present comparison. Fig. 89 compares the relative humidity variation at different depths for the hygral model adopted in this PhD and the one proposed by Havlásek [240] for the numerical simulation of S200 and P200.

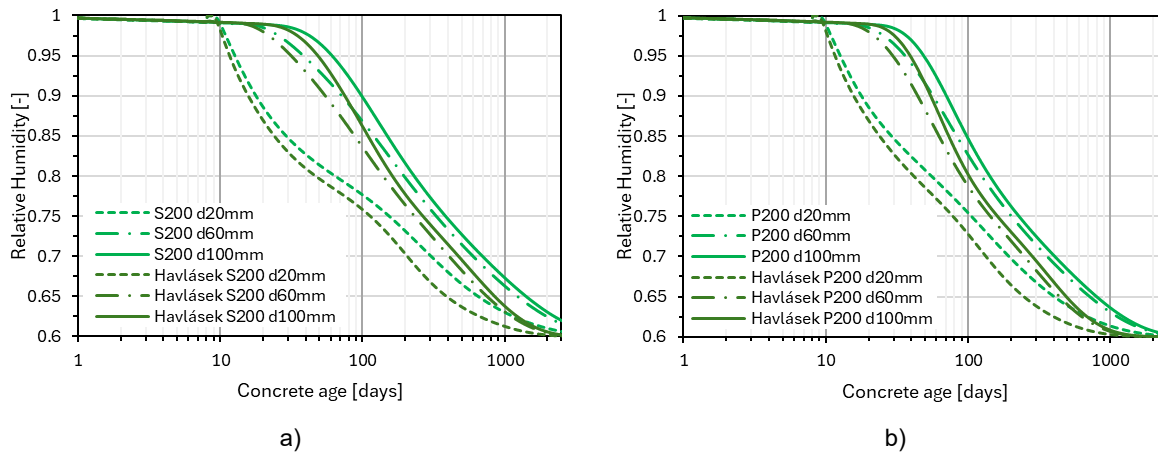


Fig. 89 – Relative humidity variation at different depths using the hygral models in Table 16 for the numerical simulation of: a) S200; b) P200.

Fig. 90 shows the comparison between the shrinkage evolution using the hygral model adopted in this PhD and the one proposed by Havlásek [240] for the numerical simulation of S200 and P200.

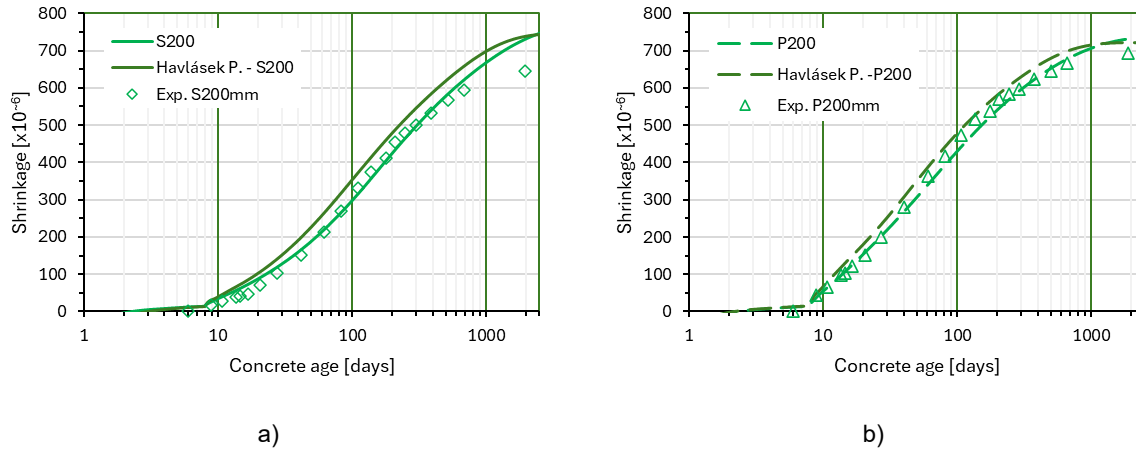


Fig. 90 – Shrinkage evolution using the hygral models in Table 16 for the numerical simulation of: a) S200; b) P200.

The results indicate similar shrinkage curves, with only minor differences in the overall behaviour. The present hygral model parameters predict slightly lower shrinkage for P200 and show a more accurate response for S200, whereas the Havlásek [240] hygral model parameters yield slightly overestimated shrinkage for both P200 and S200. Despite these differences, it is important to note that the experimental campaign includes a wider range of shrinkage tests, and the calibration must ensure reliable performance across all specimens. From this perspective, both parameter setups may be considered numerically accurate and valid for the shrinkage simulations. Although Havlásek [240] hygral and shrinkage model parameters also demonstrate a good agreement in the numerical simulation of shrinkage in other specimens, the numerical simulations presented in the following chapters are limited to the hygral model parameters calibrated in the present PhD work. Fig. 91 shows the shrinkage of the prisms, slabs and sealed specimens with different geometrical sizes.

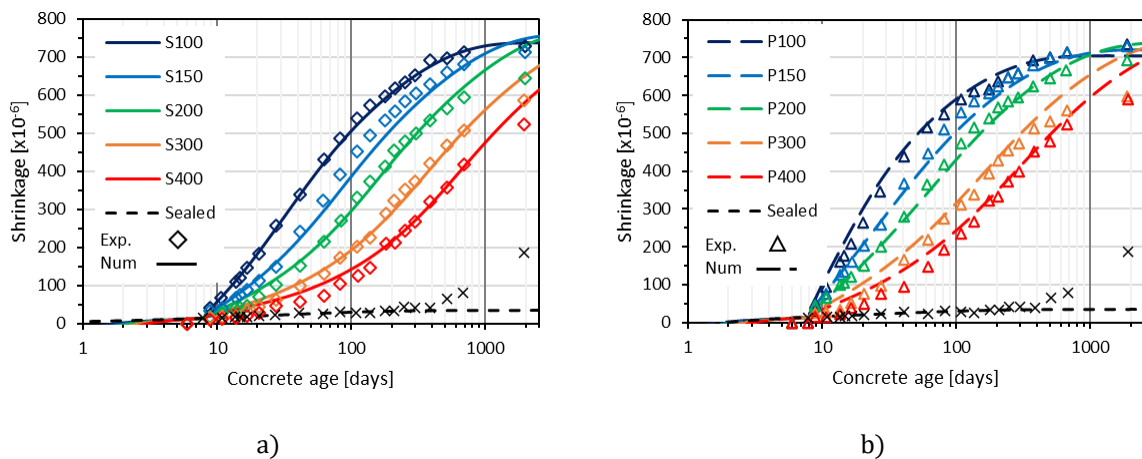


Fig. 91 - Experimental shrinkage tests with exposure to drying at 8 days: a) for slab drying; b) for prismatic drying.

The results indicate that shrinkage is more pronounced in smaller specimens due to faster drying. Prism specimens exhibit greater shrinkage than their corresponding slab specimens. The shrinkage measurements in sealed specimens show irregular behaviour after 500 days. Corrosion of the aluminium foil used for sealing was reported, compromising the accuracy of shrinkage data beyond this period.

The numerical results show good agreement with the experimental data across different element thicknesses and moisture flow directions, validating the present hygral model for the numerical simulation of the current shrinkage experimental campaign.

4.1.2.3 Creep simulation using the microprestress-solidification theory

Bažant et al. [167] observed that the MPS model does not accurately replicate the size effect identified in the experiments by Bryant and Vadhanavikkit [251]. They found that achieving a close match with experimental results required using a nonphysical value for the microprestress exponent in the relaxation function. As an alternative, they proposed separating fluidity into two components to represent the contributions of basic creep and drying creep. More recently, Rahimi-Aghdam et al. [124] introduced an extended version of the MPS theory (XMPS), which incorporates an additional parameter to account for changes in the microprestress rate. Yu et al. [148] proposed an alternative approach to the MPS theory, modifying the relationship between viscosity and microprestress by adopting a logarithmic function instead of the original power function. This subchapter re-examines the MPS theory and its improvements in simulating the drying creep observed in the experiments by Bryant and Vadhanavikkit [251]. The starting point is the original MPS theory (Chapter 2.4.3.1). A numerical algorithm was developed in MATLAB to investigate the effects of MPS parameters and formulation on the results of multiple creep tests. The objective of the proposed algorithm is to allow fast visualisation of quantitative numerical results for multiple creep test simulations when performing changes to the MPS model parameters or the MPS formulation. In the presence of several tests intended to use the same material model, every time a single property is changed, all the numerical analyses need to be executed again to check for the influence of the modified parameter in the remaining tests. For the denser meshes, the creep test analysis time can increase drastically from a few minutes to hours. The performance of

multiple finite element analyses using the pointwise THM model would be vastly time-consuming. Therefore, the calibration and investigation of the MPS theory is performed based on a simplified approach at a single integration point, where the results for multiple creep tests are simulated in seconds. This tool allows for changing parameters, the MPS formulation, or even using fitting procedures to calibrate the parameters used in the numerical model and access their results within seconds. After obtaining a good agreement between numerical and experimental results for all the experimental tests, the analyses are carried out using the pointwise THM model to validate the consistency of this simplified approach. Additionally, the present algorithm allows for validating the models implemented in the pointwise mechanical subroutine. Fig. 92 shows the algorithm employed to investigate the multiple creep tests using the MPS.

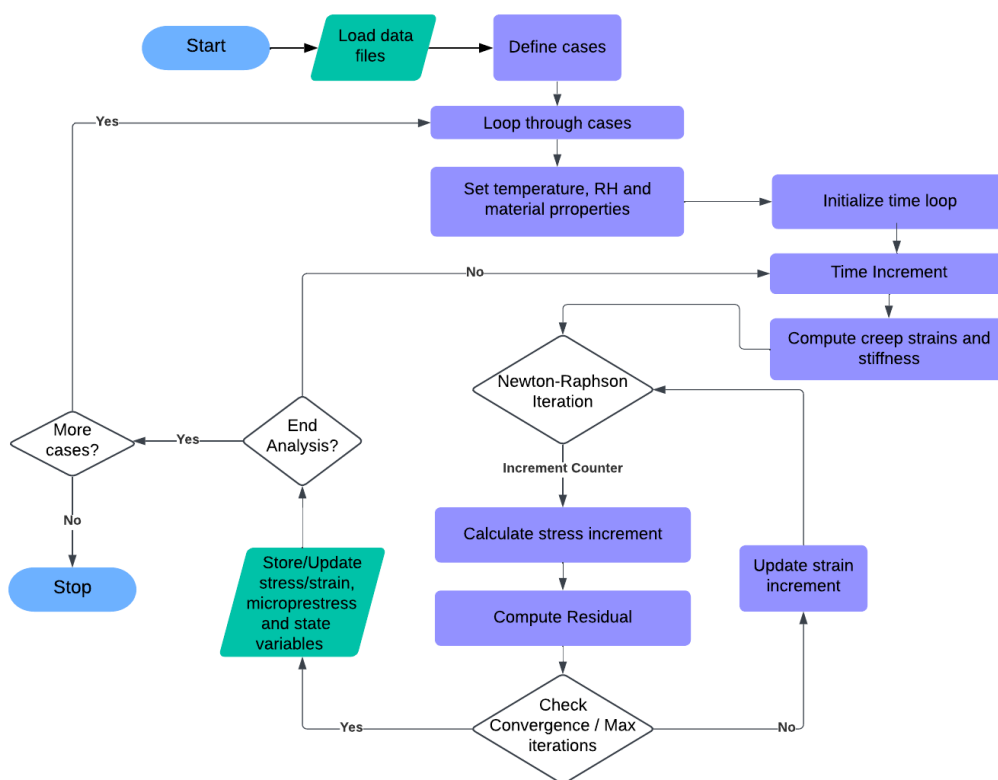


Fig. 92 - Iterative loop for investigating microprestress solidification theory creep model in multiple creep tests.

The algorithm employs the numerical model for creep calculation and linear stress calculation implemented in the pointwise THM model described in Chapter 3.7.2. However, in this case, the calculations of the stress state are applied to a single integration point. The proposed algorithm does not account for shrinkage or thermal strains. However, creep development is influenced by temperature and relative humidity histories, necessitating the establishment of representative temperature and relative humidity evolution for both. The present study assumes a constant temperature of 20°C throughout the analysis. The relative humidity is provided as input for the present algorithm.

In the numerical simulation of shrinkage tests, relative humidity exhibits nonlinear profiles across the element cross-section, making it challenging to define a unique representative relative humidity history for each slab or prism experimental setup. The approach considered for the present algorithm determines

the relative humidity through an inverse relationship with the numerical shrinkage results presented in Fig. 91, according to the following equation:

$$\dot{h} = \frac{\dot{\varepsilon}_{sh}}{k_{sh}^*} \quad (4.3)$$

Seven experimental setups are initially considered: basic creep, drying creep in prisms (P100, P200, P400), and drying creep in slabs (S100, S200, S400). A constant relative humidity of 1 is assumed throughout the analysis for basic creep tests. Fig. 93 presents the relative humidity history for the prisms and slabs with the respective experimental shrinkage results presented by markers.

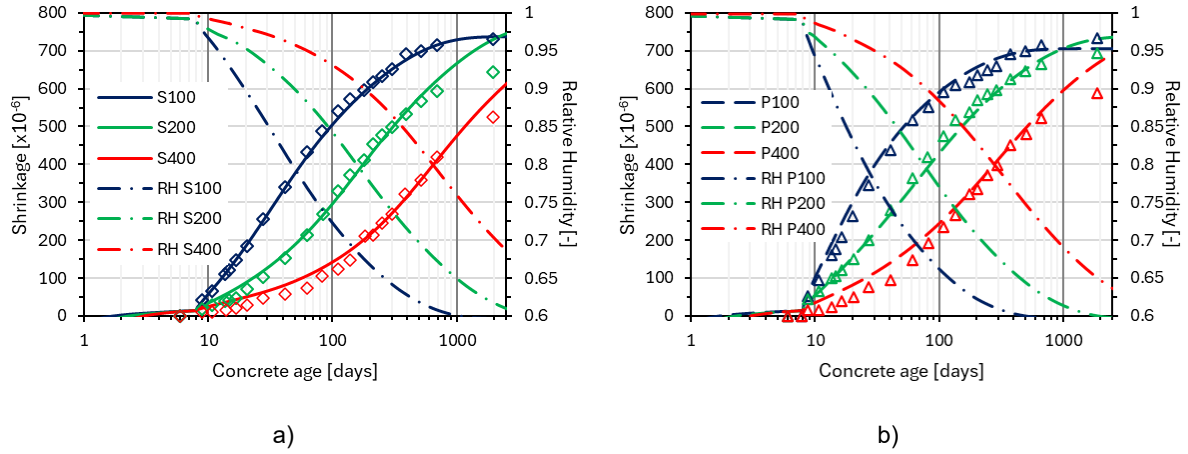


Fig. 93 - Shrinkage and relative humidity evolution: a) for slabs; b) for prisms.

Havlásek [240] conducted a calibration of the basic creep compliance. This study performs a new calibration process using the B4 model as the initial estimate. The following equation gives the basic creep compliance according to model B4:

$$J(t, t') = q_1 + c_2 \cdot q_2^* \cdot Q(t, t') + c_3 \cdot q_3^* \cdot \ln[1 + (t - t')^{0.1}] + c_4 \cdot q_4^* \cdot \ln\left(\frac{t}{t'}\right) \quad (4.4)$$

where c_2 , c_3 and c_4 are calibration parameters affecting the ageing, non-ageing and flow part of the creep compliance, respectively, and q_2^* , q_3^* and q_4^* are the model B4 parameters q_2 , q_3 and q_4 .

The calibration process adjusts the model B4 predictions using the least squares method, applied to parameters c_2 , c_3 and c_4 . This approach is more appropriate than allowing the q_i parameters to vary without constraints, as it aligns with the methodology used for calibrating creep compliance in model B4 for modern concrete mixtures containing supplementary cementitious materials (SCM) and plasticisers. The final creep model parameters are given by $q_i = c_i \cdot q_i^*$. Optimal results are obtained with $c_2 = 0.70$, $c_3 = 1.00$ and $c_4 = 1.30$. According to this calibration approach, it is possible to conclude that the present concrete presents 30% lower ageing creep and 30% higher flow creep than predicted by the model B4 formulation. Table 17 resumes the creep model parameters considered in model B4 creep compliance.

Table 17 – Creep model parameters for the Bryant and Vadhanavikkit experimental campaign simulation.

Parameter ($\mu \text{ MPa}^{-1}$)	Havlašek, Petr	Model B4	Pointwise THM model (after calibration)
q_1	9.00	23.49	23.49
q_2	75.00	110.33	77.23
q_3	28.00	5.81	5.81
q_4	6.50	6.76	8.79

The parameter q_1 remains unchanged from model B4, reflecting its physical significance as approximately 70% (60% in model B3) of the concrete's elastic modulus at 28 days ($E_{28} = 29.8 \text{ GPa}$). The other parameters are adjusted within $\pm 30\%$ of the values proposed in model B4. The calibration results indicate a reduction in the ageing component of creep and an increase in the flow creep component. Fig. 94 compares the experimental basic creep data with the numerical predictions from the calibrated model.

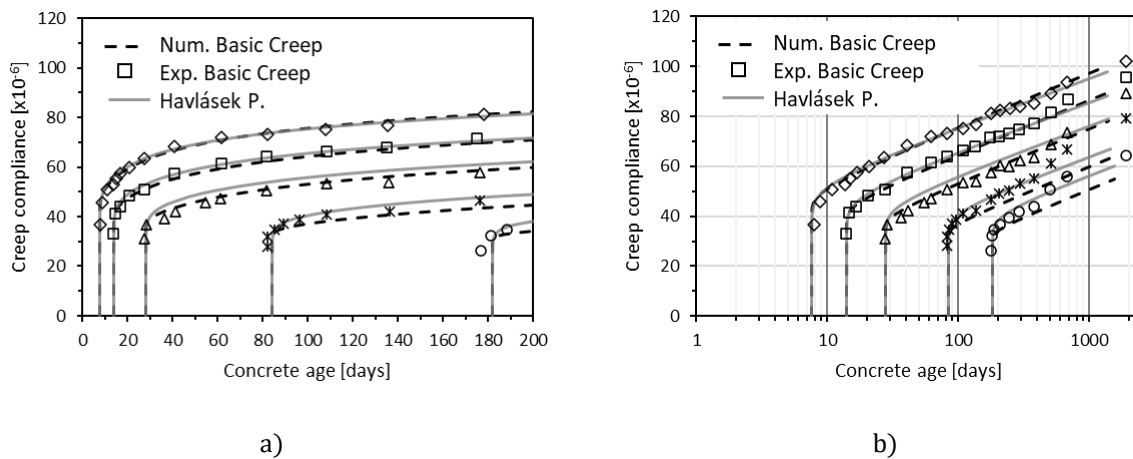


Fig. 94 - Basic creep compliance adjustment of the numerical to experimental results.

The results demonstrate good agreement between the experimental and numerical data, highlighting the model's capability to simulate concrete basic creep and ageing.

Drying creep tests, accounting for size effects, were conducted at 14 days. Since all specimens were exposed to drying at 8 days, some shrinkage had already occurred before loading was applied. The first attempt at numerical simulation of creep tests employs the MPS model (Chapter 2.4.3.1) to evaluate the error reported in the literature regarding the simulation of size effects. In the present simulations, the model parameter c_0 is considered equal to $c_0 = 0.005$, which corresponds to a microprestress of 1.6 MPa at 125 days in the absence of hygrothermal effects (see Chapter 2.4.3.1), while the model parameter k_1 is assumed equal to $k_1 = 5.25 \times 10^1 \text{ MPa}$. Fig. 95 presents the numerical results of the microprestress relaxation simulation for the slab and prismatic specimens.

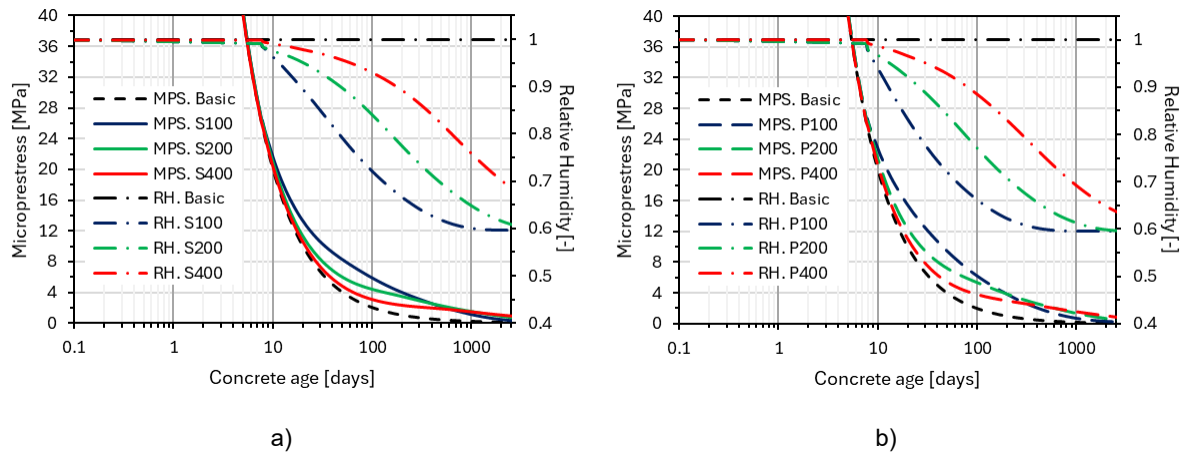


Fig. 95 - Microprestress and relative humidity evolution for: a) slab specimens; b) prismatic specimens.

The results indicate that, in the absence of drying, microprestress relaxes more rapidly than under drying conditions. This behaviour reflects the nature of the MPS relaxation equation, where variations in temperature and relative humidity drive the model towards higher microprestress values. In contrast, microprestress relaxes asymptotically to zero when such variations are absent.

In the MPS theory, the evolution of the viscosity modulus is governed by the microprestress value. Lower microprestress results in a stiffer model response, whereas higher microprestress leads to increased creep flow (assuming $c_0 \cdot q_4$ constant). Consequently, greater microprestress leads to higher expected creep flow in the model. These assumptions are consistent with the Pickett effect observed in specimens undergoing drying. Furthermore, they align with the increase in capillary stress as pore saturation decreases, as shown in Fig. 10. The increase in the capillary pressure serves as the most comparable physical quantity to microprestress, since microprestress represents the stress occurring within the nanopores of the cement gel and capillary pressure represents the stress in the capillary pores that include nanopores. Therefore, changes in the capillary pressure are supposed to be reflected similarly in the microprestress (possibly with different intensities).

Fig. 96 illustrates the evolution of creep compliance for drying slab and prismatic specimens using the MPS.

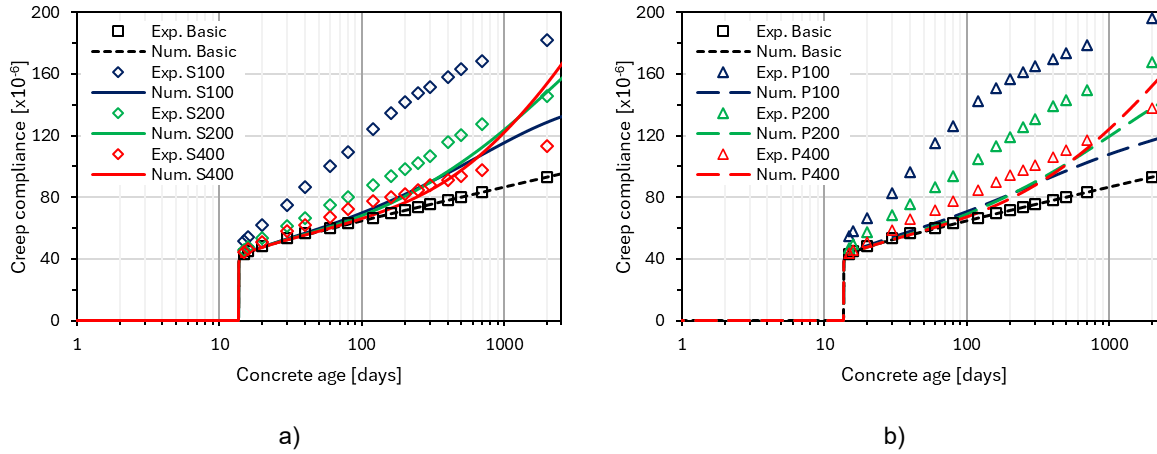


Fig. 96 – Creep strains using MPS for: a) slab specimens; b) prismatic specimens.

The numerical results confirm that the original MPS theory fails to accurately simulate the size effect on creep, as previously observed by Bažant et al. [167]. Drying creep strains exceed basic creep strains. However, in the long term, specimens S400 and P400, which undergo slower drying, exhibit greater creep strains than specimens S100 and P100. The numerical results highlight the need to update the MPS formulation for drying creep. Potential refinements encompass the modified microprestress solidification theory (MMPS) [167], the extended microprestress solidification theory (XMPS)[124] or the improved microprestress solidification theory (IMPS)[148].

The IMPS formulation for the relaxation function has a key limitation: the current model lacks an analytical solution for the relaxation function. This thesis avoids numerical solutions for evaluating microprestress whenever possible, as they significantly increase computational demand in pointwise THM analysis. Additionally, these methods are generally sensitive to time discretisation, requiring extra caution when defining the analysis time steps.

The MMPS explicitly decomposes the viscosity modulus into two components: one accounting for basic creep based on MPS relaxation and another addressing hygrothermal imbalances. However, a significant drawback of this approach is that microprestress evolution becomes independent of hygrothermal changes.

The XMPS offers a more practical alternative, preserving the traditional MPS model while introducing an additional term for drying effects. The rate of change of microprestress drives this new term in the XMPS. The viscosity modulus relationship is adjusted according to the following equation:

$$\frac{1}{\eta} = \frac{1}{\eta_n} + \frac{1}{\eta_{flow}} = c_0 \cdot q_4 \cdot S + b_{XMPS} \cdot |\dot{S}| \quad (4.5)$$

In the XMPS model, the additional viscoelastic modulus component $1/\eta_{flow}$ does not affect microprestress relaxation, preserving the original MPS relaxation equation and its analytical solution. The introduction of this additional parameter suggests that the new formulation could enhance the accuracy of creep compliance in drying specimens, as drying alters the microprestress rate.

However, the analysis of microprestress evolution in Fig. 95 shows that the microprestress rate is higher in sealed specimens than in dry ones. Consequently, applying this new formulation with a nonzero value of b_{XMPs} causes the basic creep compliance of both model B3 and model B4 to fail, since the microprestress rate remains nonzero even without hygrothermal effects. To address this issue, this PhD thesis proposes an alternative approach called refined microprestress solidification theory (RMPS): instead of focusing on the rate of microprestress change, the additional viscoelastic modulus component $1/\eta_{flow}$ is determined based on hygrothermal imbalances. This results in a slight modification, making the formulation more similar to the MMPS model, yet keeping microprestress relaxation dependent on hygrothermal effects. The adjusted viscosity modulus relationship for RMPS is given by the following equation:

$$\frac{1}{\eta} = \frac{1}{\eta_n} + \frac{1}{\eta_{flow}} = c_0 \cdot q_4 \cdot S + b_{RMPS} \cdot |\dot{s}|^{n_{RMPS}} \quad (4.6)$$

where b_{RMPS} and n_{RMPS} are new calibration parameters and $|\dot{s}| = k_1 \cdot |\dot{T} \cdot \ln h + T \cdot \dot{h}/h|$ is the hygrothermal function used in the MPS relaxation.

In the RMPS, the additional viscosity modulus term vanishes when no hygrothermal imbalances occur during the current step, while extra relaxation is introduced when such imbalances are present. The proposed adjustments ensure that the MPS theory remains consistent with the basic creep behaviour observed in models B3 and B4, while incorporating additional compliance due to hygrothermal imbalances. The parameter n_{RMPS} allows flexibility in the curve fitting of the drying creep compliance.

A good fit to the experimental data was achieved with $k_1 = 1.10$ MPa, $b_{RMPS} = 1.30 \times 10^{-3}$ and $n_{RMPS} = 1.4$. The transformed times parameters affecting the relative humidity functions given by Equation (3.24) are set to $\alpha_e = 80$, $\alpha_r = 0.80$ and $\alpha_s = 0.10$. Fig. 97 shows the microprestress relaxation obtained with this new set of parameters.

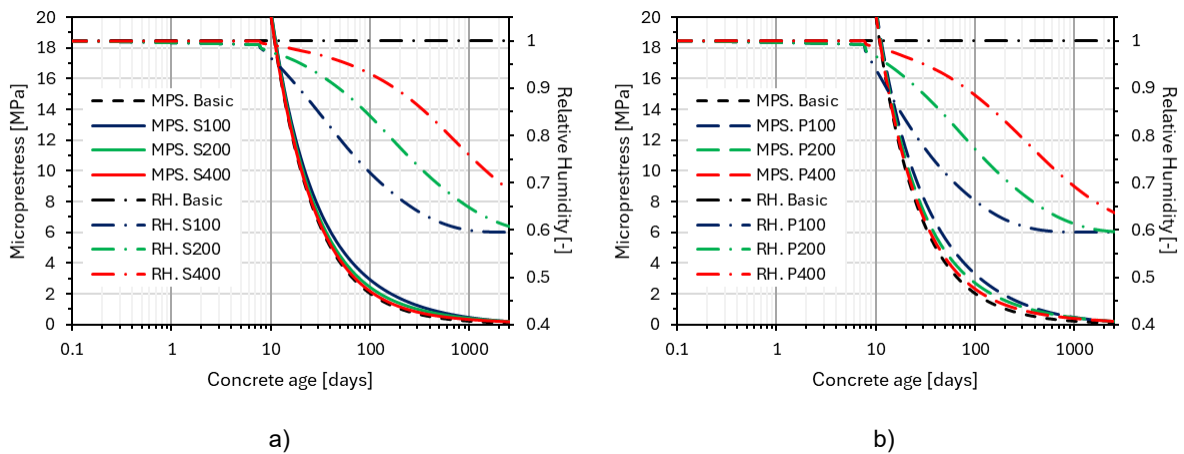


Fig. 97 – Microprestress and relative humidity evolution for: a) slab specimens; b) prismatic specimens.

In the RMPS formulation, the hygrothermal influence on MPS evolution is reduced, as it is now incorporated into the new additional viscosity modulus parameter. Fig. 98 shows the creep strains using the RMPS for slabs and prismatic specimens.

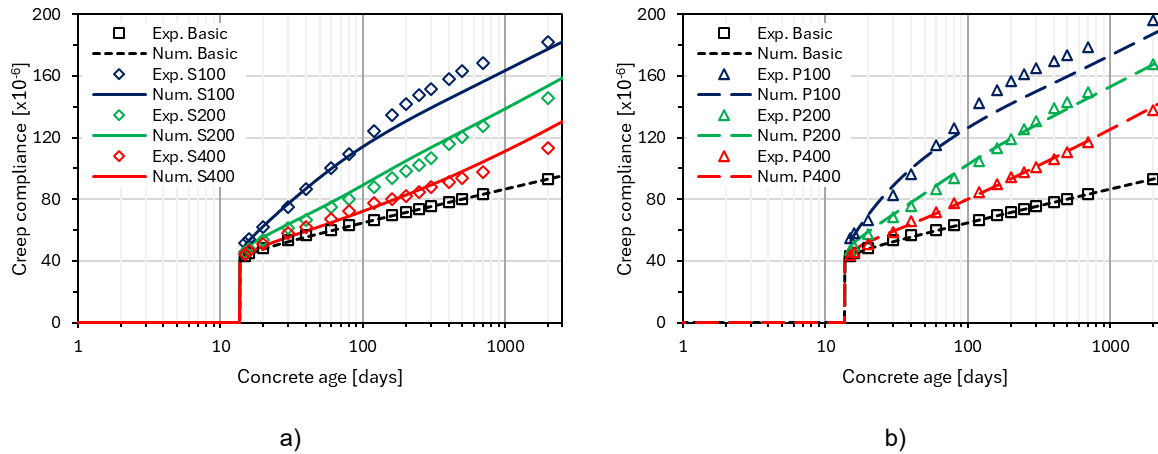


Fig. 98 – Creep strains using the RMPS for: a) slab specimens; b) prismatic specimens.

The numerical results demonstrate good agreement between the experimental and simulated data, validating the use of the RMPS for the numerical simulation of the size effect in the numerical simulation of drying creep.

The ageing effect on drying creep is investigated through simulations of drying creep tests at different ages in slabs (S150) and prisms (P150). Loading tests are conducted at 8, 14, 28, 84, and 182 days. Fig. 99 shows the drying creep compliances at different ages for slabs S150 and prisms P150.

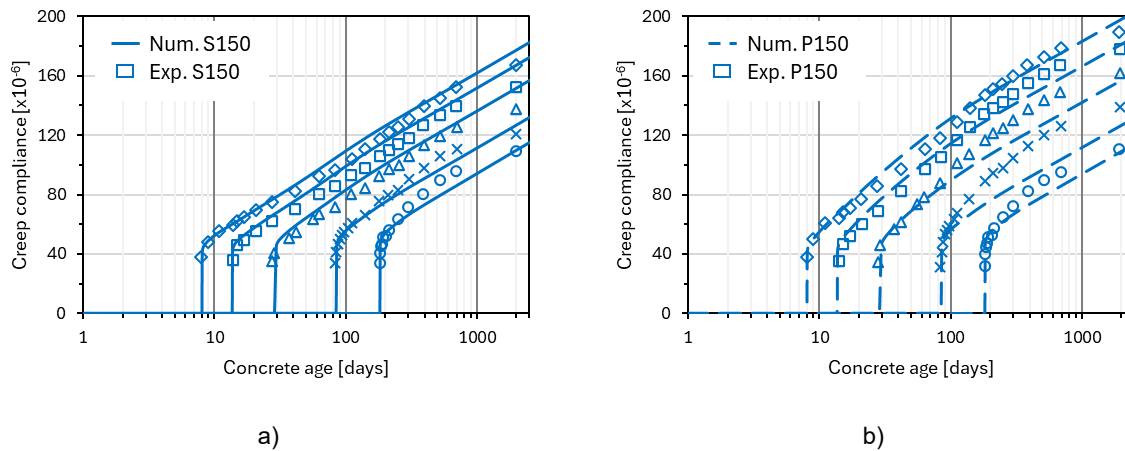


Fig. 99 - Creep compliance at different loading times for: a) slab specimens S150; b) prismatic specimens P150.

The numerical results using RMPS successfully simulate most drying creep tests across different loading ages. Microprestress is unaffected by loading age, leading to consistent flow creep regardless of loading time, provided that drying conditions remain unchanged.

4.1.2.3.1 Final considerations

The RMPS has proven effective in simulating the size effect in drying creep. However, a critical assessment of the underlying assumptions and limitations of the calibration process is necessary before its implementation in the pointwise THM model. The calibration results suggest the use of relative

humidity function parameters $\alpha_e = 80$ and $\alpha_r = 0.80$, used in Equation (3.24a) and (3.24b), respectively, which differ from the initial proposed values of $\alpha_e = 10$ and $\alpha_r = 0.10$ [65]. Fig. 100 compares the transformed time functions for relative humidity using both the traditional and newly calibrated parameters.

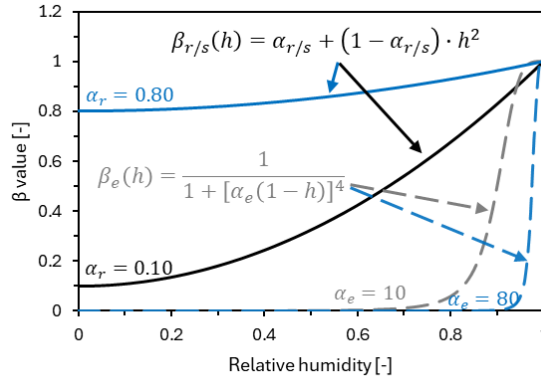


Fig. 100 – Comparison between the β_h functions used in the calibrated model and default values.

The use of $\alpha_e = 80$ reflects an increased sensitivity of cement hydration to drops in relative humidity. The assumption of a high value for α_e is primarily justified by the short-term creep observed after loading in drying specimens at later loading ages, as shown in Fig. 99, which is significantly higher than basic creep for the same loading ages, as shown in Fig. 94. This suggests that the evolution of the solidified volume nearly ceases once drying begins at 8 days. To achieve an accurate fit, a high α_e value is necessary to effectively halt ageing creep compliance after drying exposure.

It is important to note that the basic creep in Fig. 94 was simulated under the assumption of constant relative humidity ($h = 1$). For the current concrete mixture, this assumption appears reasonable, as basic shrinkage is minimal ($\sim 35 \mu\epsilon$) compared to the total shrinkage observed in drying prisms ($\sim 740 \mu\epsilon$). To investigate if the assumption of the $\alpha_e = 80$ does not significantly influence the basic creep shrinkage and to verify that the additional viscosity parameter has minimal influence under small relative humidity variations, a new simulation is conducted incorporating self-desiccation into the basic shrinkage simulations. Fig. 101 presents the results of the basic creep tests simulated with the self-desiccation model.

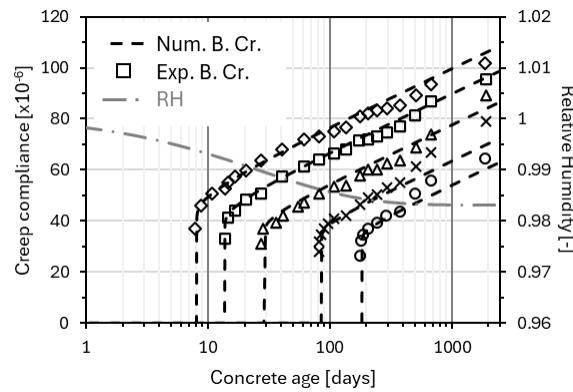


Fig. 101 - Basic creep considering the self-desiccation in the hygral model.

The numerical results show that the relative humidity drop due to self-desiccation is minimal (< 0.02), resulting in a negligible impact on the ageing component of basic creep. Consequently, the previous assumption of $\alpha_e = 80$ is deemed appropriate for this case.

The parameter $\alpha_r = 0.80$ influences flow creep through the concept of equivalent viscosity $\tilde{\eta} = \eta/\psi_r$ (see Equation (3.72) in Chapter 3.7.2.4). The traditionally expected value of $\alpha_r = 0.10$ results in a lower ψ_r , increasing the inverse of the viscosity modulus, thereby reducing flow strains at lower relative humidity. In contrast, the higher $\alpha_r = 0.80$ leads to a smaller reduction in the flow creep under lower relative humidity conditions.

A more refined approach to improve accuracy further could involve using nonlinear equations for b_{RMPS} or modify the microprestress relaxation function. However, implementing such changes requires careful investigation, which falls beyond the scope of this PhD research. Therefore, further exploration of these aspects is recommended as future work. Potential areas for investigation include drying creep in modern concrete mixtures with nonlinear sorption curves, the behaviour of drying creep under drying and wetting cycles, and the study of basic creep at different relative humidity levels, including wet ($h = 1$), intermediate ($h = 0.5$) and dried conditions ($h = 0$). In conclusion, the RMPS is considered to preserve the traditional MPS while showing good physical reasoning and avoiding numerical methods in the solution of the relaxation function, so it is implemented in the pointwise THM model.

4.1.2.3.2 Numerical simulation of drying creep tests using a pointwise THM model

The numerical simulation of creep in specimens S200 and P200 using the pointwise model is performed by replicating the full duration of the experimental creep tests. This approach incorporates both sustained mechanical loading and concurrent drying conditions. Two separate analyses are conducted for each specimen: one to evaluate shrinkage (results presented in Fig. 90) and another to simulate the creep response. A constant creep stress of 7 MPa is applied, consistent with the experimental campaign. Creep compliance is calculated by subtracting the shrinkage strain (obtained from the unloaded simulation) from the total strain observed in the creep test simulation and dividing the resulting strain by the applied stress. Fig. 102 illustrates the evolution of creep compliance for S200 and P200 using the pointwise THM model and the numerical results obtained using the algorithm in Fig. 92.

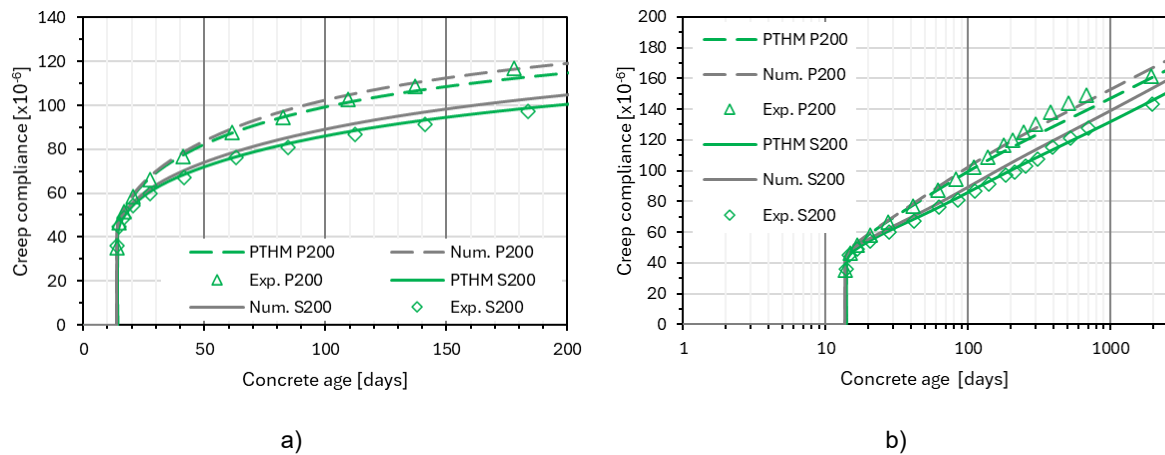


Fig. 102 – Numerical simulation of the creep compliance using the Pointwise THM model in the P200 and S200 specimens for: a) for the first 200 days; b) for 2500 days.

The results demonstrate good agreement between the creep behaviour simulated using the pointwise THM model and the experimental data. The creep compliance obtained with the pointwise THM model is only slightly lower than predicted by the numerical algorithm previously developed to investigate multiple creep tests using the RMPS theory. Such differences are explained by the complex simulation of creep in a pointwise manner, affected by local relative humidity variations and the microcracking effects occurring in the numerical model due to the drying shrinkage occurring before loading application. Fig. 103 shows the numerical simulation of creep using the pointwise THM model.

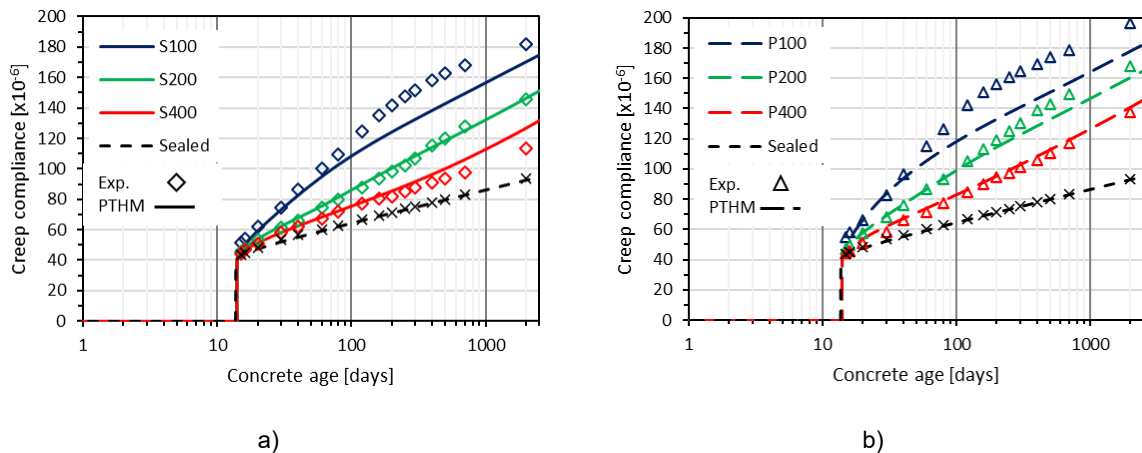


Fig. 103 – Numerical simulation of compliance using the pointwise THM model: a) for slabs; b) for prisms.

The results show a good agreement between the numerical and experimental creep, with only the slab S100 and prism P100 experiencing relatively lower creep compliance in the numerical analysis using the pointwise THM model when compared to the ones obtained in Fig. 98. The present numerical simulations validate the present creep model and the assumptions in formulating the RMPS approach to numerical modelling of concrete creep using the pointwise THM model.

4.1.2.4 Notional size in slab and prismatic specimens

The notional size, h_n , is fundamental in defining the drying rate in analytical equations, as it accounts for the element's geometry. This concept establishes a relationship between the element's total volume V_c (or cross-sectional area A_c) and the surface S_c (or perimeter μ_c) exposed to drying, as expressed by the following equation:

$$h_n = \frac{V_c}{S_c} \text{ or } h_n = \frac{A_c}{\mu_c} \quad (4.7)$$

Although straightforward to apply, the equation neglects the influence of one-dimensional (1D), two-dimensional (2D), or three-dimensional (3D) hygral flow. The present experimental campaign enables the comparison of drying rates between specimens with the same notional size, covering 1D flow (slab) and 2D flow (prism). Table 18 shows the notional size for investigated slabs and specimens using Equation (4.7).

Table 18 – Value of the notional size for the investigated slabs and specimens.

	Specimen	Notional size
Slabs	S150	150 mm
	S200	200 mm
	S300	300 mm
Prisms	P300	150 mm
	P400	200 mm

According to the results of the notional size presented in Table 18, the slab S150 has the same notional size as the prism P300. Consequently, both specimens would be expected to exhibit similar shrinkage and flow creep strains. Fig. 104 presents a comparison between the numerical and experimental shrinkage and creep compliance for slab S150 and prisms P300.

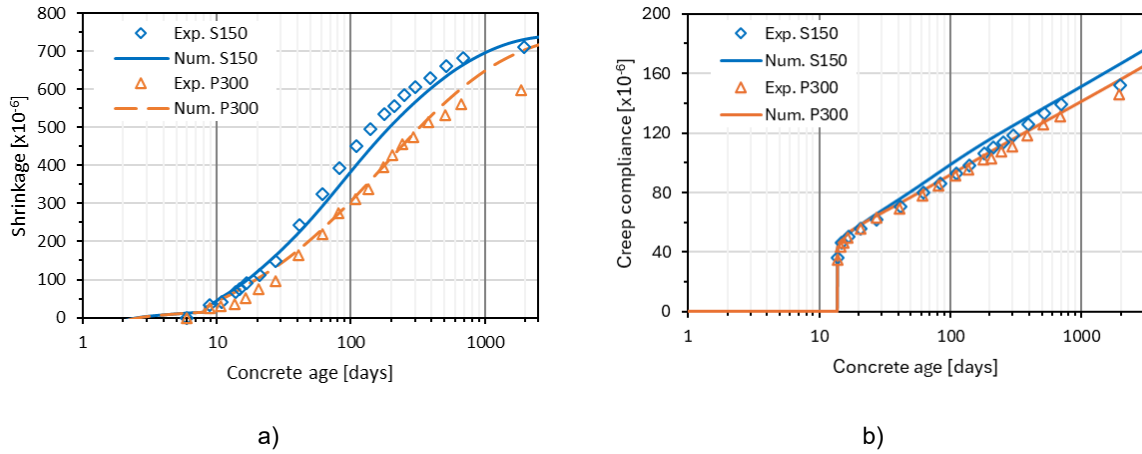


Fig. 104 - a) shrinkage of slab S150 and prism P300; b) creep compliance at 14 days for slab S150 and prism P300.

A similar comparison can be conducted for slab S200 and prism P400 mm. Fig. 105 compares shrinkage and creep compliance between slab S200 and prism P400.

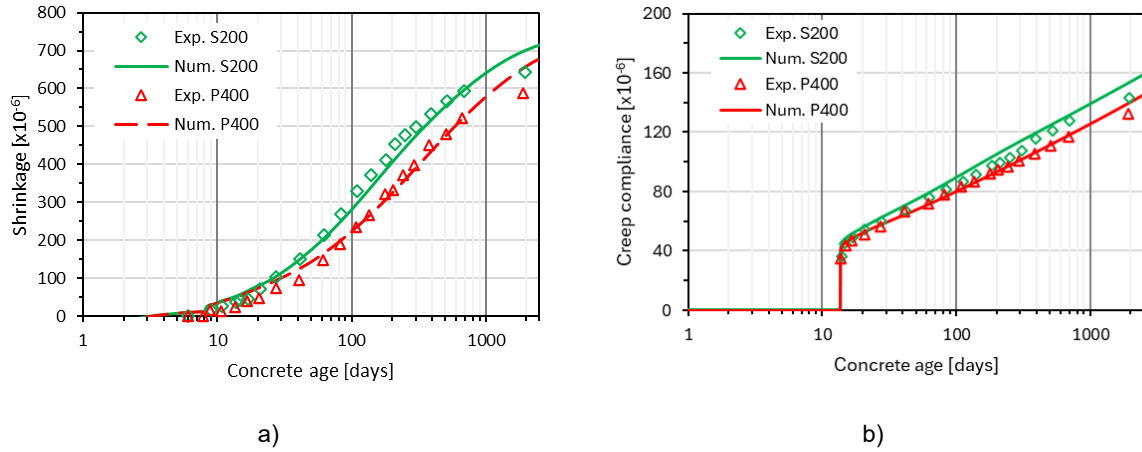


Fig. 105 - a) shrinkage of slab S200 and prism P400; b) creep compliance at 14 days for slab S200 and prism P400.

The results indicate that the shrinkage and creep strains among prisms differ despite having the same notional size. Therefore, calibration parameters must be applied depending on the element's shape (drying mechanisms). Dönmez and Bažant [252] and Abdo et al. [253] have proposed shape factors to adjust the hygral material properties relationship based on the specimen's geometry, replacing Equation (4.7) by the following equation:

$$h_n = k_s \frac{V_c}{S_c} \text{ or } h_n = k_s \frac{A_c}{\mu_c} \quad (4.8)$$

where k_s is a shape factor that is assumed $k_s = 1$ to slab-like drying specimens.

By comparing the experimental results between slabs and prisms, a closer agreement is observed when plotting the shrinkage and creep results for slab S200 and prism P300. Fig. 106 compares shrinkage and creep compliance between slab S200 and prism P300.

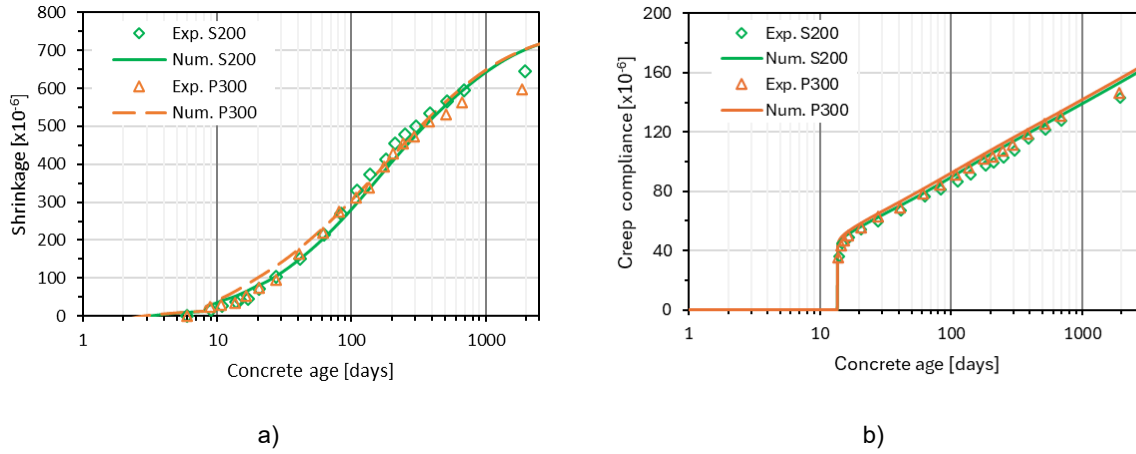


Fig. 106 - a) shrinkage of slab S200 and prism P300; b) creep compliance at 14 days for slab S200 and prism P300.

A better shape comparison for the shrinkage and creep compliance is achieved by using slab S300 and prism P400 mm. Fig. 107 compares shrinkage and creep compliance between slab S300 and prism P400.

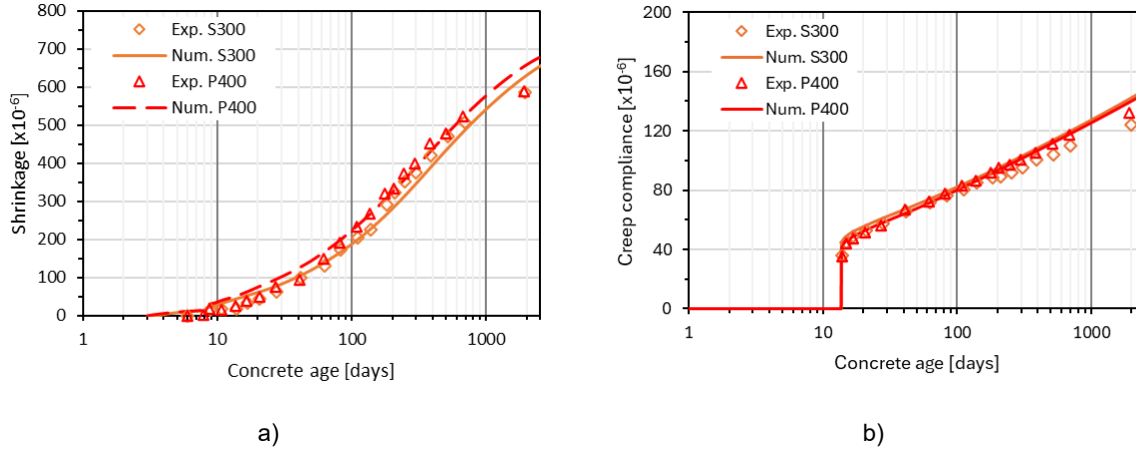


Fig. 107 - a) shrinkage of slab S300 and prism P400; b) creep compliance at 14 days for slab S300 and prism P400.

The comparison of the notional size between P300 and S200 results in a ratio of 1.5, while the comparison between P400 and S200 yields a ratio of 1.33(3). These results show that a slab experiences drying shrinkage and drying creep approximately 1.2 to 1.5 times higher than a prism with the same notional size. The range for the notional size of prisms is in agreement with the work of Dönmez and Bažant [252], which suggests that for square drying, the range between $1.17 \leq k_s(h_{amb}) \leq 1.24$. The present results are essential when dealing with the calibration of numerical models that simulate structural elements based on experimental drying data. Shrinkage and total creep are normally experimentally assessed using prismatic or cylindrical specimens, which exhibit faster drying behaviour. However, caution must be exercised when extrapolating those experimental results to simulate concrete elements, as most structural elements experience slab-like drying conditions. Using test data obtained from different drying configurations and scaling it only by notional size, without accounting for the effect of element shape, can lead to inaccurate predictions of drying shrinkage and drying creep in numerical analyses. Despite this, the pointwise THM model has demonstrated its capability to capture

shape-related effects in numerical simulations effectively. This allows it to be applied to structural elements undergoing slab-like drying, even when the model has been calibrated using prismatic specimens. Additionally, Dönmez and Bažant [252] highlight that ambient relative humidity can influence the shape factor. Future works should explore other drying shapes and the role of ambient humidity in defining or refining the notional size and its relationship to shape effects, as well as the validity of the pointwise THM to simulate those effects.

4.1.3 NUMERICAL SIMULATION OF THE SHRINKAGE IN AN UNRESTRAINED RING TEST

Menu et al. [254] studied the influence of drying shrinkage test procedure, specimen geometry and boundary conditions on the free shrinkage of two shotcrete mixtures. The study intends to investigate the common assumption that free shrinkage is the same for concrete with equal surface-to-volume ratio, regardless of specimen geometry and boundary conditions. The experimental campaign included two different specimen geometries:

- free uniaxial tests in prismatic specimens;
- unrestrained ring tests.

The prismatic specimens have 76 mm×76 mm×285 mm dimensions and were tested according to the ASTM C157 [255]. The experimental tests on prisms involved measuring basic shrinkage, drying shrinkage in unsealed conditions (labelled unsealed prism) and drying shrinkage for a partially sealed specimen, so that the specimen has the same surface-to-volume ratio as the unrestrained ring test (labelled as axial drying prism). Fig. 108 shows a schematic representation of the configuration for the unsealed prism and the axial drying prism.

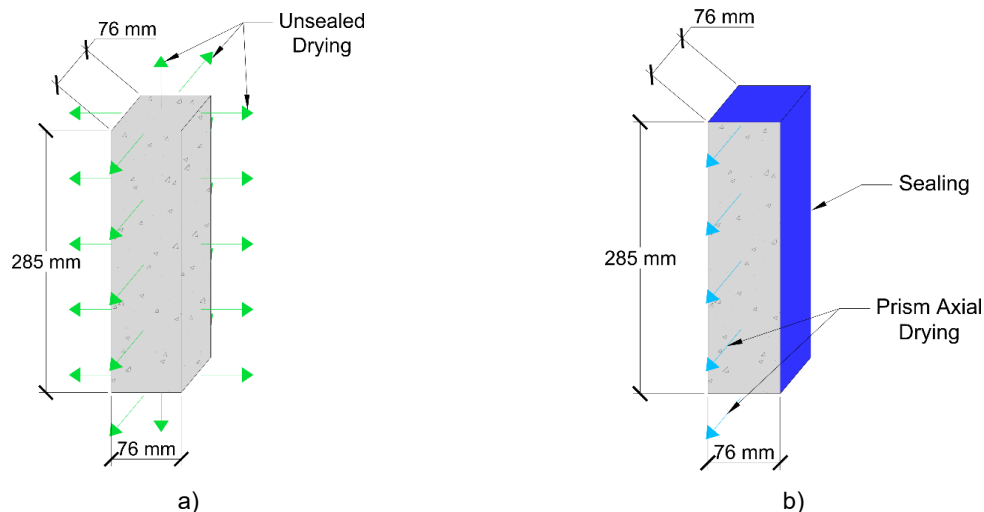


Fig. 108 - Schematic representation of the Menu et al. [254] experimental campaign: a) unsealed drying prism; b) axial drying prism;

The free ring specimen used in the experimental campaign is based on the AASHTO [256] restrained ring test specimen configuration. A 152 mm high and 76 mm thick concrete ring was cast around a polystyrene ring with a 152.5 mm radius. The authors consider the polystyrene ring restraint negligible, as it presents a modulus of elasticity of about 2.2 MPa, compared to the steel ring used in the restrained

shrinkage, which is about 200 GPa [254]. Fig. 109 shows a schematic representation of the unrestrained ring test.

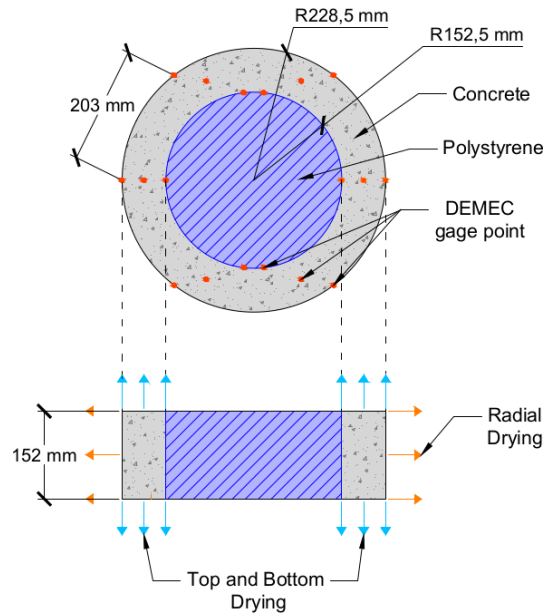


Fig. 109 - Schematic representation of the unrestrained ring test.

Two different sealing conditions are considered:

- top and bottom drying, where drying occurs from the top and bottom surfaces of the ring tests, corresponding to the blue arrows in Fig. 109;
- radial drying, where drying occurs only from the outer radius surface of the ring test, corresponding to the orange arrows in Fig. 109.

The shrinkage in the unrestrained ring tests was measured using a demountable mechanical gauge (DEMEC) at different measurement point locations:

- inner radius location, corresponding to the R152.5 mm and represented by the red dots at the interface between polystyrene and the concrete ring in Fig. 109;
- mid radius location, corresponding to R190.5 mm and represented by red dots at mid radius of the concrete ring in Fig. 109;
- outer radius location, corresponding to R228.5 mm and represented by the red dots at the outer radius of the concrete ring in Fig. 109.

The objective of considering different measurement point locations is to investigate the influence of the DEMEC gauge points' location on the measured free shrinkage for the different sealing configurations.

Both prismatic and ring specimens are cast into moulds and left for the first 24 hours covered with wet burlap and plastic sheets. After 24 hours, the exterior mould wall was removed, and specimens were cured for two more days until the test time at 3 days. The experimental measurements started at 3 days, corresponding to the test time. The specimens were exposed to drying under controlled conditions of 20°C and an environment with a relative humidity of 50%. The free drying shrinkage strain was calculated using the following equation:

$$\varepsilon_{sh} = \frac{\Delta l}{G} \quad (4.9)$$

where Δl is the change in length and G is the gauge length.

Two shotcrete mixtures were considered in the experimental campaign. One of the shotcrete mixtures featured a water-to-cement ratio typical of ordinary concrete mixtures, comprising 445 kg/m³ of Portland cement, 1790 kg/m³ of aggregates, 197 kg/m³ of water, 5 kg/m³ of superplasticiser and 0.16 kg/m³ of air-entraining admixture. In this PhD thesis, the pointwise THM model is used to simulate the present experimental campaign for the selected shotcrete mix. The objective of the present numerical simulations is to test the use of the same material model in the pointwise THM framework for the numerical simulations of different specimen geometries, for the particular case of the prism and the ring. The results are discussed in accordance with the available experimental data.

4.1.3.1 Material characterisation

The experimental campaign included compressive strength, tensile strength, and modulus of elasticity tests conducted on 3, 7, and 28 days. The compressive and tensile strength evolution is determined based on the calibration of Equation (3.86). Fig. 110 shows the evolution of numerical and experimental compressive and tensile strength.

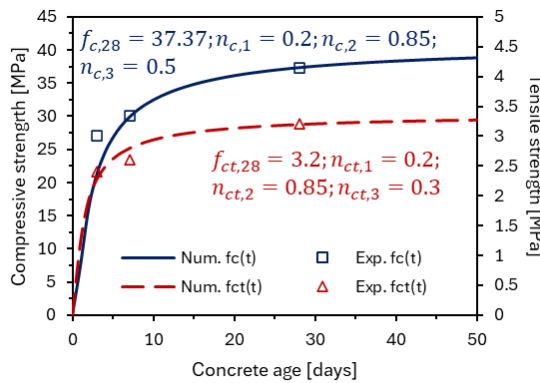


Fig. 110 – Compressive strength and tensile strength evolution.

The specimens had no relative humidity measurements, so the hygral model is calibrated with the shrinkage experimental data based on the calibration procedure used in Chapter 4.1.2.2.1. Table 19 shows the parameters used in the hygral and shrinkage model.

Table 19 - Parameters used in the hygral and shrinkage model.

Parameter	Value
α_0	0.005
D_1	$4.00 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
h_c	0.84
n_h	15
h_{env}	0.50
η_e^*	$5.00 \times 10^{-8} \text{ m s}^{-1}$
k_{sh}^*	8.44×10^{-3}
ε_{bs0}	475.00×10^{-6}
α_h	10

The shrinkage is simulated using the dKwak Equation (3.47) for the equivalent shrinkage coefficient. The creep model parameters were determined using the model B4 formulation (Equations (2.98)). Table 20 presents the creep model parameters used in the THM simulations.

Table 20 – Creep model parameters used in the numerical simulation of the Menu et al. [254] experimental campaign.

Parameter	Model B4
q_1	$24.19 \mu \text{ MPa}^{-1}$
q_2	$92.65 \mu \text{ MPa}^{-1}$
q_3	$6.01 \mu \text{ MPa}^{-1}$
q_4	$7.08 \mu \text{ MPa}^{-1}$
k_1	$5.25 \times 10^{-1} \text{ MPa}$
B_{RMPS}	0

4.1.3.2 Numerical simulation of the shrinkage prisms

The numerical simulations are carried out using the pointwise THM model. The THM analyses are performed using a staged approach consisting of the thermo-hygral analysis for determining the temperature and relative humidity distribution over the prisms and the mechanical analysis to evaluate the shrinkage deformation. The numerical simulations are carried out on one-eighth of the prismatic specimen, accounting for the 3D symmetry conditions. In the present case study, the hygrothermal mesh is equal to the mechanical mesh since drying occurs through all the specimen's surfaces for the unsealed prismatic specimen, corresponding to a 3D drying flow. Fig. 111 shows the finite element meshes used in the hygrothermal and mechanical analysis of the drying shrinkage prisms.

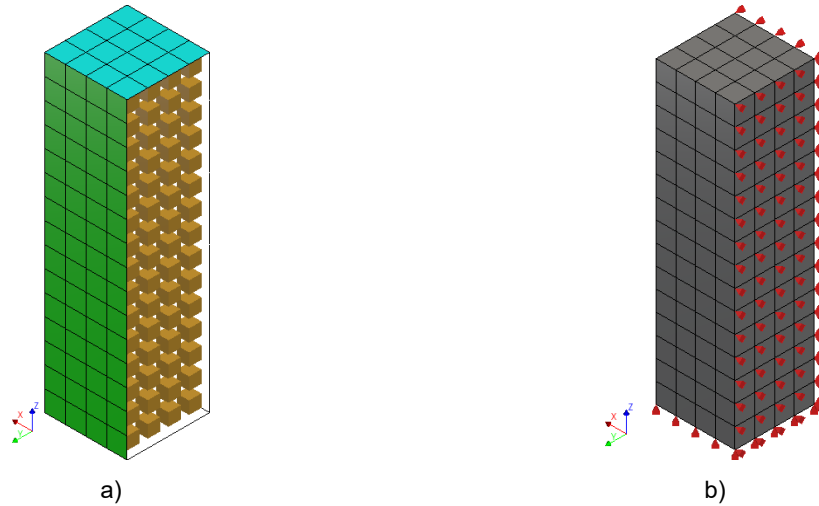


Fig. 111 – Finite element mesh for simulating the drying shrinkage prisms: a) hygrothermal analysis; b) mechanical analysis.

For the numerical simulations of the unsealed prism, drying can occur on both the blue and green surfaces in Fig. 111 (notice that there is also an additional blue surface defined in the plane orthogonal to the X direction), while for the axial drying prism, drying is only allowed by the green surface in Fig. 111. All the finite elements have the same size corresponding to $9.375 \text{ mm} \times 9.375 \text{ mm} \times 9.5 \text{ mm}$.

The numerical analyses are performed from the setting time up to 125 days to ensure the numerical simulation of the entire experimental test. The numerical results are subtracted by their value at the concrete age of 3 days to allow direct comparisons with the experimental data, where measurements only started at 3 days. Fig. 112 shows the numerical simulation of the basic shrinkage and the numerical simulation of the unsealed prism and axial drying prism.

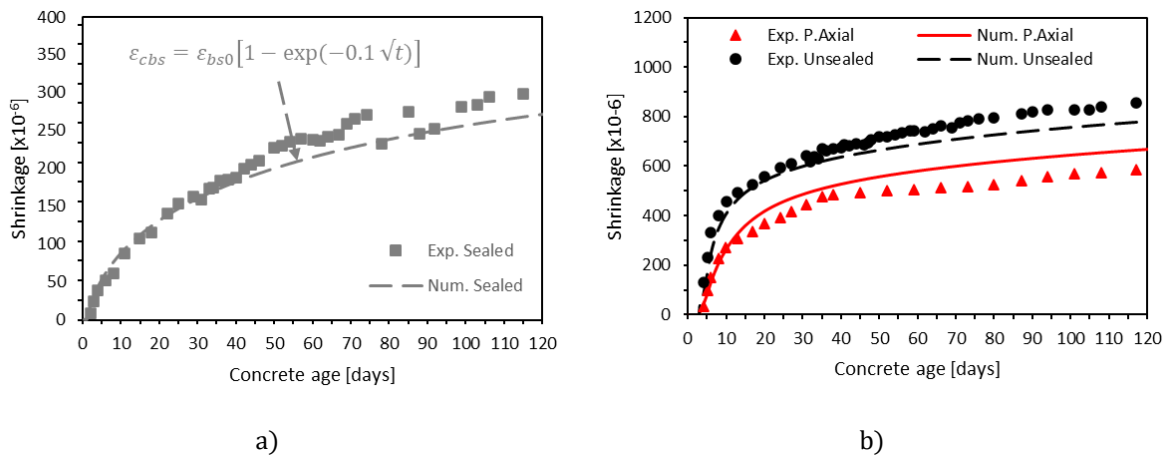


Fig. 112 - Numerical vs experimental data on prisms: a) basic shrinkage; b) total shrinkage.

Fig. 112a) shows the basic shrinkage equation used in the present study. The parameter ϵ_{bs0} is presented in Table 19. The results show a good agreement between the numerical and experimental data, despite some oscillations in the experimental data after 40 days. The final experimental measurements of basic shrinkage at 120 days show an experimental basic shrinkage strain of approximately $\sim 300 \mu\epsilon$. Fig. 112b) shows good agreement in total shrinkage simulation over the first 40 days for both unsealed and prismatic axial specimens. After 40 days, the experimental shrinkage in the unsealed specimen tends to

be higher than the numerical results, whereas the experimental shrinkage in the prismatic axial specimen is lower than the numerical results. The total shrinkage in the axial drying prisms (P. Axial) reaches $\sim 500 \mu\epsilon$, and in unsealed prisms reaches $\sim 800 \mu\epsilon$.

The basic shrinkage values are higher than expected for an ordinary concrete mixture, with a strength class of C30/37 and/or a water-to-cement ratio of 0.45. This occurs because the cement content by cubic meter of the present shortcrete mix is relatively higher than expected for a concrete with a strength class C30/37 (e.g. the concrete studied in Chapter 4.1.2 has a mean compressive strength of ~ 50 MPa with a cement content less than 400 kg/m^3). The design of shortcrete mixtures seems to increase the amount of cement and water in the mixture at the cost of decreasing the aggregate content. Such an approach may justify the observed basic and total shrinkage results. The numerical simulations provide a relatively good agreement with the experimental data. Nevertheless, the THM framework was developed to investigate drying mechanisms in mixtures where the basic shrinkage and self-desiccation represent a small share of the total shrinkage. A limitation of the present model is the simplifications regarding the microstructure evolution in the moisture transport. For the present case study, the P. Axial prisms may have developed a more sophisticated microstructure than the unsealed prism, due to slower drying mechanisms in the early ages. These differences in microstructure may explain the slower long-term drying in the axial drying prism (P. axial) compared to the unsealed prism. To improve the numerical simulations of the present case study, further investigations of the self-desiccation model and microstructure evolution effects on the hygral model are recommended as future work.

4.1.3.3 Numerical simulation of the unrestrained ring test

The numerical simulation of the unrestrained ring test is performed considering the material model used in the simulation of the prisms. The same staggered THM framework is employed in the numerical simulation of the unrestrained ring. Fig. 113 shows the finite element mesh used in the thermo-hygro-mechanical analysis of the unrestrained ring.

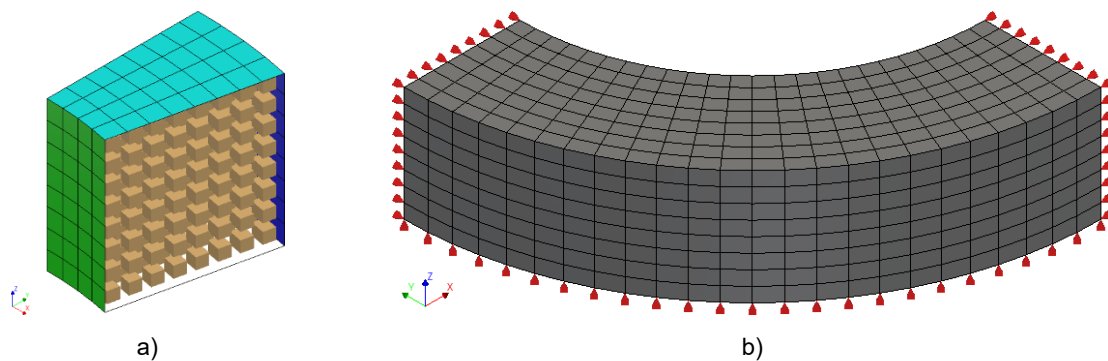


Fig. 113 – Finite element mesh for the numerical simulation of the unrestrained ring: a) thermo-hygral analysis; b) mechanical analysis.

The finite elements are $9.5 \text{ mm} \times 9.375 \text{ mm}$ in the ring cross-section and vary in the circumferential direction between $\sim 10 \text{ mm}$ for the inner and $\sim 15 \text{ mm}$ for the outer radius. Two drying configurations are considered for the unrestrained ring: top and bottom drying (ring TB), where moisture loss occurs through the top and bottom surfaces, maintaining the same surface-to-volume ratio as the axial drying

prism, and radial drying (ring Rad.), where moisture loss occurs through the outer radius surface. Shrinkage results are evaluated at three locations: the outer radius (outer), mid-radius (mid), and inner radius (inner), using the gauge points identified in Fig. 109. The numerical results for the outer and inner locations are considered at the top surface in the interior nodes of the outer and inner finite elements (nodes connected to other FE, i.e. at a distance of ~ 15 mm of the outer edge and ~ 10 mm of the inner edge), instead of the nodes at the edge of the finite element mesh. This approach is justified because the gauge points' locations are better represented by the deformation near the surface rather than the deformation at the surface, which is strongly affected by the deformations resulting from microcracking. Fig. 114 shows the comparison between the experimental and numerical results of the unrestrained ring for top and bottom drying and radial drying.

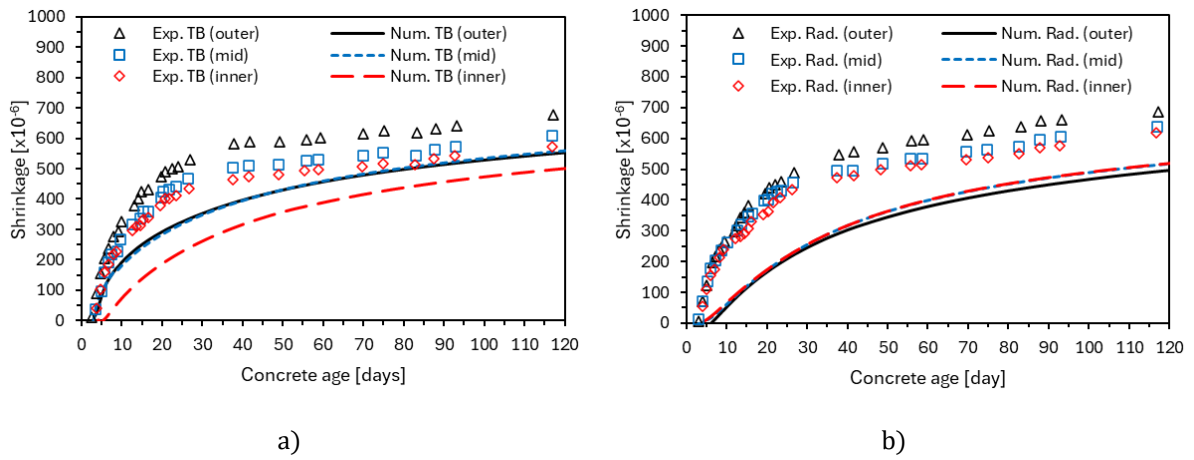


Fig. 114 - Numerical simulation of the unrestrained ring test.

The numerical results for both analyses are lower than those of the experimental data. One possible explanation for the discrepancy between the numerical and experimental results is related to the sealing of the ring specimen. The ring specimens present more complex geometry than the prismatic specimens, raising concerns about the effectiveness of the sealing adherence. Additionally, there is no information on the permeability, saturation degree or sealed conditions applied to the polystyrene cylinder shaping the inner part of the ring specimen. Therefore, moisture transport may occur through leaks on the sealed surfaces or by moisture transference at the interface between the concrete and the polystyrene cylinder. To investigate this issue, additional analyses were performed considering moisture transfereces through the sealed surfaces at a very slow pace. The following boundary conditions were considered for the previous sealed surfaces:

- in the top and bottom drying test, for the green surface in Fig. 113b), it was assumed $\eta_e^* = 1 \times 10^{-9} \text{ m s}^{-1}$ and for the dark blue surface in Fig. 113b), it was assumed $\eta_e^* = 5 \times 10^{-9} \text{ m s}^{-1}$;
- in the radial drying test, for the green surface in Fig. 113b), it was assumed $\eta_e^* = 1 \times 10^{-9} \text{ m s}^{-1}$ and for the light blue surface in Fig. 113b), it was assumed $\eta_e^* = 5 \times 10^{-9} \text{ m s}^{-1}$.

The exposed surfaces assume the surface emissivity coefficient values presented in Table 19 and used in the first analysis. Fig. 115 presents the results considering slow drying through the sealed surfaces.

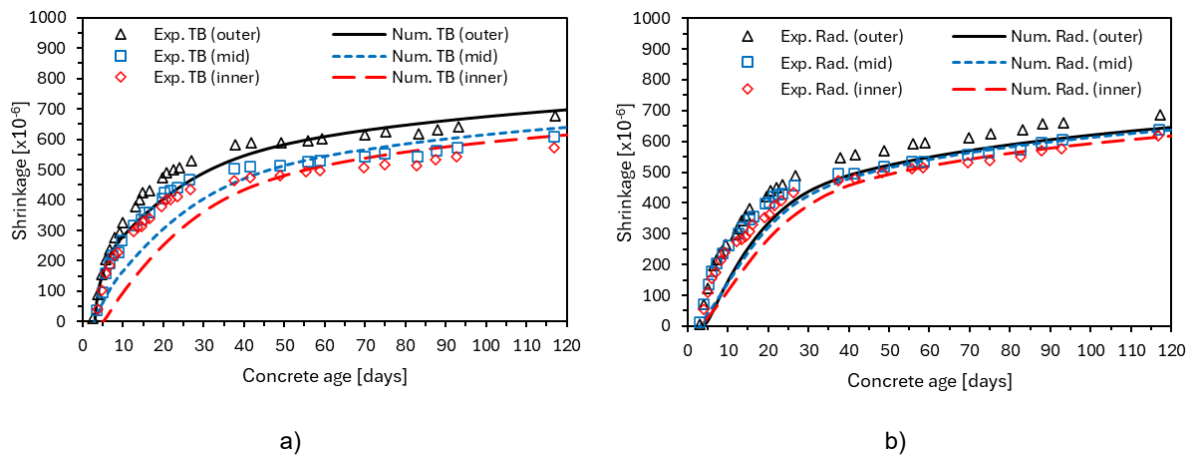


Fig. 115 - Numerical simulation of the unrestrained ring test considering small leaks in the sealing.

The comparison between experimental and numerical results shows improvements in the numerical simulation, strengthening the previous assumptions of the possible moisture loss through the considered surfaces. Fig. 115a) shows that the strain evolution at the outer radius presents higher evolution than at the inner surface. This occurs because after drying exposure, the top surface is subjected to microcracking, leading to substantial differences in the strain measurements at the different gauge locations in the top surface. In contrast, Fig. 115b) shows the strain evolution for all the measurement points to present similar values, with minor differences. This occurs because microcracking is reserved for the outer circumference surface in this drying configuration, and the measurements are all performed at the top surface. The results show that the Ring TB presents higher strain evolution in the early ages, while the Ring Rad experiences a small strain evolution rate at the early ages but higher rates in the long term.

The present findings show the importance of the surface-to-volume ratio and the shape factor in the evolution of shrinkage strains and capacities of the pointwise THM model in capturing this behaviour despite challenges in the numerical simulations. Additionally, the use of numerical simulations allowed for identifying possible moisture transport loss not initially accounted for in the experimental tests, which may be associated with sealed conditions or the moisture transferences through the polystyrene cylinder. Further investigations are required to improve the numerical simulations of shortcrete mixtures and applications of the pointwise THM model in the numerical simulation of similar experimental tests.

4.1.4 NUMERICAL SIMULATION OF THE RING TEST

The pointwise THM model is used to model the concrete behaviour in the restrained shrinkage ring tests under two distinct drying conditions, namely, top and bottom drying and radial drying. The models were calibrated using data from an extensive round-robin testing programme, which involved measurements of the time-dependent properties of a specific concrete mix. Experiments and simulations accounted for the evolution of cement hydration, moisture diffusion, mechanical and viscoelastic properties and

fracture. The modelling approach was validated using results from an unrestrained shrinkage prism test and a restrained shrinkage ring test under top and bottom drying. Insights were obtained for the behaviour of restrained concrete rings by comparing the numerical results obtained in the numerical simulation of the two distinct drying conditions.

4.1.4.1 Materials, experimental data and input parameters

The materials employed in the present case study and methods adopted in the experimental characterization of the employed materials were part of the extended round-robin testing (RRT+) programme of the COST Action TU1404 “Towards the next generation of standards for the service life of cement-based materials and structures” [257] and have been described in other publications [225, 258, 259].

The experimental data utilised for the numerical simulations of the ring tests encompassed the determination of compressive and splitting tensile strength development, elastic modulus development, creep, drying and autogenous shrinkage evolution, heat of hydration tests at different temperatures and the ring test results.

4.1.4.1.1 Tensile strength

The evolution of the strength properties of the concrete was experimentally assessed in [258, 259]. In the pointwise THM model, the tensile strength evolution is simulated through a curve fit of Equation (3.86) to the experimental data. The best curve fit was achieved using the parameters $f_{ct,28} = 4.5$ MPa, $n_{fct,1} = 0.25$, $n_{fct,2} = 0.75$ and $n_{fct,3} = 0.65$ in Equation (3.86). Fig. 116 illustrates the experimental splitting tensile strength results and the tensile strength curve used in the numerical modelling.

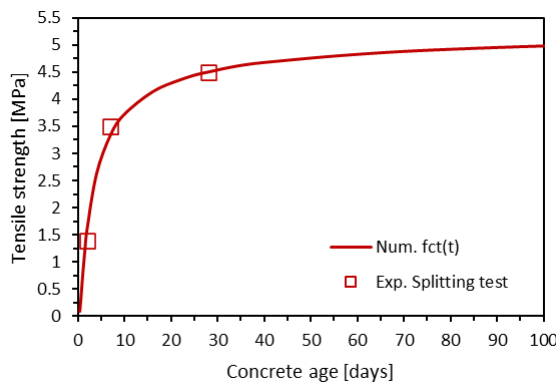


Fig. 116 – Spitting tensile strength development and best-fit curve of the tensile strength used in the numerical modelling using Equation (3.86).

4.1.4.1.2 Modulus of elasticity and creep

Experimental results for the evolution of elastic modulus and basic creep were also provided as part of the RRT+ programme, which collaborated with the EDF VeRCoRs project [260]. The concrete used in the COST Action TU1404 project was designed to be the same in proportions and materials as the concrete used in the EDF VeRCoRs project so that more data on the same concrete is generated. A small difference in CEM I used was observed, with that used on VeRCoRs reportedly having higher C₃A content than the one used by TU1404.

Static elastic modulus was measured on standard concrete cylinders, whilst the time-dependent evolution of the elastic modulus since casting was also measured using the EMM-ARM method [53].

Basic creep tests were performed as part of the VeRCoRs project on cylindrical concrete specimens of 160 mm diameter and 1000 mm length (12 MPa uniaxial stress applied at 1 and 3 days after casting). The creep model used in the numerical simulations follows the calibration process employed in Chapter 4.1.2.3. The creep model is given by Equation (4.4). The creep model parameters are initially determined based on the formulations provided by model B4. The calibration parameters c_i are calibrated to provide the best curve fit to the experimental data. In the absence of drying creep test results for these loading ages, drying creep was estimated based on the drying creep model used by Kanavaris et al. [225]. The parameters used in Chapter 4.1.2.3 were assumed for the RMPS. Table 21 shows the parameters used in the numerical simulation.

Table 21 - Creep model parameters used in the numerical simulation of concrete.

Parameter	Value	Parameter	Values
q_1	$20.19 \times 10^{-6} \text{ MPa}^{-1}$	-	-
q_2^*	$167.00 \times 10^{-6} \text{ MPa}^{-1}$	c_2	0.2
q_3^*	$7.89 \times 10^{-6} \text{ MPa}^{-1}$	c_3	1
q_4^*	$8.30 \times 10^{-6} \text{ MPa}^{-1}$	c_4	0.6
c_0	0.005	α_e	5
k_1	$1.10 \text{ MPa} \cdot \text{K}^{-1}$	$\alpha_r = \alpha_s$	0.1
b_{RMPS}	5×10^{-4}	$Q_e = Q_s$	$22.48 \text{ kJ} \cdot \text{mol}^{-1}$
p_{RMPS}	1.4	Q_r	$41.57 \text{ kJ} \cdot \text{mol}^{-1}$

The numerical analysis simulates the modulus of elasticity through the creep model. To compare the effectiveness of the creep model in the simulation of the experimental modulus of elasticity, creep tests are performed with a very short duration of 0.01 days (=14.4 min). Fig. 117a) shows the comparison between the numerical and experimental modulus of elasticity. The total creep is compared to the one used by Kanavaris et al. [225]. Fig. 117 b) shows the basic creep compliance adjustment to the experimental data and the total creep for the approaches considered.

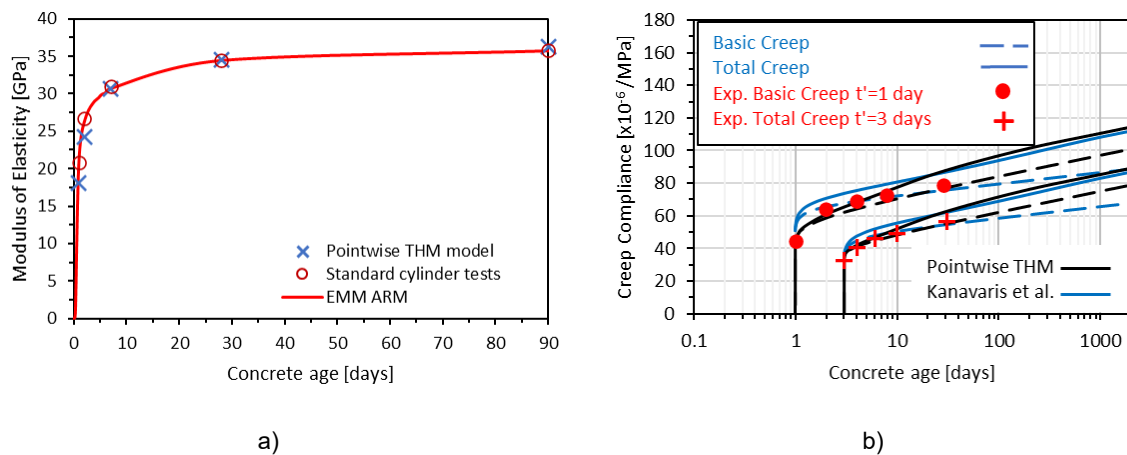


Fig. 117 – Experimental results and fitting curves for: a) modulus of elasticity; b) creep compliance.

The basic creep model demonstrates good agreement with the experimental results, although it predicts greater long-term flow strains compared to those assumed using the Kanavaris et al. [225] creep model. In contrast, the long-term total creep results (including drying creep) exhibit magnitudes similar to the experimental ones, with only minor discrepancies observed following the load application. In the current drying creep tests, drying was initiated concurrently with the application of loading.

4.1.4.1.3 Restrained shrinkage test

A 70 mm thick concrete ring was cast around a 25 mm thick steel ring (with elastic modulus of 190 GPa and Poisson's ratio of 0.30) in a plywood-based mould and left to cure totally sealed for 24 hours in a controlled environment (20 °C and 50% RH). The outer mould and horizontal plate were removed after 24 hours, and the outer circumference was sealed with a double-layer aluminium foil tape, thus permitting water evaporation only from the top and bottom surfaces. The test was conducted for 111 days at 20 °C and 50% RH, whilst no macro-crack occurrence was witnessed. This setup for the ring test also included a notch to assist with stress localisation and quicker crack occurrence. Šmilauer et al. [258] show that the notch has a negligible effect in the results of the present ring test. Fig. 118 shows the ring test dimensions and layout.

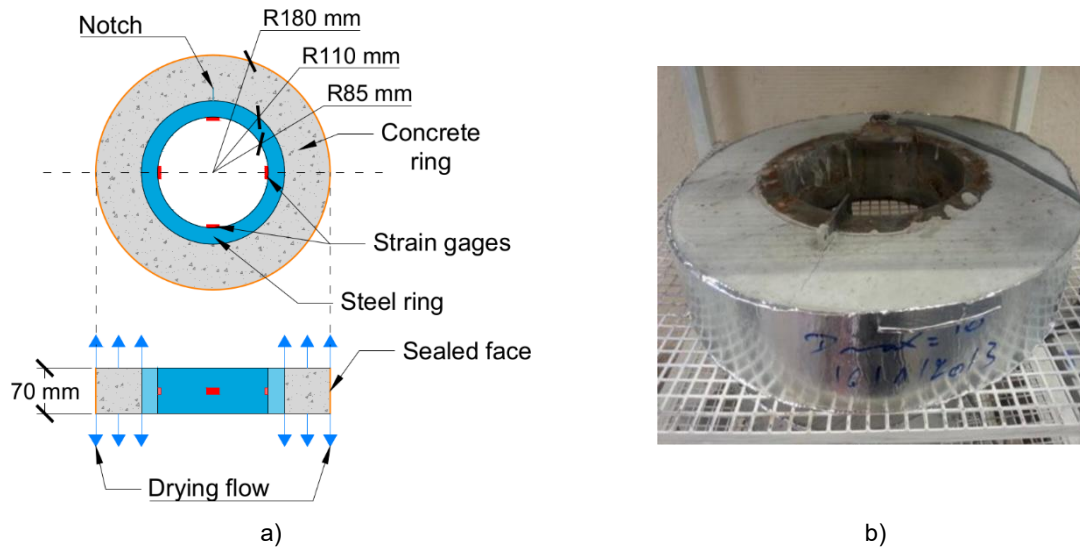


Fig. 118 – a) schematic representation of the ring test; b) an image of the ring test performed as part of the COST Action TU1404 RRT+.

4.1.4.2 Thermo-hygral model parameters

The cement hydration properties must be specified for the thermal analysis. The cement hydration is simulated considering the Affinity model given by Equation (2.7). The thermal properties of concrete were determined from experiments conducted by Azenha [5]. Fig. 119 shows the function $f(\alpha)$ for the numerical simulation of cement hydration using Equation (2.7).

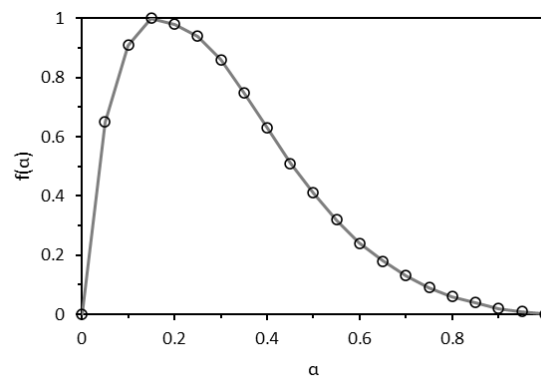


Fig. 119 – Function $f(\alpha)$ for the numerical simulation of cement hydration using Equation (2.7).

The moisture diffusion parameters required by the hygral model were selected according to previously conducted tests on a concrete with similar relevant characteristics (w/c, cement type and water content, drying kinetics) to those investigated at COST Action TU1404. The input parameters required for the thermo-hygral simulations were derived from experimental results and adapted from Kanavaris et al. [225] to the current thermo-hygral model. Table 22 shows the input parameters used in the thermo-hygral simulations.

Table 22 – Input parameters used for the THM simulations.

Model	Parameter	Value
Thermal model	k	$2.6 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$
	ρc	$2400 \text{ kJ} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$
	$h_{cr,free}$	$10 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$
	$h_{cr,moulded}$	$5 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$
	T_{env}	20°C
	E_a	$33.3 \text{ kJ} \cdot \text{mol}^{-1}$
	A^*	$3.118 \times 10^6 \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-1}$
	Q_{pot}	$3.55 \times 10^6 \text{ J} \cdot \text{kg}^{-1}$
Hygral model	α_0	0.05
	D_1	$2.71 \times 10^{-10} \text{ m}^2 \cdot \text{s}^{-1}$
	h_c	0.85
	n_h	6
	η_e^*	$5.10 \times 10^{-9} \text{ m} \cdot \text{s}^{-1}$
	$k_{sh}(\text{dKwak}) = \varepsilon_{sh,ult}$	$696 \times 10^{-6} (576\mu + 120\mu)$
	ε_{bs0}	120.00×10^{-6}
	α_h	10

4.1.4.3 Simulation of free shrinkage

The setting time for the numerical analysis was determined based on the derivative of the Modulus of Elasticity evolution through EMM-ARM tests as presented by [225]. The setting time is established as the instant when the derivative of the modulus of elasticity reaches half of the maximum value. The modulus of elasticity is simulated by the Carette and Staquet [54] equation (see Equation (2.23)). Fig. 120 shows the method adopted to determine the setting time.

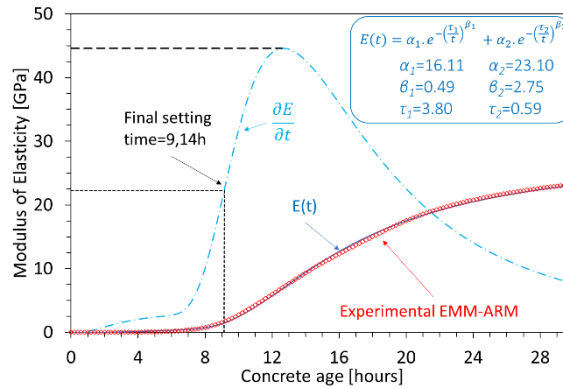


Fig. 120 – Setting time determination through the modulus of elasticity results.

The obtained setting time was 9.14 hours. To simplify the numerical inputs, the setting time used in the numerical model was considered equal to 9.5 hours.

Drying shrinkage tests were performed on 70 mm×70 mm×400 mm prisms. Four drying shrinkage tests were performed, with a duration of 120 days. The four prisms were exposed to drying (50% RH and 20 °C) at different ages, corresponding to 1, 2, 7 and 28 days after casting. Basic shrinkage was also measured from 1 to 64 days on a 70 mm × 70 mm × 280 mm specimen. The shrinkage and hygral model are calibrated based on the shrinkage tests of the prisms. The hygral analysis is performed first and is two-dimensional across the cross-section of the drying prism. The hygral analysis is followed by

the mechanical analysis, for which one-eighth of the prism was modelled (one-fourth of the cross-section and one-half of the length of the prism), taking advantage of symmetry. The numerical analysis is performed for the drying specimen at one day and at 28 days. The objective is to investigate the effects of the drying time initiation on the numerical results. Fig. 121 a) shows the adjustment of the basic shrinkage equation to the experimental data. Fig. 121 b) shows the comparison between the experimental shrinkage tests and the numerically simulated shrinkage for the different drying initiation times using the parameters in Table 22.

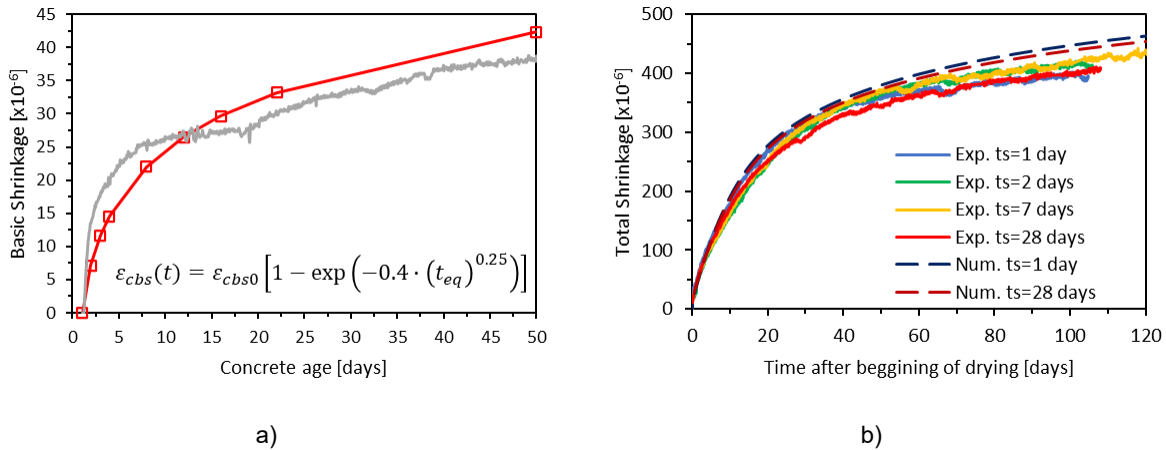


Fig. 121 – Comparison of experimental vs numerical results for: a) basic shrinkage; b) the free drying shrinkage tests.

Kanavaris et al. [225] used the direct input of the basic shrinkage in the numerical simulations. The present THM framework simulates the basic shrinkage through the self-desiccation model presented in Chapter 3.6.2.1. Therefore, the basic shrinkage given by equation (2.68) is adjusted to provide the best fit to the experimental data. Fig. 121a) shows that equation (2.68) provides slightly less basic shrinkage in the early ages but slightly higher basic shrinkage strains in the long term. In Fig. 121 b), all the experimental drying shrinkage tests show similar shrinkage evolution despite different times for drying initiation. Generally, the correlation between numerical and experimental results is satisfactory, indicating that the parameters adopted for the simulation of drying kinetics are deemed appropriate for this study. Numerical simulations of free drying shrinkage tests were conducted for two different drying initiation ages: 1 day (Num. ts=1 day) and 28 days (Num. ts=28 day). The results showed only minor differences, primarily attributable to the contribution of basic shrinkage in the measurements for the tests where drying started at 1 day.

4.1.4.3.1 Simulation of the ring test under top and bottom drying

The ring test under top and bottom drying is simulated first since experimental results are available for experimental and numerical comparison. In the numerical model, the notch identified in Fig. 118 a) was simulated by reducing the tensile strength at 28 days to $f_{ct,28} = 3.75$ MPa for two finite elements at the top surface. The weak FE were selected in order to avoid cracking localisation near the symmetry planes. The cracking model used in the pointwise THM analysis was the single-crack model (Chapter

3.8.2.6) with the Hordijk tension softening model. Fig. 122 shows the finite element meshes used in the thermo-hygral and mechanical analyses.

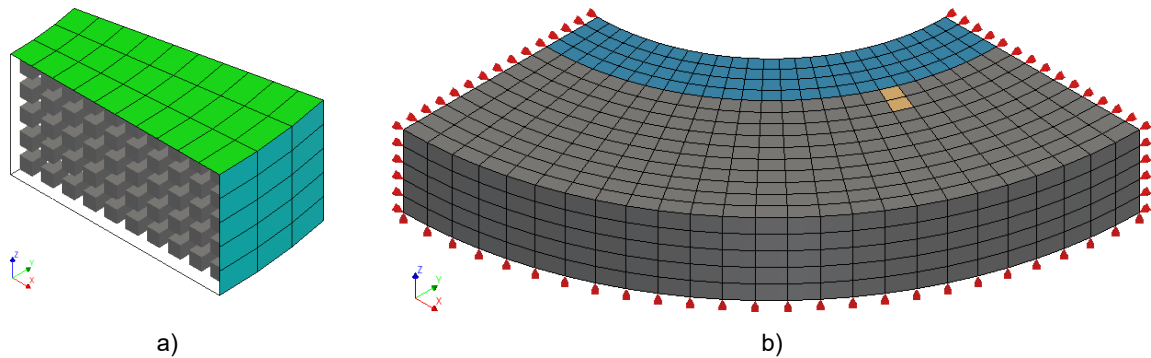


Fig. 122 – Meshed model for a) thermo-hygral analysis (3D slice of the concrete ring) and b) mechanical analysis (1/4 and 1/2 of the ring's area and thickness, respectively, due to symmetry).

The mechanical properties of concrete were presented in Chapter 4.1.4.1. The elastic properties of steel adopted were the standard properties used in structural analysis, while a perfect bond between steel and concrete was assumed.

The thermo-hygral problem is solved first and is followed by the mechanical analysis. Fig. 123 shows the temperature evolution and relative humidity distribution obtained in the thermo-hygral analysis.

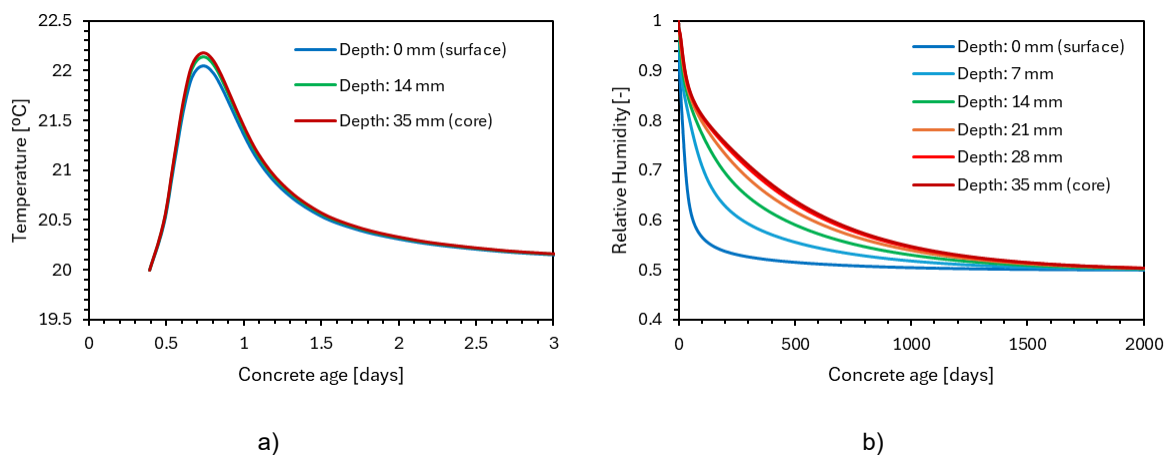


Fig. 123 – Numerical simulation: a) temperature development and b) relative humidity profiles in the ring test under top and bottom drying.

The numerical results show that the heat generated during the early stages of hydration leads to a maximum temperature of 22.25 °C reached at approximately 0.8 days after casting, and corresponds to a total temperature rise of approximately 2.25 °C, which can be neglected. This early age temperature rise was not captured in the test conducted as part of RRT+, as no temperature monitoring was involved. It should be noted that the thermal analysis results for the ring tests are very similar regardless of the drying direction employed, so they are shown only for top and bottom drying, but they also apply to radial drying. The results from the numerical thermal analysis also suggest that no thermal gradients are occurring in the concrete for this particular ring that was simulated; while it is recognised that this may not be the case for concrete rings with different thickness and different mix proportions (e.g., different cement types and contents, w/c, aggregate types) [91].

Fig. 123 b) shows the results of the hygral simulation across the thickness of the concrete ring from the top or bottom surface until the core of the element, following the symmetrical nature of the problem. A moisture gradient develops across the height of the concrete ring, with the top and bottom surfaces drying the quickest. In the present numerical simulation, the moisture equilibrium between the concrete ring and the surrounding environment in the concrete ring is achieved at approximately 2000 days (~5.5 years), with very small gradients observed after 1500 days. The relative humidity drop is expected to develop more slowly in the concrete ring than in the drying shrinkage prisms due to the difference in the exposed surface to concrete volume ratio for these two specimens: $62.1 \text{ m}^2/\text{m}^3$ for the prism and $28.6 \text{ m}^2/\text{m}^3$ for the ring under top and bottom drying.

As a strain gauge in the actual experiment is attached at the mid-height of the inner circumference of the steel perpendicularly to the vertical direction, the steel strain recorded (hoop steel strains) can be directly compared with the one simulated and serves as model validation. Fig. 124 shows the inner steel strain evolution for different time scales with and without considering cracking effects in the analyses.

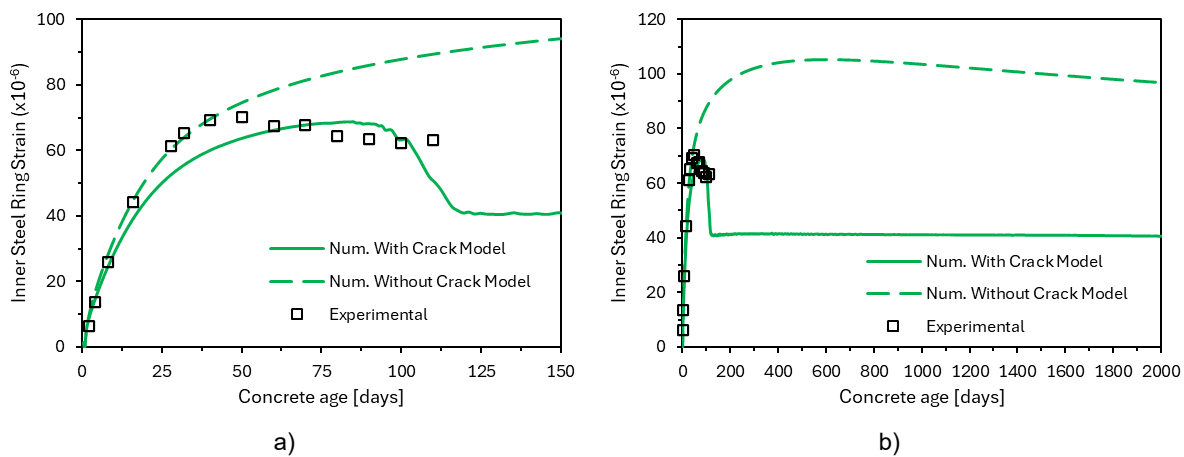


Fig. 124 – Comparison of experimental steel strains and steel strains obtained from numerical simulations with and without cracking effects for a) 150 days and b) 2000 days since casting.

There is a generally good agreement between experimental strain recordings and numerical predictions, particularly for the model considering cracking; however, the peak in steel strain and the loss in strain were not exactly matched. After 40 or 50 days since casting, an unexpected drop in steel strain started to occur in the experiment, which was not particularly anticipated as the specimen did not reportedly exhibit any macrocracking throughout the test duration. The numerical analysis considering cracking follows the trend of the recorded steel strain, suggesting that predominantly superficial microcracking may explain the drop in steel strain.

This behaviour becomes more evident if the results from the model without and with cracking are compared. In the former, there is a continuous accumulation of strain until reaching a plateau after approximately 500 days, whilst in the latter, the drop in steel ring strain can be simulated due to cracking progression. The numerically predicted steel strain with cracking continues to drop as drying evolves, until a relatively abrupt drop in strain is observed, signalling the formation of a macrocrack.

The numerical results for the analysis with the cracking model in Fig. 124 show the inner steel strains at the cross section where the macrocrack is formed. Fig. 125 shows the hoop steel strains for the modelled steel ring.

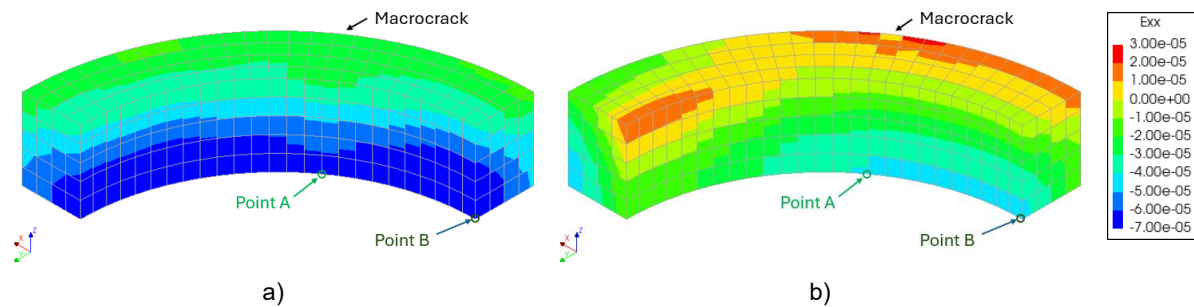


Fig. 125 –Hoop steel strains obtained from numerical simulations: a) 100 days; b) 150 days.

The steel strains vary depending on the position where they are measured. Fig. 126 compares the evolution of the steel strains for points A and B identified in Fig. 125.

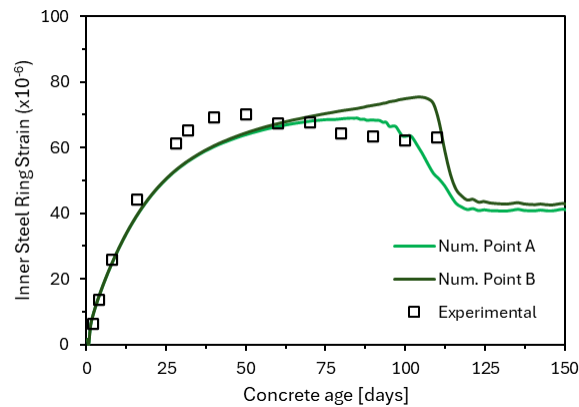


Fig. 126 – Hoop steel strains evolution at two different positions.

As the distance to the cross-section where the macrocrack is located increases, the steel hoop strain also increases during the process of crack formation. The highest differences occur immediately before the localised crack opens (~110 days). In the experiment, no crack localisation was observed during the measurement period. Therefore, the distance between the position of measurements and the section of a potential macrocrack is unknown. A further understanding of the concrete ring behaviour can be reached in an experiment if the strain is measured in various positions along the steel inner circumference.

Looking further into stress development over time will assist in understanding thermal but mainly hygral effects and changes in residual stress development before and after moisture and temperature equilibrium in the restrained concrete ring. Fig. 127 shows the development of stresses across the height of the rings at the inner and outer circumference as well as mid-section

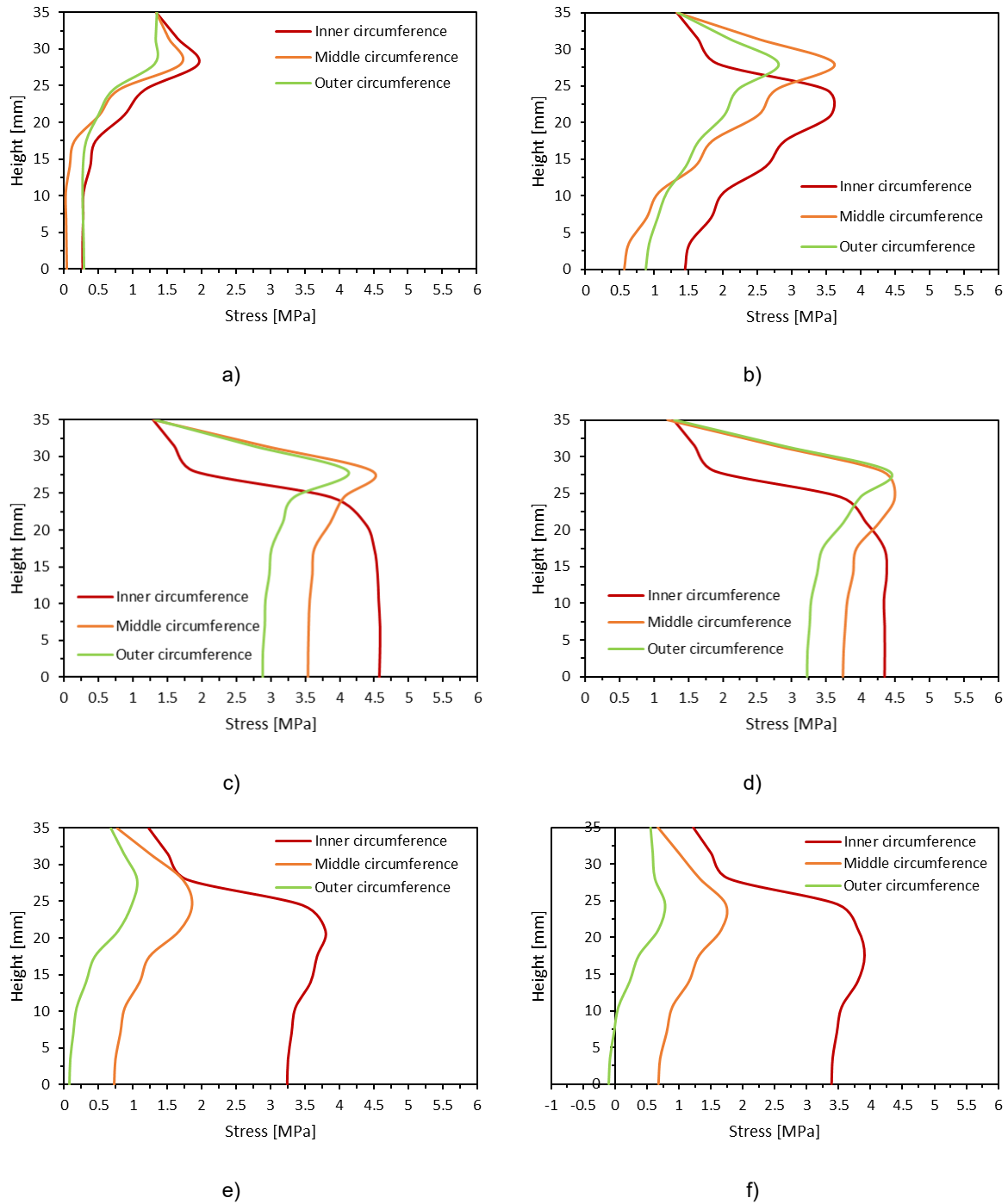


Fig. 127 – Stress profiles through the (full) height of the concrete ring at different lengths and different time instances: a) 3 days; b) 14 days; c) 60 days; d) 100 days; e) 140 days; 180 days;

The behaviour at early ages is somewhat anticipated, i.e. an increased stress generation at the top surface of the concrete due to accelerated water evaporation at this point, whilst in mid-height stresses are still relatively low. As drying continues, high stresses descend towards the mid-height of the concrete ring, see Fig. 127 (b,c,d). The maximum tensile stresses at the top and bottom surfaces reach values of 2 MPa and 3.5 MPa at 3 and 14 days, respectively, resulting in superficial microcrack initiation. Microcracking

progressively relaxes and stabilises the stresses generated, while maximum stress propagates towards the mid-height of the concrete ring. As drying evolves, a potential macrocrack, or through-crack, starts to form near the steel-concrete interface and consequently develops at full width at approximately 120 days since casting, after which strain is relieved and a stabilised stress state is observed, see Fig. 127 (e,f).

Fig. 128 shows the evolution of principal strain vectors at four distinct time instances.

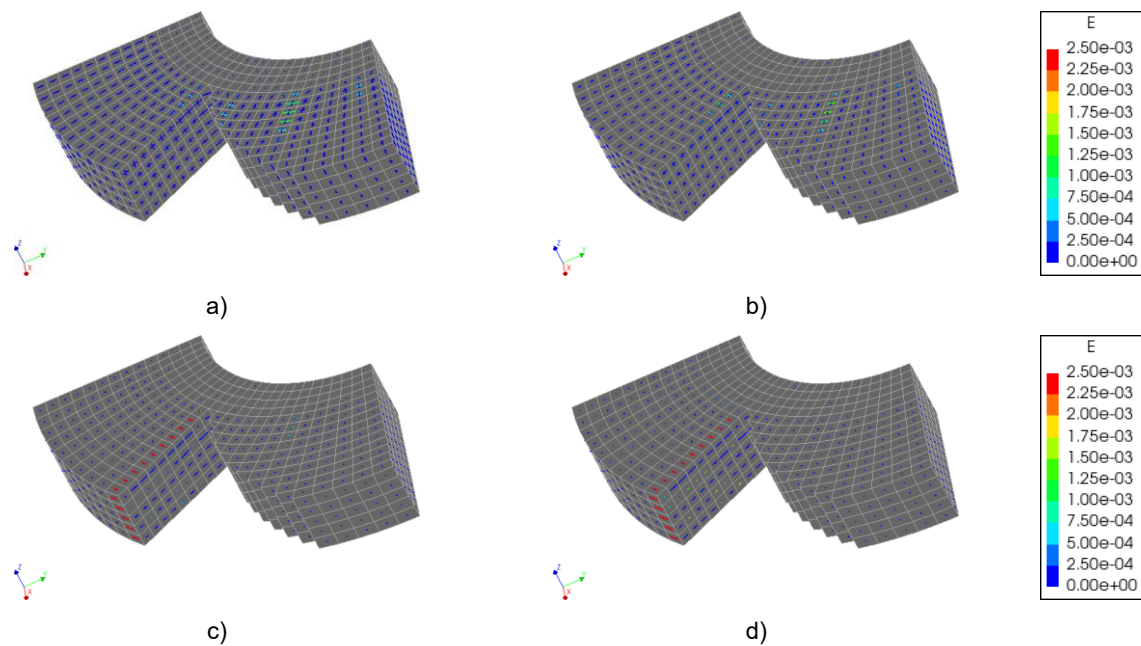


Fig. 128 – Concrete damage (principal strain vectors) at different instants of time (top and bottom drying): a) 60 days; b) 100 days; c) 140 days; d) 1500 days since casting (some FE not shown to allow viewing the internally developed damage).

The principal strain vectors are displayed up to mid-height of $1/4^{\text{th}}$ of the concrete ring due to symmetry (steel ring also included), whilst a part of them is truncated to show numerically calculated strains within the cross-section of the concrete ring. The experimental test duration was 120 days, and no macrocracking or through-cracking was observed. In the numerical simulation, it is shown that a macrocrack forms at approximately 110 days after casting. The calculated degree of restraint in the system according to [261] is approximately 70%. As indicated in [262], the degree of restraint of a ring test setup should be determined based on the anticipated shrinkage of the cementitious material to be investigated. In this case, the combination of the concrete's shrinkage and degree of restraint in the system was not enough to induce macrocracking in the specimen within a practical time frame. The crack width estimated from the simulation varies regarding the location and is approximately ~ 0.05 mm. Nevertheless, the crack width is not a relevant output of the ring test. The numerical results show that, under top and bottom drying conditions, cracking is initiated at the inner circumference of the concrete ring due to the restraint provided by the steel ring.

4.1.4.3.2 Simulation of the ring test under radial drying

The numerical simulation of the ring test under radial drying conditions is performed following the same framework as the top and bottom drying conditions. The material parameters, geometry, thermal boundary conditions, drying initiation and ambient environment conditions are described in Chapters 4.1.4.1 and 4.1.4.2. The only difference regarding the top and bottom ring-test is the drying direction, where in the present case, the exposed drying surface is the outer circumference, while the top and bottom surfaces remain sealed. Notice that radial drying conditions are also recommended by relevant ASTM and AASHTO standards [256, 263]. The simulation methodology is similar to top and bottom drying, with the same model layout, meshes, and assumptions as presented in Section 4.3. The thermo-hygral analysis is performed as a first step. The temperature results due to cement hydration reactions are no different from those under top and bottom drying, shown in Fig. 123 a). Fig. 129 shows the results for the relative humidity distribution under the radial drying conditions, with 0 mm indicating the inner concrete circumference and 70 mm the outer one.

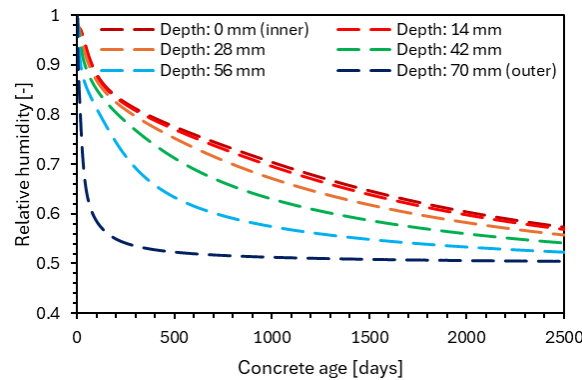


Fig. 129 – Calculated relative humidity profiles under radial drying.

The radial drying configuration produces a more pronounced moisture gradient than top and bottom drying. Drying also takes place at a slower rate than top and bottom drying, whilst the concrete will attain moisture equilibrium with the environment at more than 2500 days (6.85 years) after casting, which is substantially longer than the approximately 2000 days (5.5 years) under top and bottom drying. This behaviour can be attributed to the smaller surface-to-volume ratio for radial drying ($17.7 \text{ m}^2/\text{m}^3$), compared with the surface-to-volume ratio for top and bottom drying ($28.6 \text{ m}^2/\text{m}^3$).

Fig. 130 shows the steel strains at the mid-height of the inner circumference of the steel ring for the crack location, under both radial and top and bottom drying conditions.

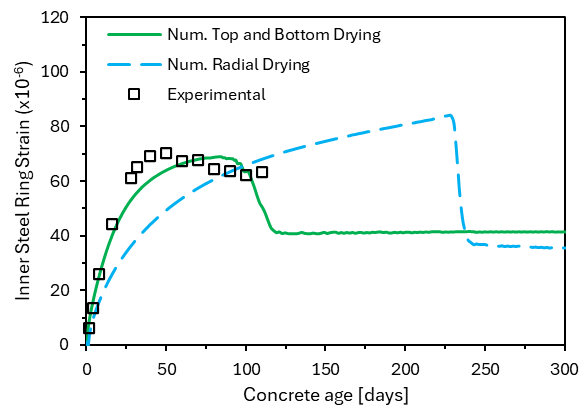


Fig. 130 – Comparison of steel strains obtained from numerical simulation for radial and top and bottom drying conditions.

There are no experimental results under radial drying, but confidence in model validity is built up from simulating the behaviour of the ring test under top and bottom drying adequately with the same approach. The numerical results show that the development of steel strain occurs at a more accelerated rate in top and bottom drying than in circumferential drying. This suggests that stress build-up in the concrete ring occurs more rapidly under top and bottom drying. In the top and bottom drying setups, cracking starts at the steel-concrete interface, while in radial drying conditions, cracking starts in the outer concrete circumference due to the self-restraining effect arising from the moisture gradient across the concrete wall thickness. In this case, stress induced by moisture gradients is more significant than that induced by the steel ring, at least at early ages. After microcracking forms at the outer circumference and subsequent stress relaxation at these locations, microcracks also form at the steel-concrete interface. A macrocrack is formed approximately 230 days, manifested by the sudden drop in steel strain under radial drying. Analysing the overall results, it is possible to conclude that the top and bottom drying conditions can result in quicker cracking manifestation than the radial drying conditions for the given geometry. Fig. 131 shows the stress profiles in the concrete ring at different times.

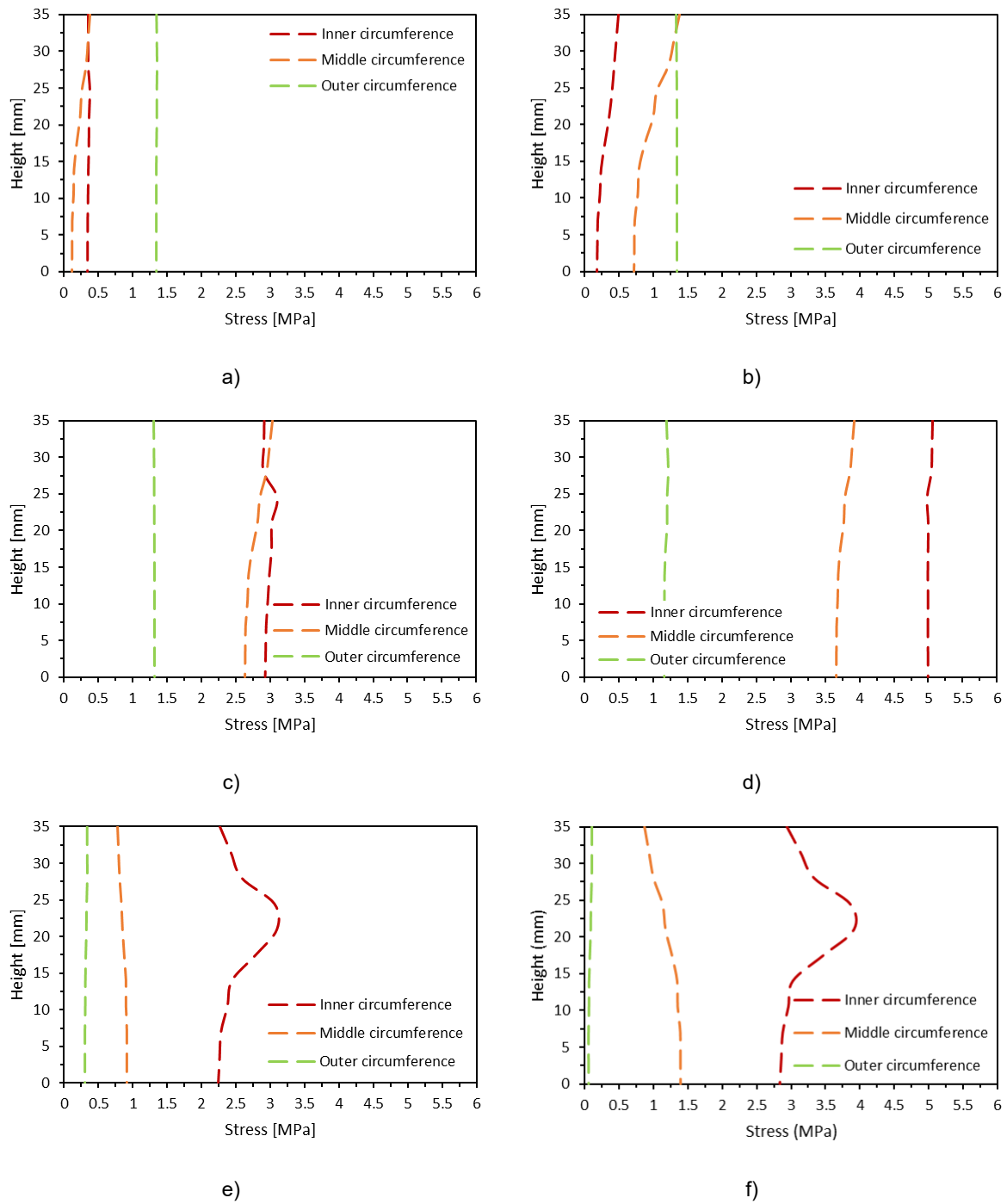


Fig. 131 - Stress profiles through the (full) height of the concrete ring at different lengths and different instants of time for radial drying conditions: a) 3 days; b) 14 days; c) 60 days; d) 180 days; e) 500 days; 1000 days;

The impact of the self-restraining effect at early ages becomes more apparent under radial drying. Maximum tensile stress is initially generated at the exposed concrete surface due to differential shrinkage, i.e. outer surfaces contract faster than the preceding concrete, resulting in a restraint effect greater than the one provided by the steel ring (see Fig. 131 (a)). Notice that in this case, the tensile strength at the outer surface corresponds to the value for 1 day evolution, which corresponds to 1.35 MPa. Once microcracking occurs in the outer circumference, tensile stresses are relaxed at these locations. However, at the inner and middle circumference, stresses continue to increase due to drying

progression (see Fig. 131 (b,c,d)). Microcracking subsequently occurs at the inner circumference, corresponding to the maximum restraint location due to the presence of the steel ring. As drying continues, the stress in the middle area rises until reaching the tensile strength, forming the macrocrack. Once the macrocrack is formed, the middle and outer circumference stresses decrease, while the inner circumference stresses remain relatively higher than the others (see Fig. 131 (f,e)).

Fig. 132 shows the evolution of the principal strain vector at 180 and 1500 days after casting.

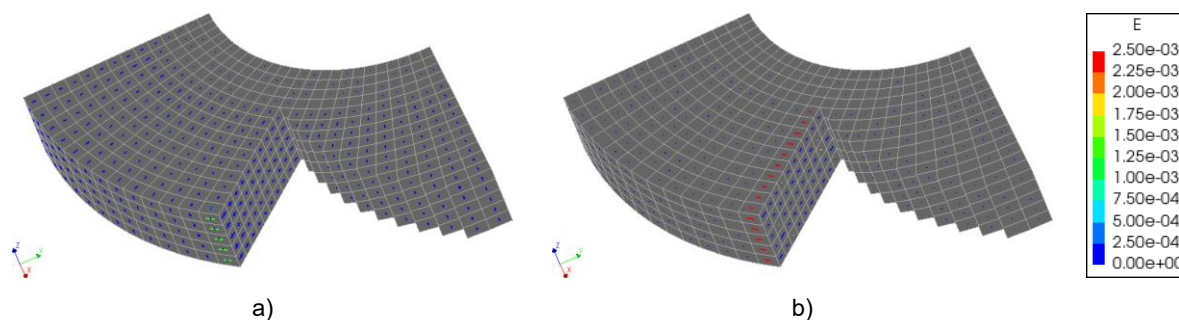


Fig. 132 – Concrete damage (principal strain vector) at different instances of time (radial drying): a) 180 days; b) 1500 days; since casting (some FE not shown to allow viewing internally developed damage).

As previously analysed, microcracking due to moisture gradient initially occurs at the outer circumference. This is then succeeded by microcrack formation in the inner circumference of the concrete ring. In the radial drying conditions, the microcracking manifestation is less pronounced than that under top and bottom drying, where distinct cracks formed at the top surface.

4.1.5 NUMERICAL INVESTIGATION OF DIFFERENT RING TEST GEOMETRIES WITH DIFFERENT DRYING CONDITIONS

4.1.5.1 Different ring test geometries and finite element meshes

Kanavaris et al. [262] conducted a critical review of the ring-test experiment, compiling various ring test geometries reported in the literature. The present study investigates four ring test geometries under top and bottom, and radial drying conditions. The selected geometries include standardised configurations and two experimental setups designed to capture geometric deviations from the standard forms. The first experimental configuration (ExpConf1) features a thin concrete ring coupled with a thick steel ring, while the second (ExpConf2) comprises a thick concrete ring paired with a thin steel ring. The ring geometries considered in the analyses are as follows:

- ASTM, standardised geometries [263];
- AASHTO, standardised geometries [256];
- ExpConf1, experimental ring test geometry [264, 265];
- ExpConf2, experimental ring test geometry [266].

Fig. 133 shows the schematic representation of each of the ring test geometries considered in the numerical analysis.

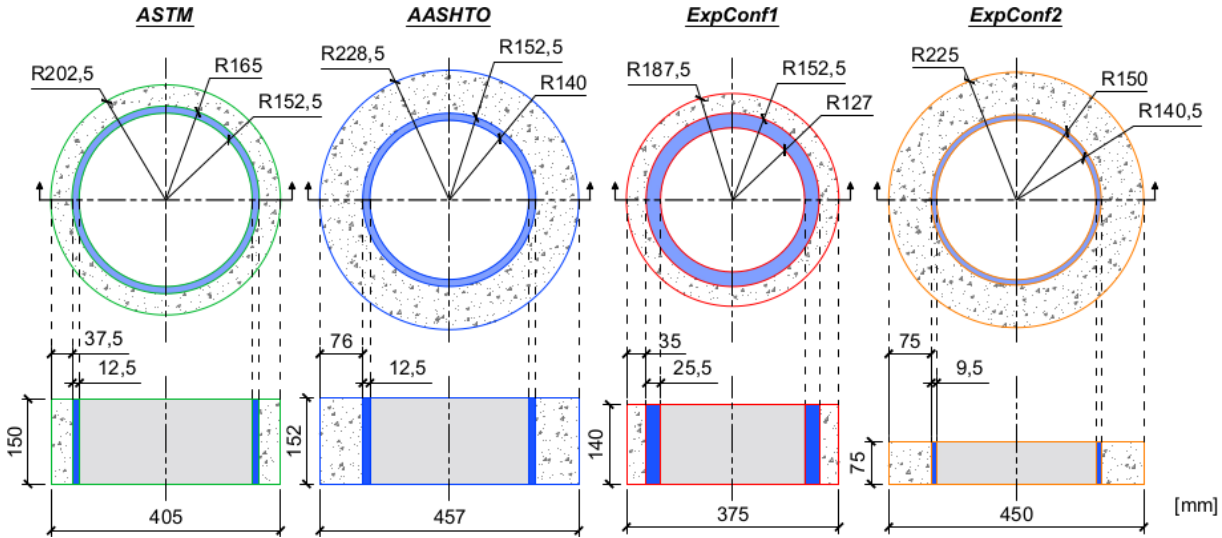


Fig. 133 – Different ring geometries considered in the analyses (dimension in mm).

The different ring-test configurations result in different exposed surfaces and concrete and steel ring volumes. Table 23 presents the concrete and steel volumes, exposed surface area and surface-to-volume ratio for the considered ring-test geometries under different drying conditions.

Table 23 – Exposed drying surface area and surface-to-volume ratio.

Geometry	Drying conditions	Exposed Surface (m ²)	Concrete Volume (m ³)	Exposed Surface / Concrete Volume (m ⁻¹)	Steel Volume (m ³)	Concrete Volume / Steel Volume
ASTM	TB	0.08659	0.006494	13.3	0.001870	3.47
	R	0.1909	0.006494	29.4	0.001870	3.47
AASHTO	TB	0.1819	0.01383	13.2	0.001746	7.92
	R	0.2182	0.01383	15.8	0.001746	7.92
ExpConf1	TB	0.07477	0.005234	14.3	0.003135	1.67
	R	0.1649	0.005234	31.5	0.003135	1.67
ExpConf2	TB	0.1767	0.006627	26.7	0.0006503	10.2
	R	0.1060	0.006627	16.0	0.0006503	10.2

The pointwise THM model is used to investigate the differences between each ring test geometry and drying configuration to determine the respective advantages and disadvantages. The investigation is performed only for one concrete mixture, presented and validated in Chapter 4.1.4. Other mixtures may lead to different results.

The FE meshes were generated to get similar finite-element sizes. The finite-element side is generally close to 7mm, resulting in enough FE to capture the gradients of imposed strains and the variation of stresses and cracking patterns throughout the concrete cross-section. Only 1/8th of the ring-test was modelled (1/4th of the ring and 1/2nd of the height of the ring), taking advantage of symmetry. Fig. 134 shows the FE mesh for each ring configuration for the THM analyses.

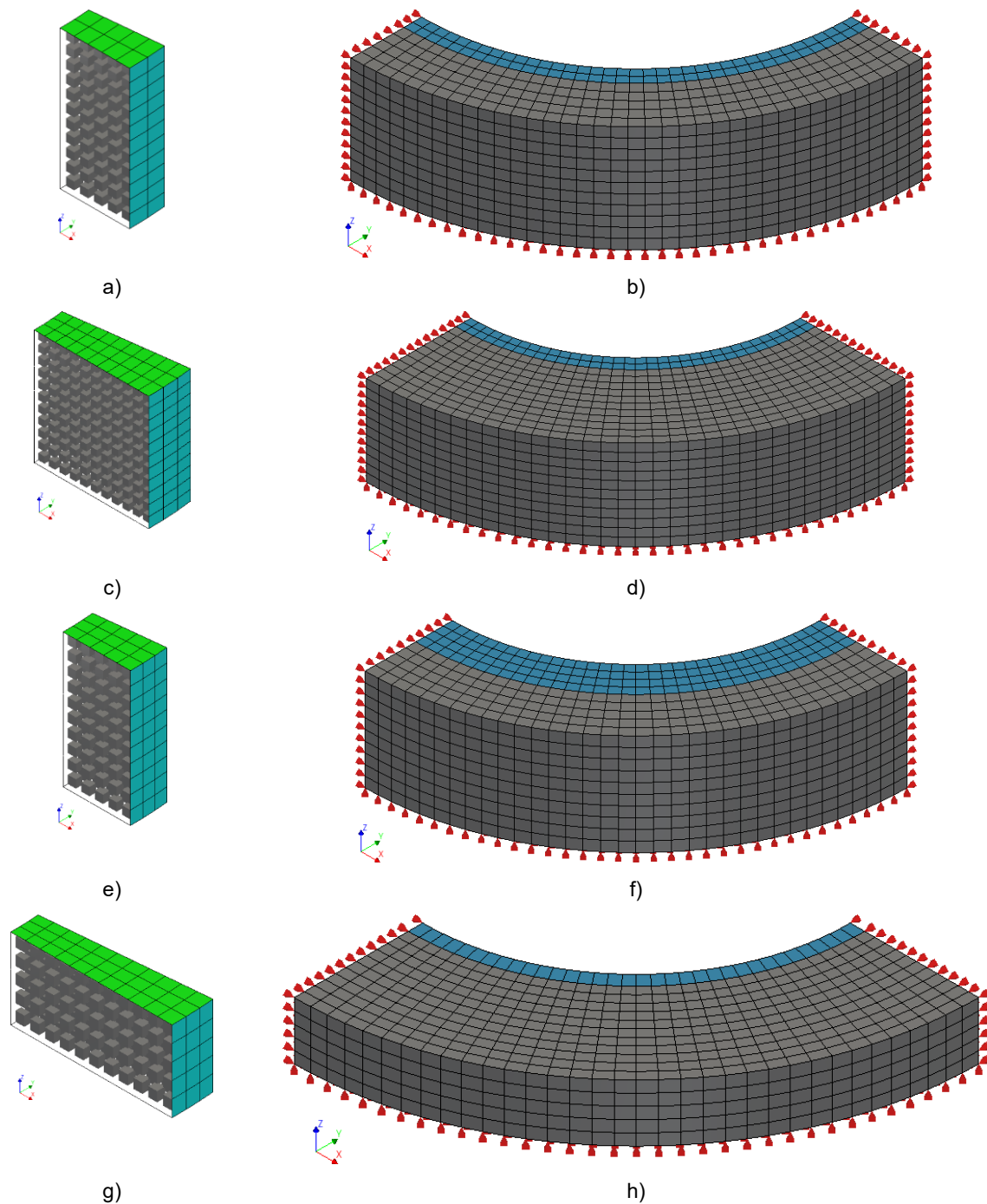


Fig. 134 – FE meshes for each ring configuration: a–b) ASTM: a) thermo-hygral, b) mechanical; c–d) AASHTO: c) thermo-hygral, d) mechanical; e–f) ExpConf1: e) thermo-hygral, f) mechanical; g–h) ExpConf2: g) thermo-hygral, h) mechanical.

4.1.5.2 Numerical results and discussion

4.1.5.2.1 Temperature and potential shrinkage

The temperature history due to cement hydration is investigated for each ring geometry. Fig. 135 a) shows the temperature variation for the different concrete rings geometries. The temperature is presented at the core of the ring element near the steel ring for only one drying configuration (radial drying in the

present case). As shown in Chapter 4.1.4, considerable temperature gradients over the element cross-section are not expected due to the small dimensions of the ring test. The potential drying shrinkage is also investigated for the different ring-test and drying configurations. The potential drying shrinkage is determined based on an average free shrinkage over the element's cross-section. While this approach neglects the internal restraint of concrete due to moisture gradients, it also provides a good comparative tool to assess the drying rate in the different ring geometries. Fig. 135 b) shows the potential drying shrinkage, calculated based on the shrinkage calculation from the moisture field obtained in the hygral analyses, averaged over the concrete cross-section.

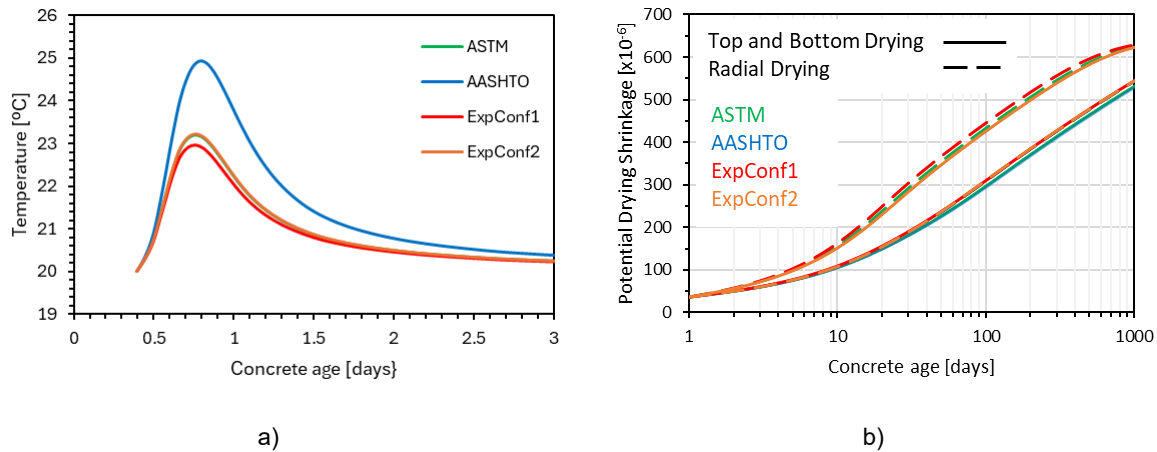


Fig. 135 – a) Temperature evolution; b) Potential shrinkage strains for the different ring test configurations.

The temperature results indicate that the AASHTO ring test configuration exhibits the highest temperature rise, reaching nearly 25°C, whereas the other geometries maintain maximum temperatures around 23°C. This behaviour is expected, as the AASHTO configuration has the most significant concrete volume (see Table 23), while the other configurations have comparable volumes, resulting in similar thermal responses. Despite these variations, the observed temperature increases are of minor importance. Therefore, drying shrinkage is still the dominant mechanism driving cracking in those ring specimen configurations. Nonetheless, it can be concluded that the AASHTO configuration is more susceptible to temperature rises due to cement hydration and may thus yield different results when considering concrete mixtures with high cement content.

The potential drying shrinkage results indicate that, despite the diversity of ring geometries and drying configurations considered in this study, the evolution of potential drying shrinkage across the eight configurations can be categorised into two distinct groups:

- Group 1: Configurations exhibiting the fastest evolution of average drying shrinkage, comprising ASTM (radial drying), ExpConf1 (radial drying), and ExpConf2 (top and bottom drying). These setups have an exposed surface-to-concrete volume ratio ranging from 26.7 to 31.5 (see Table 23).
- Group 2: The remaining five configurations, comprising ASTM (top and bottom drying), AASHTO(top and bottom drying), AASHTO(radial drying), ExpConf1 (top and bottom drying) and ExpConf2 (radial drying). These setups exhibit a slower evolution of average drying shrinkage, with surface-to-volume ratios between 13.2 and 16.0 (see Table 23).

These findings confirm that the drying rate is more pronounced in specimens with a larger boundary surface area exposed to drying. Specifically, concrete rings with smaller radial thicknesses dry faster under radial drying, while concrete rings with reduced height dry more rapidly under top and bottom drying conditions. This behaviour is consistent with physical principles governing moisture transport: water dissipation through exposed surfaces occurs significantly faster than moisture transport through the pore network. The latter is slow when the diffusion processes control moisture transport, which occurs for lower local relative humidities (see Chapter 2.2.3).

The fact that the ring-test configurations can be grouped into only two distinct groups is advantageous for systematically comparing the effects of varying ring-test setups, steel ring restraint and drying configurations.

4.1.5.2.2 Degree of restraint

The outcomes of the ring test are notably influenced by the degree of restraint imposed by the steel ring. CIRIA C766 [189] provides an analytical approach to determine the degree of restraint for axially restrained elements given by:

$$r = \frac{1}{1 + \frac{E_c A_c}{E_s A_s}} \quad (4.10)$$

where r is the degree of restraint, E_c and E_s are the modulus of elasticity for concrete and steel, and A_c and A_s are the cross-sectional areas for concrete and steel.

A value of $r = 1$ corresponds to full restraint, while $r = 0$ is obtained in the case of free deformation. Table 24 shows the degree of restraint using Equation (4.10) and assuming $E_c = 35$ GPa (modulus of elasticity at 28 days for the concrete under analysis, see Fig. 117 a)) and $E_s = 190$ GPa.

Table 24 – Degree of restraint estimated based on the concrete modulus of elasticity at 28 days.

Geometry	r
ASTM	0.64
AASHTO	0.47
ExpConf1	0.79
ExpConf2	0.41

Another approach to determine the degree of restraint is to evaluate the ratio between the restrained strain developed in the concrete cross-section and the corresponding free (or potential) strain. This leads to the following expression:

$$r(t) = \frac{\varepsilon_r(t)}{\varepsilon_{pot}(t)} = \frac{\varepsilon_{pot}(t) - \varepsilon_c(t)}{\varepsilon_{pot}(t)} \quad (4.11)$$

where ε_r is the average restrained strain in the concrete cross-section, ε_c is the average strain in the concrete cross-section and ε_{pot} is the potential total strain deformation (see Fig. 126 b)).

The potential total strain deformation ε_{pot} , requires the numerical simulation of the ring-test without the inner steel ring test. A simplified approach is adopted by decreasing the steel ring stiffness to 1.9 MPa (negligible value). Fig. 136 shows the degree of restraint evolution calculated based on Equation (4.11).

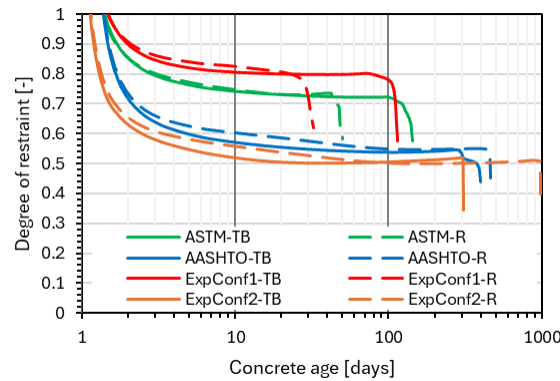


Fig. 136 – Degree of restraint for the different ring-test geometries.

The degree of restraint takes a higher value in the early ages, while it decreases over time with the increase of the stiffness of the concrete element. The high values for the degree of restraint observed at one day result from the basic shrinkage and temperature variations owing to cement hydration (see Fig. 135a). These deformations occur when the stiffness in the concrete element is very low, leading to restraint values near the full restraint. Additionally, despite the steel ring not being simulated in the thermal analysis, heat conduction occurs through the steel ring. Therefore, in the mechanical analyses, the temperature history of the nodes at the interface between the concrete and the steel ring is applied equally to all the nodes of the steel ring. These temperature variations also contribute to the increase in the degree of restraint during the first days. The numerical results show that ExpConf1 provides the highest degree of restraint (~ 0.80), and ExpConf2 provides the lowest one ($0.5 \leq r \leq 0.6$). The ASTM experiences a degree of restraint between $0.7 \leq r \leq 0.8$, while the AASHTO experiences a degree of restraint of $0.55 \leq r \leq 0.6$. Overall, the drying conditions have a negligible effect on the degree of restraint, with similar values obtained for each test under the top and bottom and radial drying conditions. At certain times, it is possible to observe a sudden drop in the degree of restraint due to the appearance of a through crack. This drop occurs early in the ExpConf1 and ASTM tests due to the high restraint in these specimens, leading to earlier cracking than other configurations. The long-term degree of restraint results obtained using Equation (4.11) based on the numerical analysis results are closely related to the degree of restraint calculated analytically with Equation (4.8) and presented in Table 24.

4.1.5.2.3 Inner steel ring strains

The main results obtained in the experimental ring tests are the hoop strains measured at the mid-height of the inner steel ring. As shown in Chapter 4.1.4.3.1, the measurements may be affected by the distance between the measurement point and the crack location. Therefore, the calculation results are measured at two points, one at the section away from the macrocrack and the other at the section near the macrocrack. Fig. 137 shows the inner steel ring strains for the different ring test configurations.

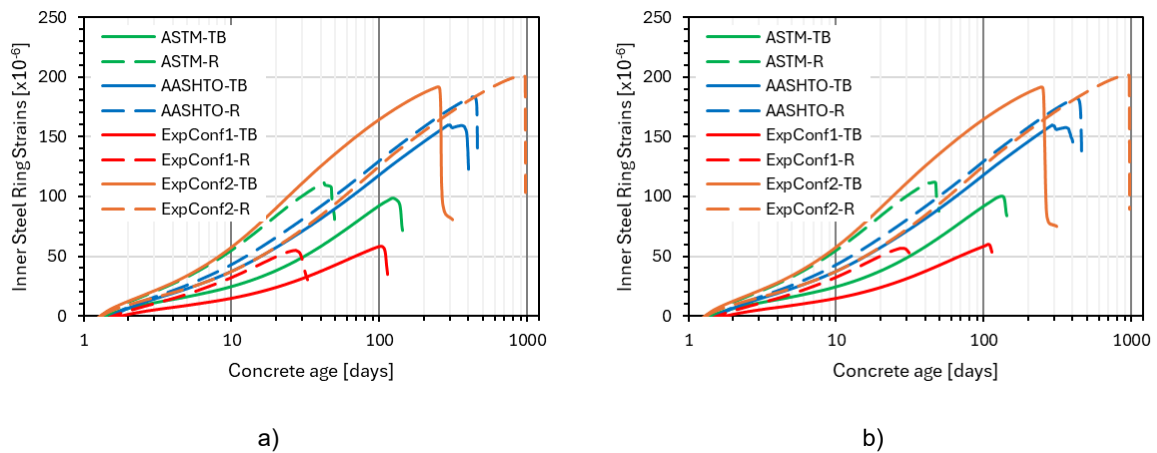


Fig. 137 – Inner steel ring strains: a) at the section away from the macrocrack; b) at the section near the macrocrack.

The results show that the overall response of the evolution of the inner steel ring strains follows the same profile for the results evaluated at the section away and near the macrocrack. As expected, the differences are only noticeable in the instants before the macrocrack opening, where the inner steel strains measured near the macrocrack present a softening behaviour represented by a concave curve before the opening of the macrocrack, while in the results measured away from the macrocrack, the strains drop abruptly after cracking.

The inner steel hoop strain magnitude is inversely related to the degree of restraint in Fig. 136. For the tests with a higher degree of restraint (ExpConf1 and ASTM), the inner steel ring strains are smaller, while in the tests with a lower degree of restraint (ExpConf2 and AASHTO), the inner steel ring strains are higher. This relationship does not yield any relevant practical consequence, except that the experimental tests made with the setups with lower inner steel ring strains, or a high degree of restraint, like ExpConf1 and ASTM, require a high-resolution and accurate strain measurement system, so that the hoop strain can be accurately detected.

The radial drying conditions provide a higher rate for the inner steel strain development for the ASTM, AASHTO and ExpConf1 test. The exception is the ExpConf2 test, where the top and bottom drying conditions present the higher rate of inner steel strains. These findings agree with the potential shrinkage results presented in Fig. 135 b). The ASTM, AASHTO, and ExpConf1 setups have a small radial concrete thickness, and therefore, the drying mechanisms are more accentuated under the radial drying setup. In contrast, a low-profile ring test geometry, like ExpConf2's, has a higher rate of steel strains in the top and bottom drying configuration.

4.1.5.2.4 Concrete stresses in the ring test

The rate of variation of the tensile stress in concrete is one of the variables that govern the time of occurrence of cracking. In an experimental ring test, concrete stress is usually indirectly estimated by assuming a uniform stress distribution in the concrete and steel cross-sections. Therefore, the following equation can be used to determine the concrete stress based on the experimental results of the ring test:

$$\sigma_c = \frac{\varepsilon_s E_s A_s}{A_c} \quad (4.12)$$

where ε_s is the measured hoop steel strain, E_s is the modulus of elasticity of the steel, A_s is the cross-sectional area of the steel and A_c is the cross-sectional area of concrete (see Table 23). This expression assumes a uniform distribution of concrete stresses in the cross section and uniform stresses in the steel.

The concrete stresses can also be evaluated, based on the numerical analysis results, as the average stress results for the element's cross-section. Fig. 138a) shows the average concrete stresses for each ring test geometry, and Fig. 138b) shows the calculated stresses according to Equation (4.12), based on the calculated hoop steel strains.

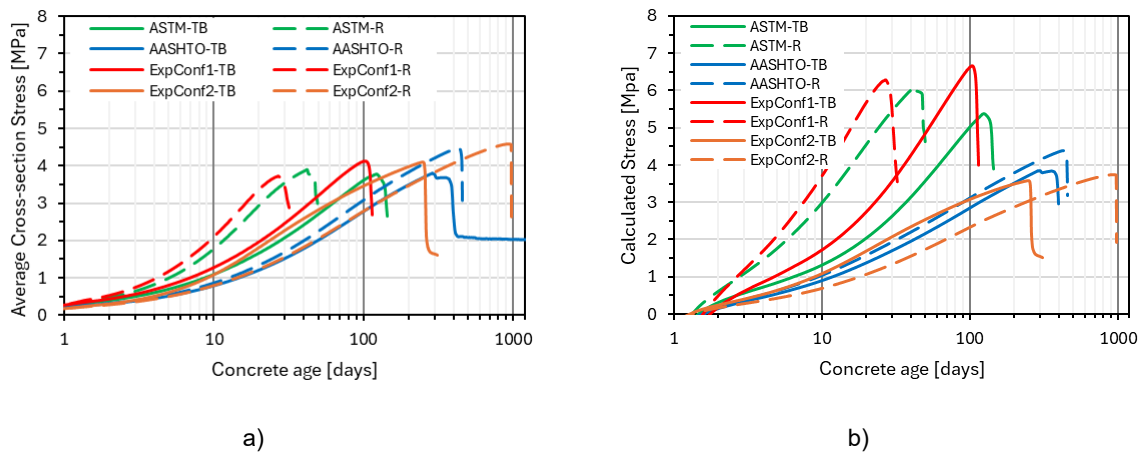


Fig. 138 – a) average concrete stresses from the numerical analysis; b) concrete stress indirectly calculated based on the steel hoop strain.

Comparing both figures, one observes that the approach using Equation (4.12) yields high values of concrete stresses for the ASTM and ExpConf1, while good approximations are achieved for the AASHTO and ExpConf2. The discrepancies in the results of Fig. 138b) may be related to the fact that the ASTM and ExpConf1 present a low value for the concrete volume divided by steel volume (see Table 23), resulting in a higher degree of restraint, which would not lead to a reasonable stress distribution over the element cross-section. In contrast, high concrete volume divided by the steel volume, which is the case of the ExpConf2, would lead to an estimate in the lower range of the stress state.

Equation (4.12) simplifies important physical phenomena, like non-uniformity of creep and shrinkage in the cross-section, an effect which is included in the numerical simulations using the pointwise model. Nevertheless, the equation may be useful to provide an approximate calculation of the stress state without numerical analysis based only on experimental results of the ring test. The calculation of concrete stresses based on Equation (4.12) can be improved if an additional factor is introduced to account for the experimental test setup. The following equation shows the update of Equation (4.12):

$$\sigma_c = k_R \frac{\varepsilon_s E_s A_s}{A_c} \quad (4.13)$$

where k_R is a factor introduced according to the test used.

The factor k_R can be determined by calculating the ratio between the numerically obtained stresses shown in Fig. 138a) and those calculated using Equation (4.12) shown in Fig. 138b). Of particular interest are the values corresponding to the typical duration of a ring test, which is generally considered to be until crack formation, usually before 120 days. Fig. 139 presents the evolution of the factor k_R , determined by dividing the numerical stress results shown in Fig. 138a) by the calculated stresses shown in Fig. 138b).

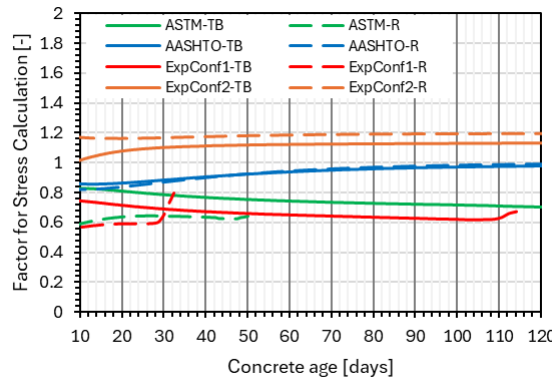


Fig. 139 – Factor for the analytical stress calculation dependent on the ring test setup.

The results indicate an approximately constant k_R factor over time for most test setups, except for ASTM-TB and ExpConf1, which exhibit a decreasing trend. To facilitate the use of a representative constant value for k_R , a weighted average is taken during 120 days, or up to the time of cracking in the numerical analyses, where cracking occurred before 120 days. The factor k_R seems to be related to the degree of restraint. The following analytical equation is proposed to evaluate the value of k_R :

$$k_R = \frac{0.48}{r} = 0.48 \cdot \left[1 + \frac{E_c A_c}{E_s A_s} \right] \quad (4.14)$$

Table 25 shows the values obtained for $k_{R(num)}$ in Equation (4.13) and the values for k_R using Equation (4.14).

Table 25 – Factor for stress calculation.

Geometry	Drying conditions	$k_R(num)$	r (Equation (4.10))	k_R (Equation (4.14))
ASTM	TB	0.77	0.66	0.73
	R	0.63	0.66	0.73
AASHTO	TB	0.97	0.48	1
	R	0.97	0.48	1
ExpConf1	TB	0.68	0.81	0.59
	R	0.59	0.81	0.59
ExpConf2	TB	1.13	0.55	1.14
	R	1.19	0.55	1.14

The results for k_R using equation Equations (4.14) are in the range of the numerical results obtained. Fig. 140 shows the updated concrete stress indirectly calculated based on the steel hoop strain, applying the factors k_R (Equations (4.14)) in Table 25 in Equation (4.13).

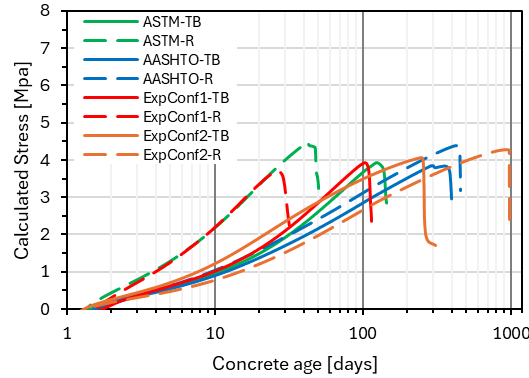


Fig. 140 – Updated concrete stress indirectly calculated based on the steel hoop strain.

The figure now shows improved agreement with the numerical average stress results presented in Fig. 138a). An even closer match could be obtained by using the numerical $k_R(num)$ values in Equation (4.13). However, Equation (4.11) aims to estimate stress based solely on experimental results of the inner steel strains, making an analytical approach preferable without any dependence on specific drying conditions. The current formulation appears suitable for this study's ring-test geometries, concrete mixtures, and drying conditions. Nevertheless, further validation is necessary for its application to other geometries, material compositions, or environmental conditions. In particular, incorporating the influence of drying conditions across all ring-test configurations would be ideal, as discussed in Chapter 4.1.3.

4.1.5.2.5 Suitability of the different ring test geometries

The crack's occurrence time is an important feature in choosing the correct ring-test setup. Table 26 summarises the time of crack formation for all numerical analyses and the hoop steel strain peak value.

Table 26 – Summary of the crack formation for all numerical analyses

Geometry	Drying conditions	Time of peak occurrence for the Macrocrack (days)	Hoop steel strains peak value ($\mu\epsilon$)
ASTM	TB	123.00	98.4
	R	42.25	112.0
AASHTO	TB	298.0	160.0
	R	430.0	183.0
ExpConf1	TB	103.50	58.6
	R	27.00	55.3
ExpConf2	TB	306.7	191.8
	R	945.00	201.1

The ASTM and ExpConf1 configurations exhibit the shortest times to macrocrack formation, particularly under radial drying conditions, 27 days for ExpConf1 and approximately 42 days for ASTM. In contrast, the ExpConf2 and AASHTO configurations with radial drying show significantly delayed cracking, occurring at around 945 days and 430 days, respectively. This behaviour is expected due to the lower degree of restraint and the substantial concrete ring thickness in these setups, which results in slower drying rates.

Given that the primary purpose of the ring test is to compare the cracking risk of different concrete mixtures under the same setup, the following conclusions can be drawn:

- fast-cracking configurations (ExpConf1 and ASTM) may be suitable for testing concrete mixtures where drying shrinkage is the main driving force for cracking, as these geometries allow for rapid shrinkage development at early ages. Radial drying in these setups can lead to fast cracking before a significant portion of the total shrinkage strain has developed, while Top and bottom drying conditions exhibit a low rate of drying shrinkage. The ExpConf1 presents small values of the inner steel strains compared to ASTM, requiring more precision in the measurement of the hoop steel strains;
- low-restraint configurations (AASHTO and ExpConf2) lead to excessively long cracking times for the concrete mix used in this study. These configurations may be more appropriate for testing concrete or mortar mixes that exhibit substantial basic shrinkage and hydration-induced thermal effects, where drying shrinkage plays a secondary role. They may also be suitable for evaluating mortars or high-shrinkage concretes that exhibit very high deformation after drying initiation, and internal restraint effects may play an important role in cracking development. These setups also allow for more accurate investigation of the stress distribution since they present a more stable degree of restraint than the other compared mixtures and a slower stress rate evolution.

4.2 ADJUSTABLE RESTRAINING FRAMES FROM TU GRAZ

Avoiding or limiting crack widths in massive concrete elements can be a challenging problem owing to the physical phenomena inherent to hardening processes occurring at early ages. In restrained elements, the increase of temperature at an early stage, due to the heat of hydration of cement, and the consequent cooldown at a stiffer stage, results in tensile stresses, which may lead to cracking or reduce the tensile capacity to sustain additional loading in the long-term. A recurrent set of questions, made by designers and scientists, is: *Do the long-term concrete stresses due to hydration heat relax? or Do they need to be superposed to the stresses owing to long-term effects and applied loading? and, Do the hydration heat effects influence the long-term crack widths?*

The Adjustable Restraining Frames (ARFs) were developed at the Graz University of Technology (TU Graz) to investigate the behaviour of massive concrete elements since casting, including additional imposed deformations to help answer these questions [203]. However, a different set of questions persists: *How accurate are finite element methodologies in predicting the developed concrete stresses and crack widths from the early ages until the long-term of analysis?*

The present chapter intends to show the application of the pointwise THM model in the numerical simulation of the ARF experimental campaign conducted at TU Graz and discuss the comparison between experimental and numerical analysis results.

4.2.1 EXPERIMENTAL CAMPAIGN

The ARF consists of a steel frame comprising two head girders and two supporting struts, incorporating hydraulic cylinders and load cells. The tested specimen is a RC tie with a 3.7 m length and a cross-section of $25 \times 25 \text{ cm}^2$ cast directly into the steel frame and tied to the head girders. The steel frame configures a passive restraining system with constant stiffness, providing nearly full restraint immediately after the concrete setting and a degree of restraint of about 0.65 for hardened concrete for the adopted material and concrete geometry. Fig. 141 shows the schematic illustration of the ARF from TU Graz.

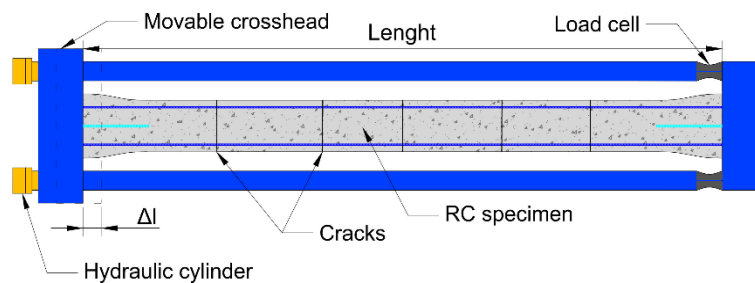


Fig. 141 – Schematic illustration of the passive phase and active phase of the adjustable restraining frames from TU Graz (adapted from [203]).

The tested RC tie is reinforced with four rebars having a diameter of 14 mm, yielding a reinforcement ratio of $\rho_s \approx 1\%$. A linear widening of the tie's cross-section in the area of the crossheads until a cross-section side of 35 cm ensures that cracking does not occur near the specimen extremities. Additional connection reinforcement at the extremities make sure that the force application area is as short as possible.

The restraint forces are measured through the two load cells installed at one of the extremities of the experimental setup. The RC specimen's average deformation is measured by LVDT (measuring the length spanning between both head girders). The temperature in concrete is measured at the core and the concrete surface. Crack widths are measured with high-strain transducers (DD1) applied to the surface of the concrete tie. Fig. 142 show the ARF experimental setup at TU Graz.

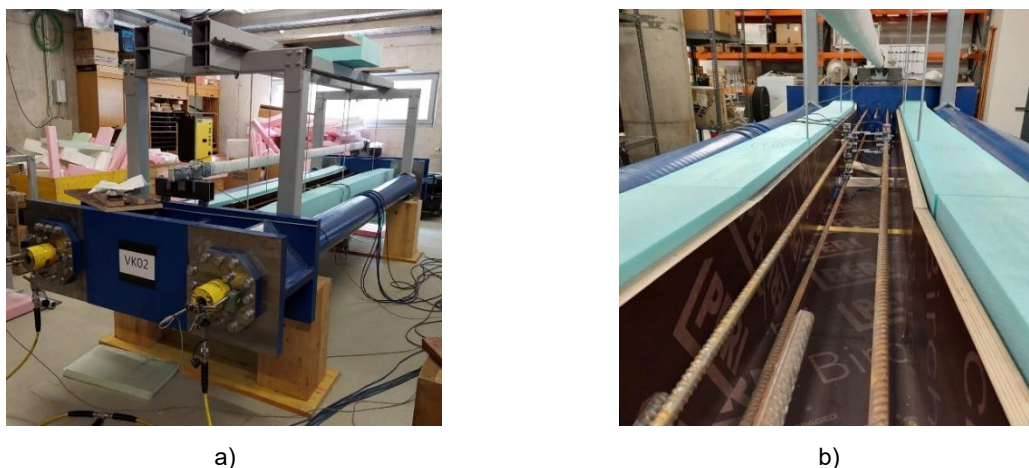


Fig. 142 – Adjustable Restraining Frames at TU Graz: a) Experimental framework; b) formwork, reinforcement and transducers setup before casting.

Turner [196] performed five series of tests, where, in each series, two specimens were tested simultaneously. Since the RC tie cross-section is not relatively thick to spontaneously generate a temperature history conventionally found in massive concrete elements, the semi-adiabatic conditions are obtained using thermal insulation. The temperature drop effect is investigated by removing the thermal insulation at different times. Additionally, an aluminium foil moisture barrier is applied to some specimens to limit the experimental campaign's drying effects. Table 27 summarises the test duration, the thermal insulation duration and the moisture barrier assumption on each ARF test.

Table 27 – Series of ARF experimental tests [267].

	Serie 1		Serie 2		Serie 3		Serie 4		Serie 5	
	T1	T2	T1	T2	T1	T2	T1	T2	T1	T2
Duration (days)	28	28	168	168	231	231	287	287	196	378
Thermal Insulation	72h	264h	72h	336h	336h	336h	72h	72h	No	No
Moisture barrier	No	No	No	No	No	No	Yes	Yes	No	*

The tests were performed in a laboratory room at an ambient temperature of 20°C and an average relative humidity of 40%. The concrete used is of strength class C35/45, with a measured average modulus of elasticity of 34.1 GPa and a measured tensile strength at 28 days between 2.5 and 3.2 MPa. Table 28 presents the concrete composition.

Table 28 – Concrete mixture used in the ARF from TU Graz.

Material	Quantity (kg/m ³)
CEM III/A 32.5 N Holcim	300
Aggregates (0/16)	2000
Superplasticiser BV ViscoCrete 1051 PCE	3
Water	145

The cement considered in this experiment was a CEM III/A 32.5N. This type of cement has 36-65% ground granulated blast-furnace slag (GBFS). Such an addition has been reported in the literature to increase long-term shrinkage, especially in the case of a high water-to-cement ratio [268, 269].

4.2.2 NUMERICAL SIMULATION OF THE ARF TESTS

The numerical simulation of this experimental campaign considers the same geometry and material for all the tests. Four tests were selected for the numerical simulation:

- Test 1: corresponding to series 2 T2 in Table 27;
- Test 2: corresponding to series 2 T1 in Table 27;
- Test 3: corresponding to series 4 T1 in Table 27;
- Test 4: corresponding to series 5 T1 in Table 27.

The temperature and applied elongation used in the numerical analyses were input based on the experimental measurements. Due to the effectiveness of the thermal insulation and the small cross-section size of the RC tie, the gradient of temperatures between the core and the surface can be dismissed in the numerical simulations, with only the temperature at the core being considered as input. Fig. 143 shows the temperature input and elongation for the tests considered in the numerical analyses.

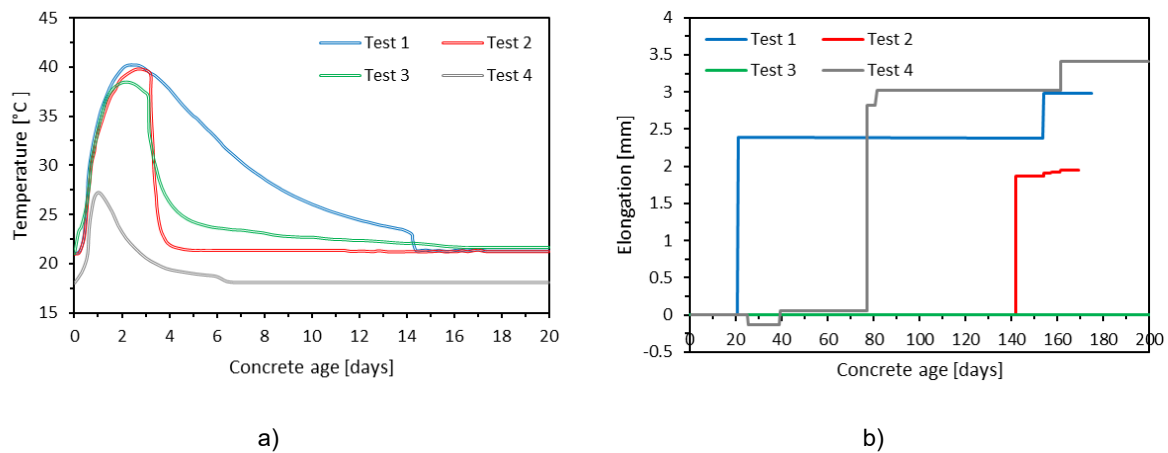


Fig. 143 – Experimental data: a) concrete temperature; b) imposed elongation.

Test 1 and Test 2 investigate the interaction between the temperature rise due to cement hydration and the concrete's viscoelastic behaviour by varying the thermal insulation removal time. In Test 1, the

insulation was removed at 336 hours, while in Test 2, it was removed at 72 hours, corresponding approximately to the time the maximum temperature was reached. Test 3 replicates the setup of Test 2. However, in this case, a moisture barrier was applied following the removal of thermal insulation. This modification enables the assessment of shrinkage effects on the long-term behaviour of the RC element. Test 4 consists of a numerical simulation of the RC element without thermal insulation, serving as a reference case. In Tests 1 and 4, elongation was applied until a stabilised crack pattern was achieved, whereas in Test 3, no additional imposed elongation was included in the experimental setup.

4.2.2.1 Numerical model

The experimental campaign benefits from the fact that the concrete composition and geometry are equal for all series. Therefore, the material model and FE mesh are the same for all tests, with differences limited to the input of the temperature history and imposed elongation as shown in Fig. 143. Fig. 144 shows a schematic representation of the geometrical model considered for the numerical analysis.

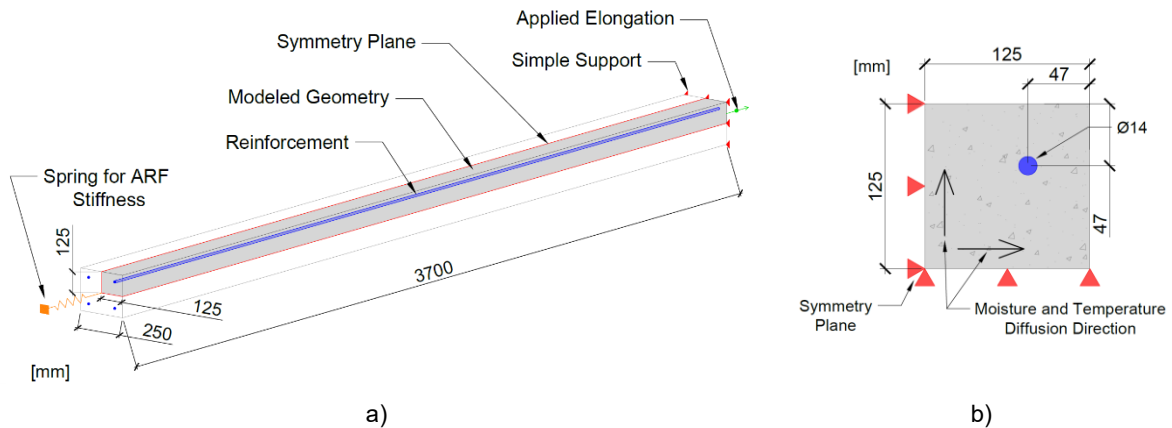


Fig. 144 – Numerical model for the simulation of ARF: a) geometry; b) cross-section.

Only one-fourth of the cross-section was discretised due to the symmetry conditions. The full length of the RC tie is modelled because the occurrence of cracks is not symmetrical along the bar length. The stiffness of the restraining steel frame is simulated by considering an elastic spring applied at one of the RC tie extremities. The boundary conditions in that extremity impose that the cross-section is kept plane (equal longitudinal displacement in all the cross-section nodes). The opposite RC tie extremity is supported in the longitudinal direction, and this is the position where the imposed elongation is applied as a prescribed support movement in all the cross-section nodes. Along the symmetry planes, the node displacement is prevented in the direction perpendicular to the plane. Fig. 145 shows the FE mesh for the cross-section at the notch location.

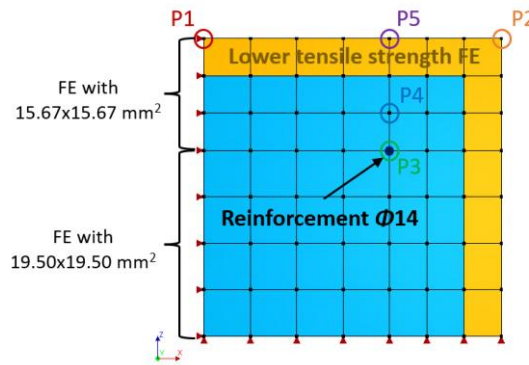


Fig. 145 – FE mesh for the cross-section at the notch location.

Three layers of FE are used to discretise the concrete cover so that the variation of the crack width throughout the concrete cover can be captured. The FE edges have a different size in the concrete cover portion and the core portion, so that the centre of the $\phi 14$ mm reinforcing bar can coincide with a line of nodes. In the longitudinal direction, the FE edge has a size of 18.5 mm, so each FE is approximately cubic.

The widening effect at the ends of the RC tie is simplified by keeping the cross-section geometry constant, with a tensile strength of concrete equal to 110% of the current value, along a distance of 390 mm from the tie end. The reinforcement is simulated using truss elements. The bond-slip between concrete and reinforcement is simulated using interface elements that employ a bond-slip law for the shear tractions. Given that the calculated concrete stresses are uniform in the whole model before the first crack occurs, some perturbation is needed to induce the localisation of the first crack. This was made by simulating a notch in a cross-section 800 mm apart from one of the RC tie ends. In that section only, the superficial layer of FE is modelled with reduced tensile strength, equal to 90% of the current value, as shown in Fig. 145.

4.2.2.2 Material parameters

The basic shrinkage is simulated through Equation (2.68) and is affected by the temperature effects using the transformed times (see Chapter 3.5.2.1). The total basic shrinkage is $\varepsilon_{cbs,0} = 90.1 \times 10^{-6}$. Turner [196] reported seasonal variations in the relative humidity of the lab: RH=30% for winter and RH=80% in summer. Since Test 1 and Test 2 were performed from winter to spring, the numerical simulations considered RH=40%. No experimental drying shrinkage tests are available for numerical calibration of the hygral and shrinkage model. Therefore, the total drying shrinkage is determined based on the strength properties according to the MC2010 formulation, which gives a value of $\varepsilon_{cds,0} = 314.5 \times 10^{-6}$. The parameters used in the hygral model in Chapter 4.1.1 were adopted for the present hygral simulations and are presented in Table 12. The dKwak shrinkage model (Equation (3.47)) is assumed for the numerical simulation of shrinkage. The selection of the hygral and shrinkage models for this study is based on the similarities of the present concrete mix with concrete mixes that incorporate admixtures and plasticisers. These models have previously shown good performance in simulating the behaviour of similar concrete types, as demonstrated in Chapter 4.1.1. Since no creep

tests have been performed in the experimental campaign, the creep parameters assumed in the numerical simulations were determined from model B4 based on the concrete mix proportions and cement type. The RMPS model is used considering the parameters in Chapter 4.1.2. However, the temperature and relative humidity function parameters are kept equal to the proposed default values. Table 29 shows the creep parameters used in the simulation of the ARF.

Table 29 – Creep parameters used in the simulation of the ARF.

Parameter	Value	Parameter	Values
q_1	$22.55 \times 10^{-6} \text{ MPa}^{-1}$	-	-
q_2^*	$120.58 \times 10^{-6} \text{ MPa}^{-1}$	c_2	1
q_3^*	$4.65 \times 10^{-6} \text{ MPa}^{-1}$	c_3	1
q_4^*	$5.57 \times 10^{-6} \text{ MPa}^{-1}$	c_4	1
c_0	0.005	α_e	10
k_1	$1.10 \times 10^{-1} \text{ MPa} \cdot \text{K}^{-1}$	$\alpha_r = \alpha_s$	0.1
b_{RMPS}	5.0×10^{-4}	$Q_e = Q_s$	$33.26 \text{ kJ} \cdot \text{mol}^{-1}$
p_{RMPS}	1.4	Q_r	$33.26 \text{ kJ} \cdot \text{mol}^{-1}$

The steel frame has a longitudinal axial stiffness of $k \approx 1053 \text{ kN} \cdot \text{mm}^{-1}$, which was simulated by springs at one extremity of the numerical model.

4.2.2.3 Numerical results

A preliminary analysis was made to get an estimate for the setting time, t_s , which may affect stress development due to heat of hydration and autogenous shrinkage. Based on the recorded concrete temperatures, it seems plausible that the t_s value, for all the tests, is between 6 h and 10h. The present study considers different values for the setting time: 6h, 8h and 10h after the mixture, for Tests 1 and 2. The setting time corresponds to the time that cementitious material changes from fresh to hardened and defines the time zero of the employed material models. The presence of reinforcement was disregarded in these particular analyses. Fig. 146 shows the calculated early-age evolution of the concrete stresses, as well as the respective temperature history.

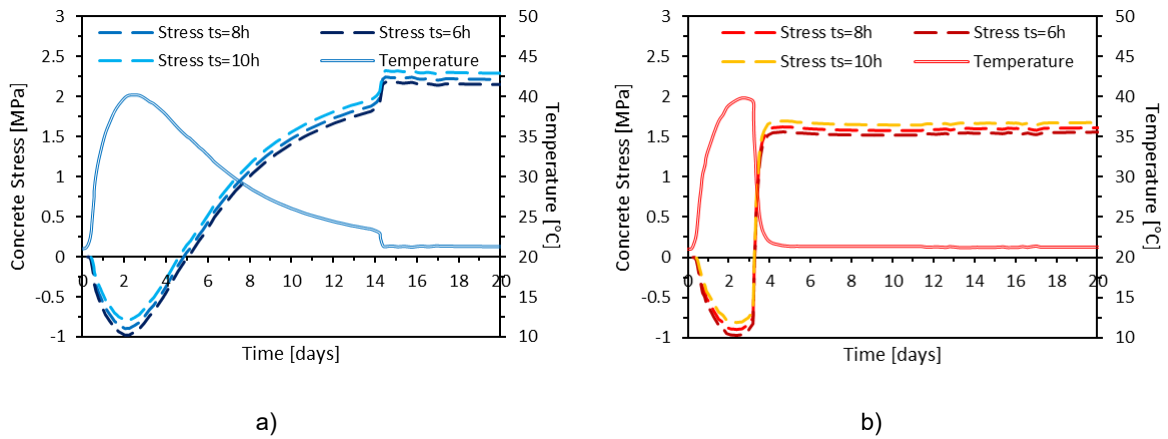


Fig. 146 – Influence of the assumed concrete setting time in the early-age concrete stresses: a) Test1; b) Test2.

Assuming an earlier setting time ($t_s = 6h$) implies that the concrete has a stiffer response during the initial temperature rise, thus increasing the maximum compressive stress and decreasing the tensile stress after the temperature in the concrete equals the ambient temperature. The opposite occurs for a later setting time ($t_s = 10h$). Most importantly, in the context of this particular study, one concludes that the variation of t_s in the interval of 6h to 10h is not determinant, because the calculated maximum stresses only varied 0.25 MPa. Consequently, it seems reasonable to make the subsequent analyses of the RC ties considering a medium value for the setting time, $t_s = 8h$. Fig. 147 shows the evolution of the axial restraining force (N) in the RC specimen, divided by the concrete cross-section area (A_c).

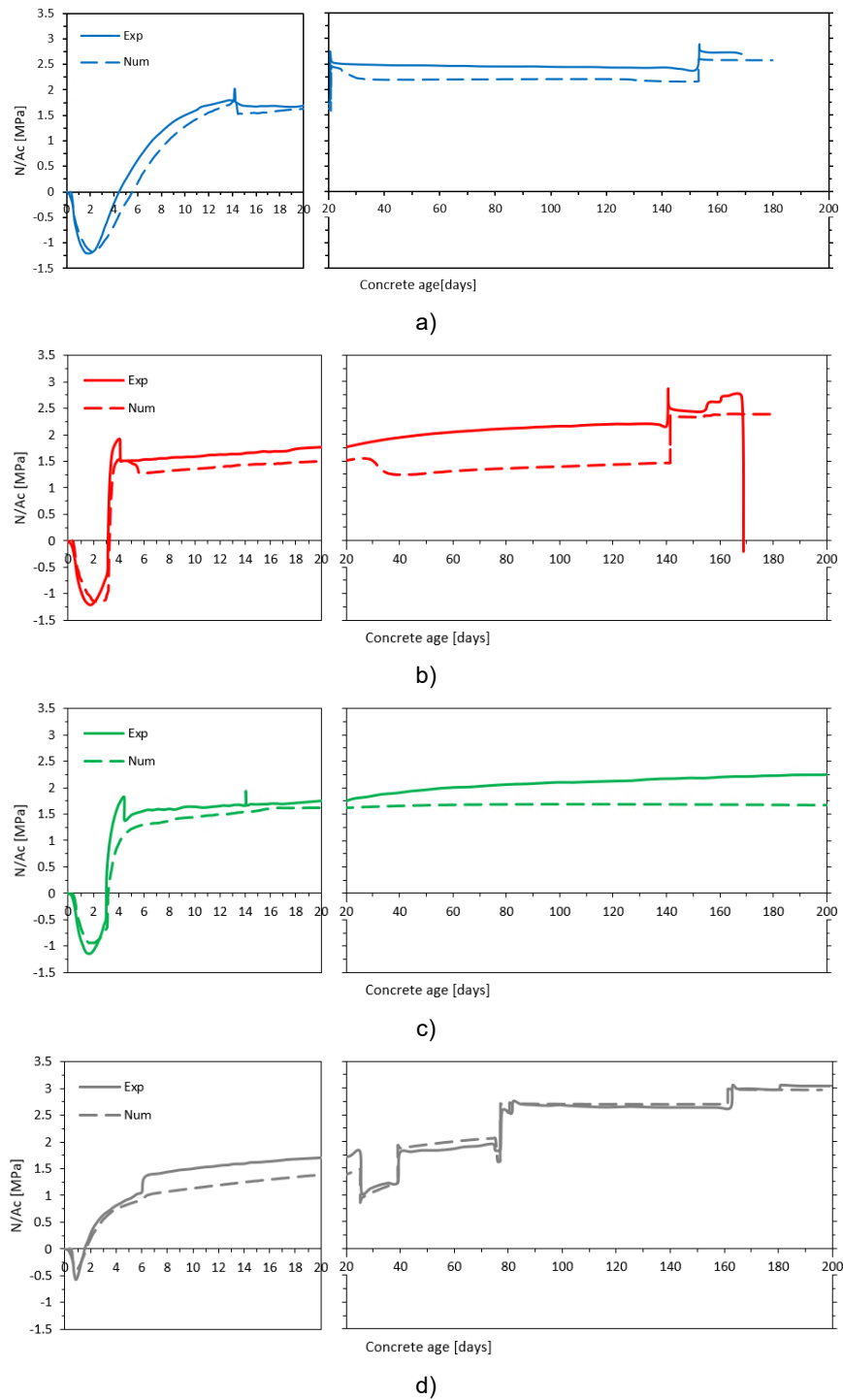
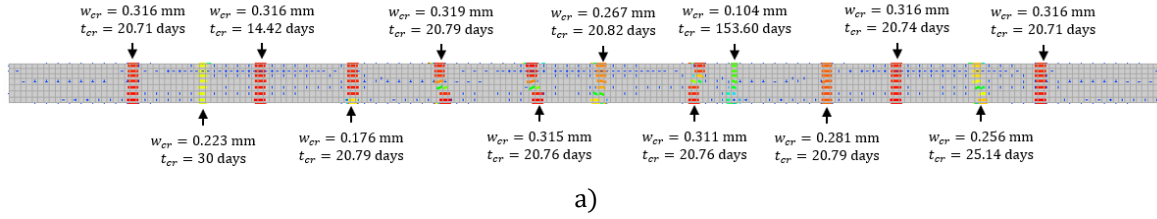
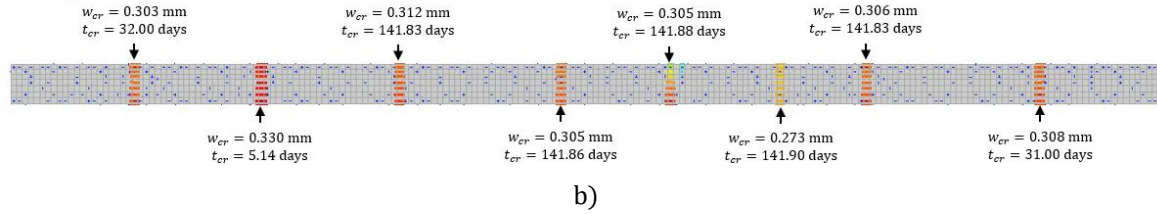


Fig. 147 – Experimental and calculated results for the restraining force, normalised with respect to the cross-sectional area of concrete. From top to bottom: a) Test1; b) Test2; c) Test3; d) Test4.

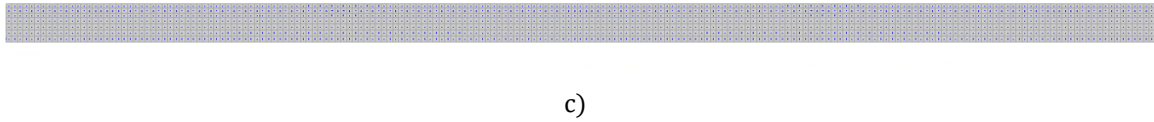
Fig. 148 shows the numerical crack pattern for the analysed tests at the exterior surface of the specimen. The crack widths are calculated based on the deformations between the nodes of the cracked finite element and the length of the finite element. The time of appearance of each crack, t_{cr} , and the crack width calculated, w_{cr} , at P1 (see Fig. 145) at the end of the tests are presented in each image.

Test 1 (180 days)


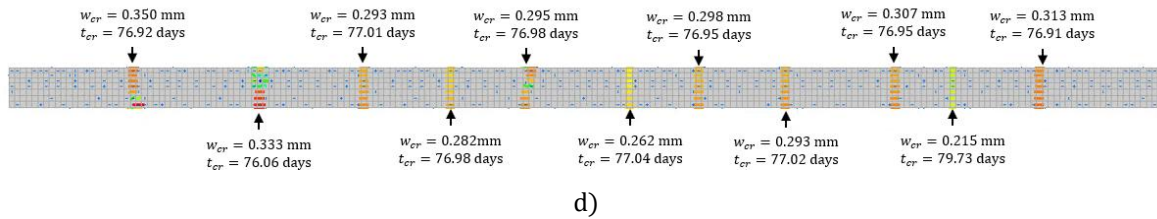
a)

Test 2 (180 days)


b)

Test 3 (200 days)


c)

Test 4 (200 days)


d)

Fig. 148 – Calculated crack patterns, with the indication of the crack width (w_{cr}) in the position P1 at the end of the analysis, and the time (t_{cr}) when each crack is formed.

In Test 1, a comparison between the experimental and numerical N/A_c , shows a delayed response in the numerical results during the cooling period. At ≈ 14 days, there is a drop in the experimental restraining force owing to the appearance of a crack in the experimental tests. In the numerical simulation, cracking also initiates at 14 days. At ≈ 20 days, a stabilised crack pattern is imposed in Test 1 by applying an elongation. The last formed crack, presented in green in Fig. 148, occurs at ~ 154 days owing to additional imposed deformation. All the cracks present a similar crack width value at the end of the test of ~ 0.320 mm, except the last formed crack, which presents a crack width of 0.104 mm.

In Tests 2 and 3, the thermal insulation is removed when the maximum temperature is reached. This leads to a temperature drop in Test 2, while the temperature in Test 3 decreases at a slower rate. After the temperature drops, the experimental N/A_c drastically changes from negative to positive values. In both experimental tests, a small drop in the N/A_c occurs due to cracking. In Test 2, the numerical N/A_c show a drop at 6 days, resulting from the formation of a through crack. In Test 3, the numerical N/A_c is smaller than the experimental values, and no drops were observed, meaning there was no crack. In the long term, the experimental restraining forces of Tests 2 and 3 increase over time. In the numerical analysis, the restraining forces for Test 2 also increase due to the restrained shrinkage until the formation of a new crack at ~ 30 days. In contrast, the numerical restraining forces for Test 3 remain almost constant

over time. Fig. 148 shows that in Test 2, a full crack is generated at ~ 5 days. Two more cracks are formed at ~ 30 days. Additionally, the elongation applied in Test 2 at 142 days leads to the appearance of five more cracks. At the end of the test, the cracks of Test 2 present a width of ~ 0.310 mm.

In Test 4, the temperature history reaches smaller values due to the absence of thermal insulation (see Fig. 143 a). Consequently, the compressive and tensile restraining forces observed in the early ages are decreased. Due to the restrained shrinkage, the experimental and numerical N/A_c continue to increase over time. Between ≈ 25 and 40 days, the RC tie of Test 4 is subjected to contracting imposed deformation, resulting in a drop in the tensile stresses. At ~ 77 days, a stabilised crack pattern is imposed in Test 4 by applying an elongation.

The experimental results in all the tests show that the stresses in the concrete remain relatively high after the temperature stabilises, and these stresses continue over the long term with minimal relaxation. This effect reduces the ability of the concrete element to withstand additional loads without cracking and shows the importance of considering the effects of early ages when simulating the long-term behaviour of concrete elements.

Fig. 149 presents the evolution of the experimental and numerical crack widths for the first formed crack in Tests 1 and 4. The numerical crack width is evaluated at different points as presented in Fig. 145.

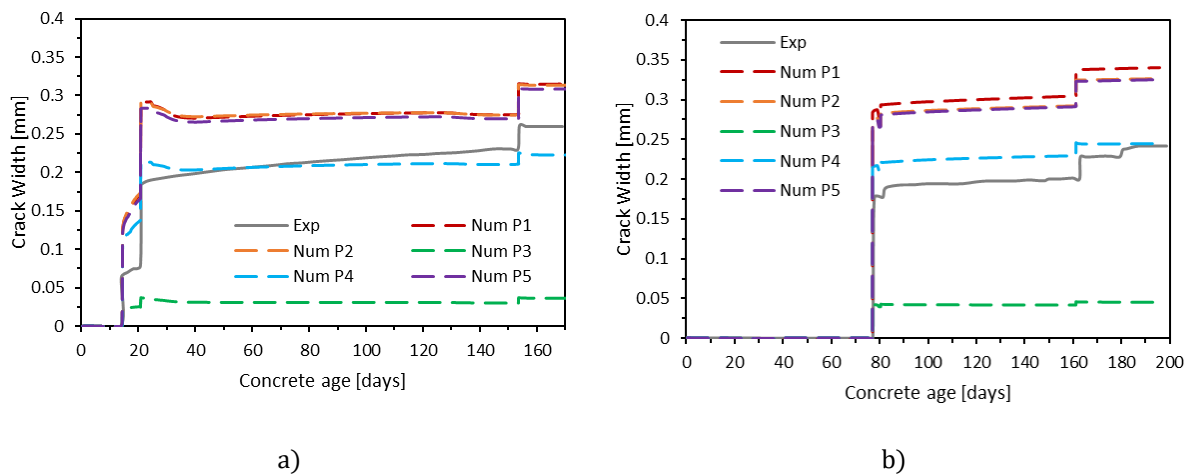


Fig. 149 – Experimental and numerical crack widths: a) Test 1; b) Test 4.

The numerical results show that the experimental crack width at the surface of the RC tie, points P1, P2 and P5, presents similar values. Point P3, which corresponds to the reinforcement location, presents a smaller crack width. The numerical results at point P4, located at 15.67 mm from the reinforcement, resemble a crack width value close to the one measured experimentally. The application of the elongation is directly associated with the crack width opening. The simplifications regarding the numerical simulation of reinforcement using truss elements and bond-slip using interface elements lead to increased crack strains in the present case study. These results can be associated with combining the bond law for the interface and the fracture model for concrete. Krenn and Schlicke [270] performed an explicit simulation of the bond between reinforcement and concrete and explored the effects of fracture in the bond slip. They consider rigid connections between reinforcement and concrete to observe that the slip is associated with cracking at the interface between them, which may indicate that, in some

cases, using a bond-slip law in the numerical simulations may lead to the underestimation of the bond-slip stiffness. Additionally, using truss elements to simulate reinforcement results in the concentration of the reinforcement volume and bond effects in a single point of the element cross-section, which is not the best modelling option for 3D numerical simulations. Future work should investigate better strategies to numerically simulate the bond between concrete and reinforcement, considering solid finite elements for the reinforcement and investigating the bond law between reinforcement and concrete.

The present case study shows the capacity of the pointwise THM model to simulate the early age stresses typical of thick RC elements. Moreover, these stresses extended into the long term, reducing the RC elements' capacity to withstand additional deformations without cracking. The magnitude of the stresses at an early age is important for the time of crack occurrence and early age cracking risk. After cracking, the crack width is affected by the reinforcement installed and the bond between the concrete and reinforcement. In all the numerical tests, the same reinforcement and bond-slip were used, resulting in similar crack width values at the end of the analyses where the crack occurred, independently of the crack location, the extent of the imposed deformations and the time of cracking occurrence. The model also shows that the crack widths vary drastically depending on the location where the crack widths are being evaluated. The simplifications regarding the volume occupied by the reinforcement being reduced to a line (truss elements) may therefore have an important effect on the crack width over the element cross-section. Krenn and Schlicke [270] performed the numerical simulation of the crack width by modelling the reinforcement rebar, showing that considering a bond-slip law in the numerical simulation of bond-slip simplifies complex bond behaviour that is not captured in the present numerical analysis. Further work should aim to improve the numerical simulation of the ARF by improving the numerical simulation of the reinforcement and bond-slip according to the recent findings.

4.3 MODIFIED FRAME AND CRACK PATTERNS IN THICK MEMBERS

Schlicke et al. [203] investigated the crack patterns of thick concrete members using the modified frame. The principle of the experimental campaign is to impose an axial deformation in a panel with only one reinforcement rebar at each side, leading to the generation of one primary crack at half-length of the specimen, plus secondary cracks at both sides of the primary crack. Fig. 150 shows the schematic representation of the experimental procedure and an image of the test frame.

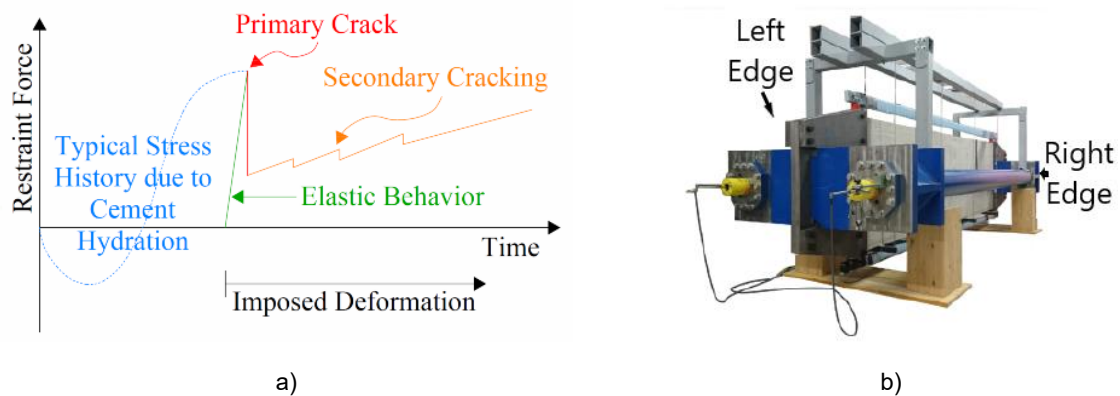


Fig. 150 – Modified frame developed at TU Graz for experimental assessment of the crack-formation in thick restrained RC members: a) Schematic representation of the experimental procedure; b) image of the test frame (adapted from [203]).

4.3.1 EXPERIMENTAL CAMPAIGN

The modified frame represents a variation of the ARF intended to allow the application of imposed elongation to generate the typical crack pattern in thick RC elements. The experimental campaign intends to investigate the cracking in a 1.028 m thick RC member, by considering a concrete panel that represents a slice of a thick wall or slab with these dimensions. The tested concrete panel is 1.028 m thick, 3.5 m long and 0.1 m wide and is reinforced with two rebars with 14 mm located one at the top and the other at the bottom of the panel (symmetry conditions at half thickness) with a concrete cover of 37 mm measured from the concrete surface to the rebar centre. Fig. 151 shows the schematic representation of the modified frame.

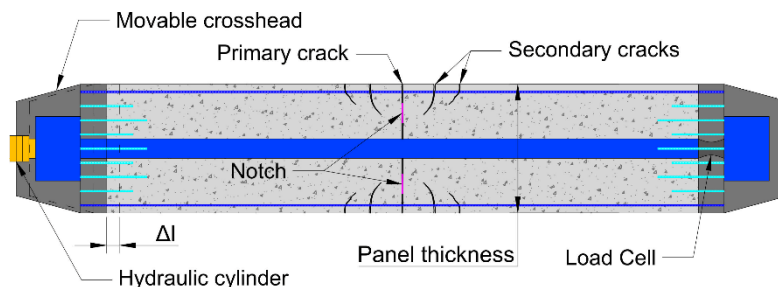


Fig. 151 – Schematic representation of the modified frame.

The experimental test used the same concrete mixture as the ARF presented in Table 28. The panel was cast outside the frame and then carefully installed for testing. This experimental test was a short-duration test, applying imposed deformation until the desired crack pattern was achieved. Two thin steel plates work as a notch to induce the primary crack at the half-span. The total imposed deformation is 2.4 mm ($\approx 0.7\%$). LVDT as well as DD1-strain gauges, are located at the panel surface and in the middle span, allowing to measure the crack width of the primary crack and secondary cracks during the total time of the experiment. Extra measurements are performed at the uncracked concrete zone to evaluate the concrete strains. Fig. 152 shows the LVDT and DD1 locations and the base-length values for deformation measurements and an approximate representation of the crack pattern in the experimental test.

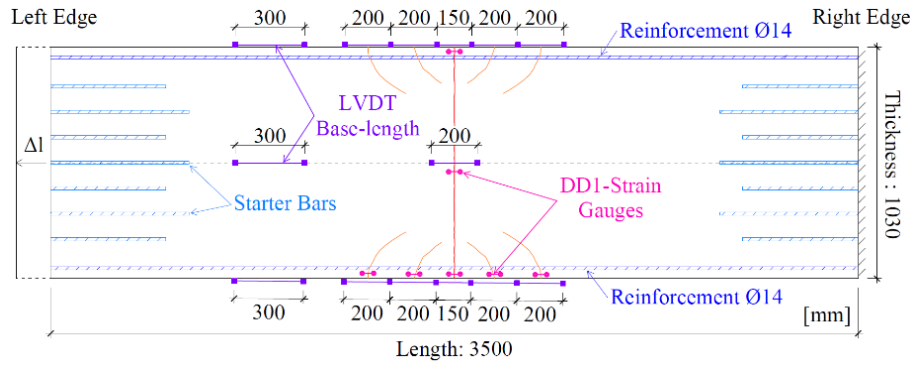


Fig. 152 – Position of the DD1 and LVDT transducers for measurements of crack widths, base length for LVDT measurements [mm] and reinforcement position.

4.3.2 NUMERICAL MODEL

Preliminary analyses were performed before the pointwise THM model was developed, considering the total strain cracking models [201]. Since the pointwise THM model is applicable in time-controlled analyses, concrete maturity was simulated at a constant temperature of 20°C and high relative humidity. This approach is based on the fact that the concrete panel was stored under controlled environmental conditions to ensure proper curing and was only installed in the experimental setup on the day of testing. The numerical simulation was carried out by applying an elongation of 2.4 mm over 3 hours at a concrete age of 28 days. The same material models used in the numerical simulation of the ARF in Chapter 4.2 are used in the numerical simulation of the modified frame. The notch is simulated by reducing the tensile strength to 2/3 of the current value in a vertical column of finite elements. The crack width assumed for switching between the rotating to fixed crack is 0.01 mm. The shear retention factor is assumed to be $\beta = 0.01$, corresponding to a value typically used in the literature [230]. The bond-slip parameter τ_{bm} in Equation (3.162), and the bond stiffness modulus were calibrated based on experimental results for the crack widths and were taken as 13 MPa and 206 N/mm³, respectively. Fig. 153 shows the FE mesh used in modelling the modified frame.

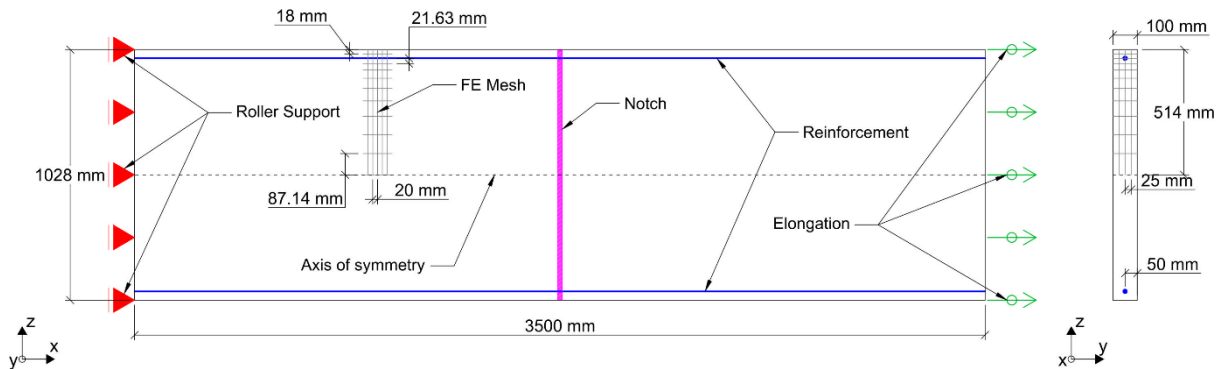


Fig. 153 – FE mesh used in the modelling of the modified frame.

Additional supports were introduced in the y and z directions to prevent rigid body movements.

4.3.3 NUMERICAL RESULTS

Fig. 154 shows the numerical crack pattern, the tensile strain contours in the longitudinal (EXX) direction and the normalised FE deformation at the end of the numerical analysis.

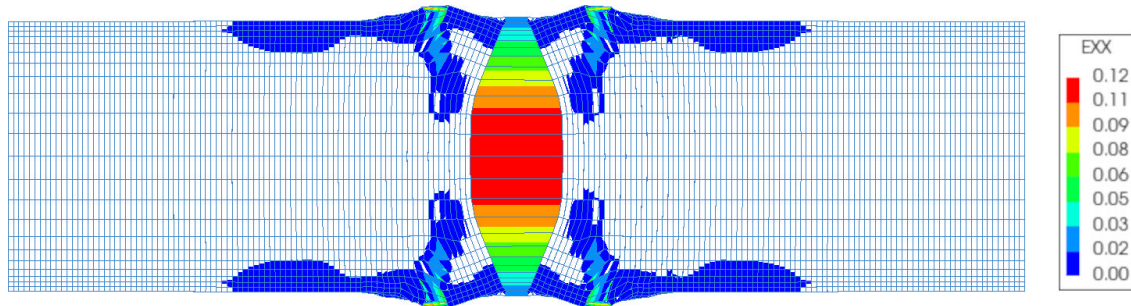


Fig. 154 – Numerical crack pattern of the modified frame experiment.

The deformed mesh shows the primary crack propagation, exhibiting larger crack widths at the core and narrower ones at the surface. Near the primary crack on the surface, secondary cracks develop and propagate towards the core, inclined at an angle to the primary crack. These secondary cracks exhibit wider crack widths at the surface than the primary crack. The primary crack is concentrated in a column of finite elements, while the secondary cracks show deformations distributed over several finite elements. This is due to the complexity of the mechanics associated with the transfer of stresses from the reinforcement to the concrete, resulting in the appearance of secondary cracks. Switching between rotating and fixed crack models is important in the numerical simulation of secondary cracks. The secondary cracks initiate in the vertical direction parallel to the primary crack. The eccentric transference of bond stresses in the vicinity of the primary crack generates principal stresses in the direction of the primary crack, hereby directing the development of secondary cracks towards the primary crack. The rotating crack model enables the rotation of the secondary cracks in accordance with the directions of the principal stresses. Since crack development is also influenced by aggregate interlock in the inclined secondary cracks, it is important to fix the secondary crack to provide more realistic shear transferences at the cracking location and avoid further crack rotation due to stress changes. Despite the absence of a perceptible second pair of secondary cracks, the morphology of the crack pattern in the numerical analysis resembles crack patterns observed in the present experimental test (see Fig. 152), thus validating the capability of the pointwise THM model for simulating cracking patterns in such elements.

Fig. 155 a) compares the sum of the crack widths at the top side with the width of the primary crack at the core, and Fig. 155 b) shows the evolution of crack widths at the top side of the experimental setup.

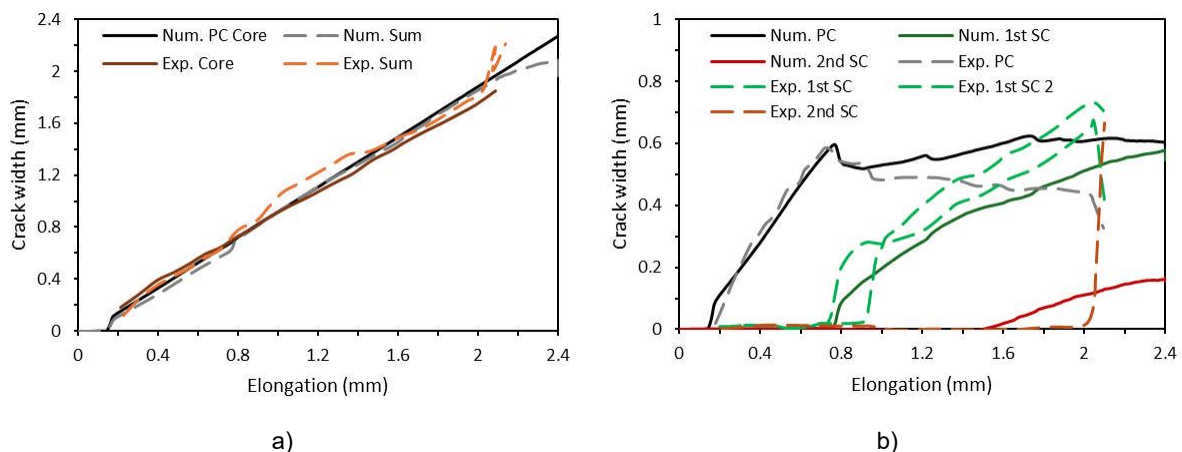


Fig. 155 – a) sum of the crack widths at the surface and the core of the element; b) primary (PC) and secondary (SC) crack width at the panel's surface.

Fig. 155 a) shows a good agreement between the numerical and experimental results, reflecting the strain compatibility between the crack in the core and the sum of the cracks at the element's surface. Fig. 155 b) shows that the width of the primary crack increases until the first pair of secondary cracks is generated. Subsequently, the crack width in the primary crack decreases. With further elongation, the crack width of secondary cracks widens, reaching values that may exceed the crack width of the primary crack. The width of the secondary crack in the numerical results is evaluated based on the total strains over a length of 200 mm, comprising the top surface FE where the secondary crack is located. This approach is consistent with the one used in the experimental work, where crack widths were evaluated based on the deformation over the same controlled length. The evident difficulties in the numerical crack localisation of secondary cracks over the considered length show the complexity of the numerical simulation of the thick concrete members. Nevertheless, the numerical simulations using the pointwise THM model show good qualitative agreement with the evolution of crack widths observed in the experimental test. Further investigation is required to enhance the numerical simulation of cracking in thick members, particularly the bond interaction between concrete and reinforcement.

4.4 RC TIE RESTRAINED SINCE THE EARLY AGES

The present chapter involves the numerical simulation of a 0.50 m thick RC tie. Prior to the development of the pointwise THM model, the layered approach was used to perform parametric analysis of the present case study. The objectives were to investigate the long-term deformation, stresses and cracks from casting up to 50 years, considering the complex interplay of cement hydration, temperature variations and shrinkage. The layered approach subdivides the finite element mesh into layers (groups of finite elements) constituted by finite elements that share the same temperature histories, relative humidity and mechanical properties. For each layer, a material model is calibrated and specified based on the relative humidity and temperature variations. The material model is applied to all the finite elements in the same layer based on the respective nodes' average relative humidity and temperature. This approach leads to different mechanical properties, temperature variations, shrinkage and creep models through the element thickness owing to the number of layers considered to account for the non-

uniform temperature distribution and relative humidity variations. The layers approach presents some inconveniences:

- increasing the number of layers in the numerical analysis can become extensively time-consuming and impractical, posing difficulties in the numerical simulation of complex geometries;
- despite the mesh subdivision into layers, the material models at each layer are determined based on the average relative humidity and temperature over the finite element nodes representative of the layer;
- small changes in the hygrothermal conditions automatically required the calibration of the material models for all the layers.

The pointwise THM model developed in this PhD work, overcomes these difficulties by evaluating the mechanical properties internally based on the temperature and relative humidity at each integration point. Nevertheless, the layered approach was utilised successfully in parametric analyses of a 0.50 m RC tie to investigate the amount of reinforcement, degree of restraint, RC tie length, bond-slip law and drying creep models. These results can be consulted in the reference [224].

The objectives of the present study are to investigate and compare the performance of the pointwise THM model developed in the scope of the present PhD work with other numerical approaches. Three numerical approaches are considered:

- the pointwise THM model;
- the layered approach;
- the average approach, which consists of assuming a uniform material model for all FE.

The average approach neglects the self-equilibrated stresses generated by localised hygrothermal imbalances, and it is considered to highlight the importance of THM analysis in the simulation of structures sensitive to hygrothermal effects.

4.4.1 MATERIAL BEHAVIOUR IN THE POINTWISE THM MODEL

The concrete material used in the numerical analyses conducted in the present chapter corresponds to a mix previously characterised in an extensive laboratory experimental campaign described by Azenha et al. [91]. Table 30 shows the concrete composition used in the numerical simulation of the 0.50 m RC tie.

Table 30 – Concrete mixture used in the numerical simulations of the 0.50 m RC tie.

Material	Quantity (kg/m ³)
CEM II 42.5 R	280
Fly ash	40
Water	145
Aggregates (0/16)	1926
Water reducing admixtures	6

The mechanical simulation was based on the assumption of a concrete of C30/37 grade, according to EN 1992-1-1 [51], justified by the obtained average cube compressive strength of 48.4 MPa at 28 days [91]. The tensile strength evolution is simulated using Equation (3.86) with $f_{ct,28} = 2.9$ MPa, $n_{fct,1} = 0.20$, $n_{fct,2} = 0.50$ and $n_{fct,3} = 0.65$. The MC2010 bilinear tension softening model is used for the numerical simulation of fracture, considering $G_f = 0.14$ Nmm⁻¹ and the crack bandwidth of 25 mm (FE size). Azenha et al. [91] validated the hygral model through comparison between numerical and experimental measurements of the relative humidity at different depths for three different geometries drying in a slab-like flow:

- specimen H10, with the dimensions 10 cm × 10 cm × 40 cm;
- specimen H15, with the dimensions 15 cm × 15 cm × 60 cm;
- specimen H20 with the dimensions 20 cm × 20 cm × 60 cm.

The hygral model was calibrated to provide an accurate representation of the relative humidity variation for all the specimens. Table 31 shows the parameters adopted from Azenha et al. [91] and assumed in the present thermo-hygral simulations.

Table 31 – Thermo-hygral properties used in the numerical simulation of the 0.50 m RC tie.

Model	Parameter	Value
Thermal model	k	$2.6 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$
	ρc	$2400 \text{ kJ} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$
	$h_{cr,free}$	$10 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$
	$h_{cr,moulded}$	$5 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$
	T_{env}	20°C
	E_a	$38.38 \text{ kJ} \cdot \text{mol}^{-1}$
	A^*	$2.645 \times 10^7 \text{ m}^3 \cdot \text{kg}^{-1} \cdot \text{s}^{-1}$
	Q_{pot}	$3.55 \times 10^6 \text{ J} \cdot \text{kg}^{-1}$
Hygral model	α_0	0.0967
	D_1	$3.08 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$
	h_c	0.80
	n_h	2
	η_e^*	$4.81 \times 10^{-8} \text{ m s}^{-1}$
	$\varepsilon_{sh,ult}$	$595.2 \times 10^{-6} (539\mu + 56.2\mu)$
	$k_{sh}(\text{dKwak})$	3.3837×10^{-3}
	ε_{bs0}	56.20×10^{-6}
	α_h	10

The relative humidity specimens were cast and continuously kept in a climatic chamber with a temperature of 20 °C and a relative humidity of 60%. After casting, the specimens' free surfaces were covered by plastic films to ensure adequate sealing conditions. A plywood board was placed over the top free surface. After 7 days, the moulds and board were removed, and four surfaces of each specimen were sealed with paraffin wax (over 2mm thick) to ensure a 1D moisture flow. The relative humidity measurements were performed using the Vaisala® HM44 probe following the measurement procedure specified in Chapter 4.1.1. The measurements were performed at 2 cm, 4cm and 5 cm for the H10 specimen, 2 cm, 4 cm and 7.5 cm for the H15 specimen and 2 cm, 4 cm and 10 cm for the H20 specimen. The numerical simulations of the relative humidity tests are carried out using the parameters in Table 31. The finite element mesh consists of a vertical column with a height equal to the height of the specimen dimension in the flow direction. All the finite elements have the size of 10 mm × 10 mm × 10 mm for all analyses, with one finite element in the H15 mesh with the dimensions of 15 mm to match the experimental measurements at 7.5 cm. Fig. 156 shows the comparison between the hygral simulation results and the relative humidity measurements.

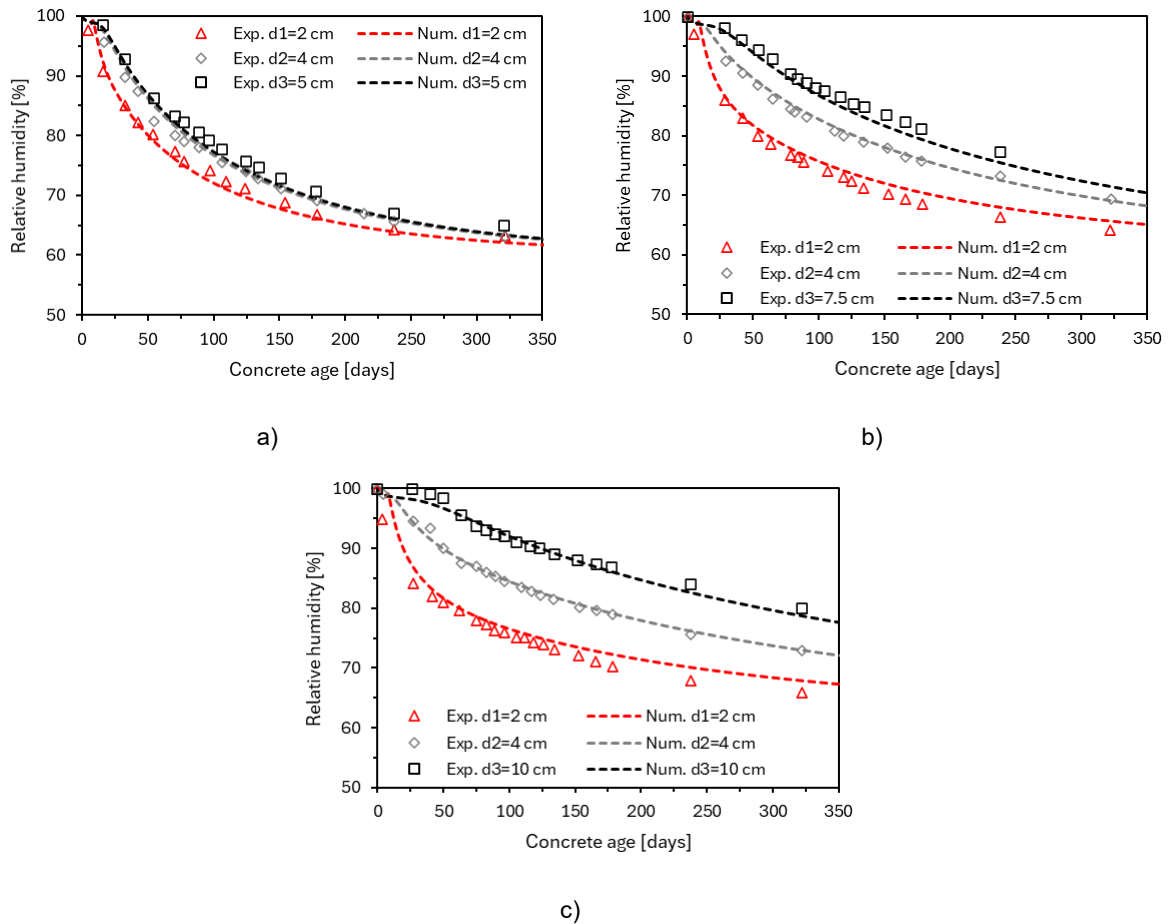


Fig. 156 – Numerical simulation of the relative humidity measurements performed by Azenha et al. [91]: a) H10; b) H15; c) H20.

The results show a good agreement between the experimental and the numerical simulations. Azenha et al. [91] performed the hygral analysis after drying initiation, which starts at 7 days. The authors despise the self-desiccation that occurs over the first 7 days. The numerical simulations performed in this chapter

commence at the setting time, with the thermo-hygral model incorporating the relative humidity drop due to self-desiccation, as described in Chapter 3.6.2.1. Therefore, before the initiation of drying at 7 days, the numerical results show a slight drop in relative humidity for all the presented depths.

Additionally, Azenha et al. [91] simulated the drying shrinkage through the Kwak equation (Equation (2.79)) estimating a value of 539μ for the drying shrinkage of the investigated concrete. In the present simulations, the drying shrinkage is combined with the basic shrinkage ($539\mu + 56.2\mu$) and the dKwak equation (Equation (3.47)) is used in the numerical simulations.

4.4.2 HYGROTHERMAL ANALYSIS OF THE 0.5 m RC TIE AND DEPENDENT PROPERTIES OF HYGROTHERMAL RESULTS

The case study is a 0.5 m RC tie that dries in a slab-like flow, similar to the relative humidity tests presented in Fig. 156. Given that the current hygral model accurately simulates the relative humidity profiles for H10, H15 and H20, it is hypothesised that the same numerical model will also provide a representative relative humidity profile for the 0.5 m (H50) element considered in the case study. Therefore, the same thermo-hygral model, boundary conditions, and drying start time of 7 days are considered, with the only variation being an increase in the element thickness. Due to the increased element thickness, the temperature resulting from the thermal analysis becomes more important for the present numerical simulations. Fig. 157 shows the thermo-hygral model results for the numerical simulation of the 0.50 m thick tie.

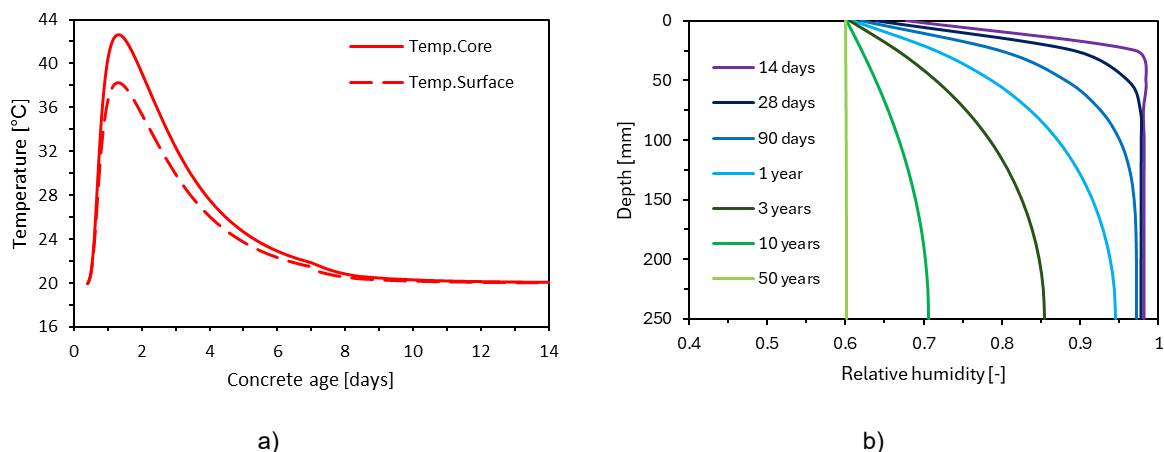


Fig. 157 – Thermo-hygral results: a) temperature evolution; b) relative humidity distribution for different concrete ages.

The temperature at the core reaches a maximum value of approximately 43 °C, while the temperature at the surface reaches a maximum value of approximately 38 °C. These maximum temperatures occur 1.5 days after casting. The relative humidity distribution shows a noticeable drop at the surface (depth of 0 mm) by 14 days, approaching the ambient relative humidity of 0.6. In contrast, the core (depth of 250 mm) retains high relative humidity, which decreases gradually over time as drying progresses. Simulation results indicate that drying at the core continues for up to 10 years, with equilibrium shown

only for the 50-year results, highlighting the inherently slow nature of moisture transport in concrete structures.

The creep parameters were determined based on model B3 (Equations (2.97)) through the concrete composition and compressive strength. Table 32 presents the creep model parameters used in the numerical simulation of the 0.50 m RC tie.

Table 32 – Creep model parameters used in the numerical simulation of the 0.50 m RC tie.

Parameter	Value	Parameter	Values
q_1	$20.56 \times 10^{-6} \text{ MPa}^{-1}$	-	-
q_2^*	$117.46 \times 10^{-6} \text{ MPa}^{-1}$	c_2	1
q_3^*	$2.32 \times 10^{-6} \text{ MPa}^{-1}$	c_3	1
q_4^*	$5.31 \times 10^{-6} \text{ MPa}^{-1}$	c_4	1
c_0	0.005	α_e	10
k_1	$5.25 \times 10^{-1} \text{ MPa} \cdot \text{K}^{-1}$	$\alpha_r = \alpha_s$	0.1
b_{RMPS}	0	$Q_e = Q_s$	$33.26 \text{ kJ} \cdot \text{mol}^{-1}$
p_{RMPS}	0	Q_r	$41.57 \text{ kJ} \cdot \text{mol}^{-1}$

In the layered approach, drying creep was simulated using the numerical model proposed by Benboudjema et al. [149] (see Chapter 2.4.3.5), calibrated to match the cross-sectional deformation of the B3 drying creep compliance model. The pointwise THM model considers the MPS with $k_1 = 5.25 \times 10^{-1} \text{ MPa} \cdot \text{K}^{-1}$, which would lead to long-term drying creep strains similar to those considered in the layered approach. Differences in the development of the drying creep strains are expected to be minimal, as the MPS (used in the pointwise THM model) and model B3 drying creep (used in the layered approach) share the same theoretical and numerical calibration background [2]. Fig. 158a) shows the free shrinkage at both the surface and core of the element, and the resultant average shrinkage calculated through either a linear or a cracking model for an unrestrained 0.50 m thick tie using the pointwise THM model. Fig. 158b) shows the evolution of creep compliance at two integration points, one at the surface and the other at the core of the element, alongside the corresponding evolution of relative humidity.

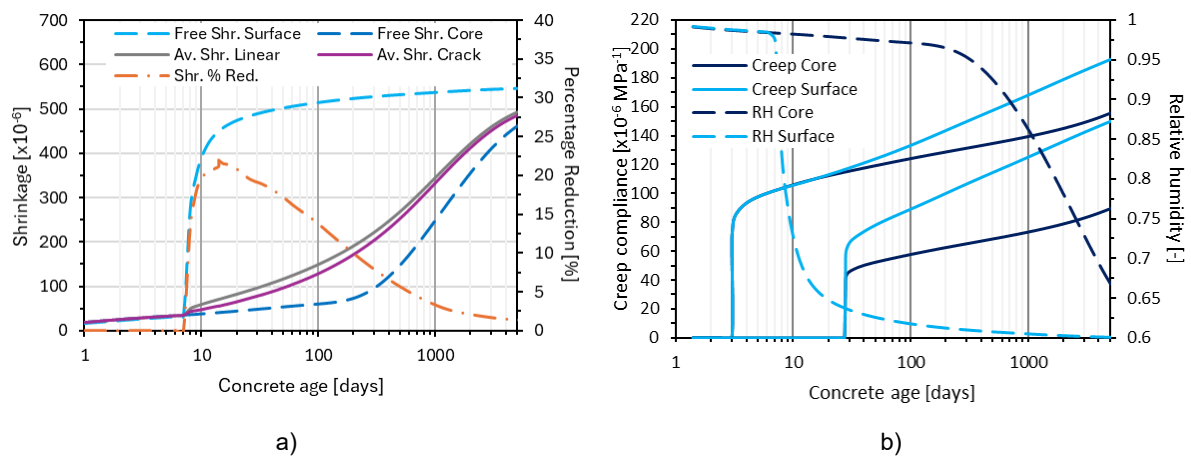


Fig. 158 – a) Comparison of different shrinkage approaches; b) free creep compliances at the surface and core of concrete.

In Fig. 158, the free shrinkage at the surface (Free Shr. Surface) increases rapidly due to the drop in relative humidity, whereas at the core (Free Shr. Core) it evolves more slowly. The average shrinkage

in the analysis with the cracking model (Av. Shr. Crack) shows smaller shrinkage values than the analysis without cracking (Av. Shr. Linear). This occurs due to the microcracking at the surface of the RC tie, which is caused by a sudden drop in the relative humidity at the surface after drying initiation. Microcracking relaxes the self-equilibrated stresses over the element cross-section that lead to the strain compatibility, justifying the smaller average shrinkage values in the analysis with cracking. The orange dashed-dot line indicates the numerical shrinkage percentage reduction due to cracking (Shr. % Red.), showing that it can exceed 20% in the days after drying initiation, but slowly decreases over time with drying progression. The result of the Av. Shr. Crack analysis is more representative of the real shrinkage of the structural element than the Av. Shr. Linear, making it a more accurate indicator of the shrinkage expected in experimental tests or in the design code shrinkage formulations [51]. For the subsequent analysis of RC tie, whenever the average approach is considered, the shrinkage input is defined by the average shrinkage shown in Fig. 158a) (Av. Shr. Crack) for all the finite elements.

In Fig. 158b), the two creep compliance curves for loading at 3 days reveal similar behaviours after the load is applied, with long-term creep compliance in the surface elements tending to increase over time due to rapid drying effects. In the creep simulations performed at 28 days, the free creep compliance curves diverge after loading, demonstrating that the elements exposed to drying exhibit higher free creep strains than those in the core. This discrepancy arises because drying started at 7 days, affecting the maturity of the concrete at the surface of the element. Consequently, the free creep compliance at 28 days for the surface element resembles the behaviour of concrete with an effectively younger age than the concrete in the core. These results highlight the differences in the local behaviour of the concrete when using the pointwise THM model that evaluates material behaviour locally, contrasting with classic models that typically consider a generalised creep model equal to all finite elements.

4.4.3 NUMERICAL SIMULATION OF THE 0.50 M THICK RC TIE

The reinforced concrete tie is 0.50 m thick, 2 m long and 0.1 m wide. The RC tie incorporates reinforcement installed at both the top and bottom surfaces, with a total area of $A_s = 24.94 \text{ cm}^2/\text{m}$. The degree of restraint is set to $R = 2/3$, determined for a scenario without cracking or creep at 28 days. The degree of restraint represents the ratio of restrained deformation to the free deformation of concrete and is modelled using springs with uniform stiffness. The stiffness of the springs is determined through the following equation:

$$k_{total} = \sum_{i=1}^{n_s} k_i = \frac{R}{1-R} \frac{E_c A_c}{L} \quad (4.15)$$

where A_c is the cross-sectional area of concrete, n_s is the number of springs and k_i is the stiffness of each spring.

Azenha et al. [91] performed experimental tests for the modulus of elasticity at 7, 14 and 28 days, obtaining 27 GPa, 30 GPa and 32 GPa, respectively. The modulus of elasticity at 28 days of 32 GPa is used to calculate the springs' stiffness. A tying condition is prescribed at the spring nodes to ensure that

all the nodes have the same displacement in the restraint X direction (plane section condition). Good bond-slip conditions were assumed, according to MC2010 [50] (see Equation (3.162)), resulting in $\tau_{bm} = 15.41$ MPa. The cracking model switching from rotate to fixed cracks is used with a switching threshold corresponding to 0.01 mm crack width. The RC tie is only subjected to the temperature and relative humidity histories (shown in in Fig. 159), resulting in thermal strains and shrinkage strains without any additional external loading. The analysis are carried out since the setting time up to 50 years. Fig. 159 shows a schematic representation of the FE mesh used in the mechanical analysis of the 0.5 m RC tie.

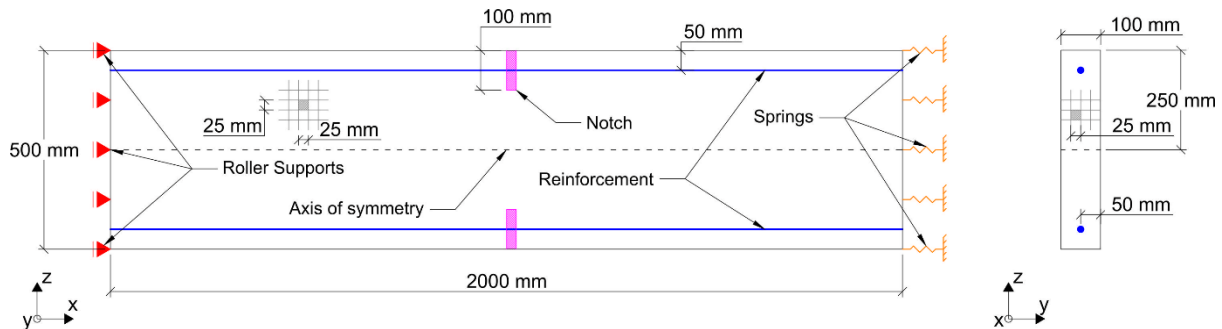


Fig. 159 – Schematic representation of the FE mesh used in the mechanical analysis of the 0.50 m RC tie.

Additional supports were introduced in the y and z directions to prevent rigid body movements.

Only half of the height (500 mm) of the RC tie is simulated due to the symmetry conditions. The previous parametric studies conducted with the layered approach were performed for a plane stress analysis (2D). Since the present pointwise THM model was developed for a 3D analysis, the numerical model is set to a tie slice with the reinforcement spacing dimensions corresponding to 100 mm.

4.4.4 RESULTS AND DISCUSSION OF THE NUMERICAL SIMULATIONS OF THE 0.5 M RC TIE

The support reactions were determined at the restraint extremities of the numerical model. The results are presented for all the element thicknesses, corresponding to twice the total forces of the symmetric model. Fig. 160 compares the evolution of the resultant support reactions for the entire element thickness for the three numerical approaches considered.

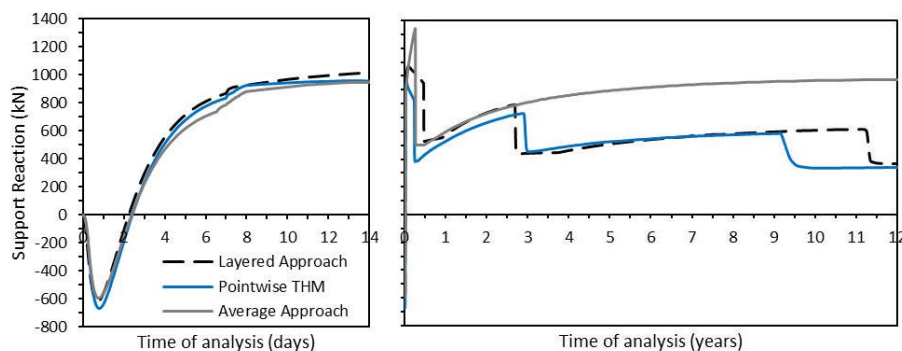


Fig. 160 – Evolution of the results and support reaction for the entire element thickness (0.50 m).

The results indicate a good agreement between the evolution of support reactions for the layered approach and the pointwise THM model. During the early ages, compressive forces are generated due to the rise in temperature owing to cement hydration. A maximum compressive force of -600 kN is reached at approximately one day. Following temperature cooldown, the compressive support reactions start to decrease and turn into tensile forces. At 7 days, before drying initiation, the support reactions are approximately 800 kN. Fig. 157 shows that the temperature reaches equilibrium at 7 days, resulting in residual tensile forces. The appearance of this residual tensile force occurs due to the temperature rise in the early stage and cooldown in a much stiffer phase, as investigated in detail in Chapter 4.2. The differences in the support reaction evolution for all analyses during the first 14 days are very small and can be justified by small changes in the creep model. Over the long term, a reduction in the reaction force due to crack formation is observed at approximately 0.5 years. As drying progresses, more through-cracks appear, represented by a sudden reduction in support reactions occurring at approximately 3 years and between 9 and 12 years. The differences in the age and support reaction forces at the cracking occurrence for the layered approach and pointwise THM model are relatively minor. In contrast, while showing similar behaviour in the early stages, the average approach can only develop one through-crack throughout the analysis, occurring under higher support reaction forces than in the other analyses. Fig. 161 shows the crack pattern at the end of the analysis, 50 years, for the average approach and the pointwise THM model (showing the total element thickness with no symmetry considerations).

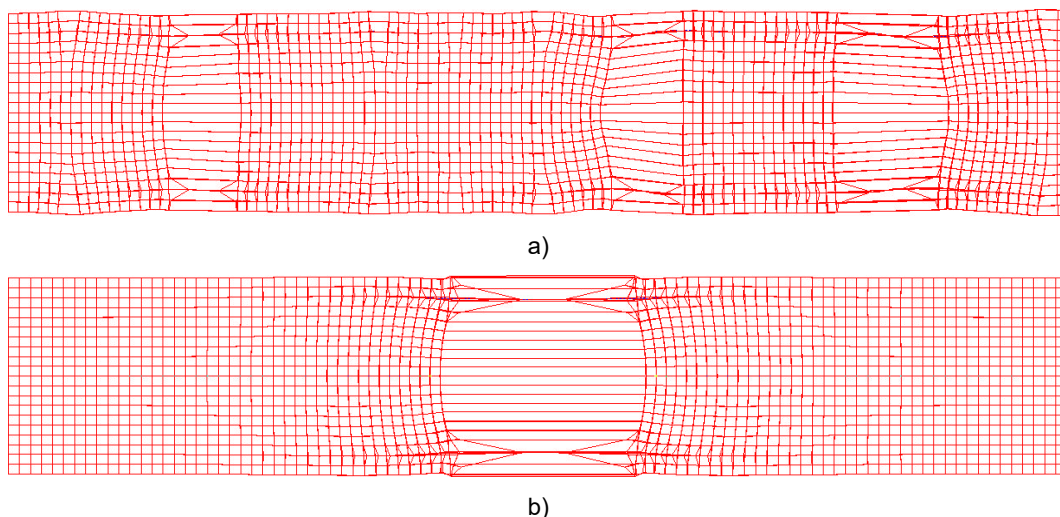


Fig. 161 – Deformed meshes at 50 years: a) pointwise THM model; b) average approach.

The differences are pronounced in terms of crack patterns. The deformed mesh of the numerical analysis using the pointwise THM model presents three through-cracks and several drying cracks exhibiting a triangular shape, limited to the mesh top and bottom finite elements. The drying cracks in triangular shape are generated due to drying progression as the through-cracks; however, due to the opening of the through-cracks in the vicinity of those, the degree of restraint of the concrete between two through-cracks decreases, and halts the cracking progression of those cracks. Similar deformed meshes are obtained using the layered approach. In contrast, the average approach deformed mesh does not exhibit drying cracks, with deformation localised only at the first through-crack. Fig. 162 shows the crack width evolution at the surface for the first through-crack of the three analyses.

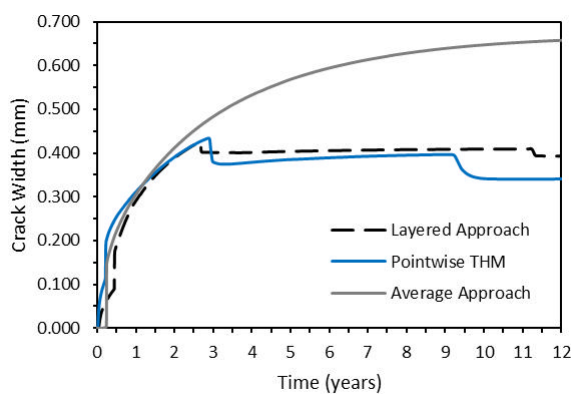


Fig. 162 – Crack width evolution at the surface for the three analyses.

The results show similar crack widths for both the pointwise THM and the layered approach, where the crack width increases over time until the formation of a second through-crack. Subsequently, the crack width decreases slightly and remains almost constant throughout the analysis. When a new through-crack forms, the crack width slightly drops and remains constant throughout the analysis. In contrast, the crack width in the average approach continues to increase over time, reaching values that are 1.5 times larger than those observed in the other analyses. This is due to the absence of self-equilibrated

stresses, which hinder the formation of new drying cracks and concentrate all the deformation in the existing through-crack.

Overall, the results show similar numerical predictions between the pointwise THM model and the layered approach, validating the use of the former for numerical simulation of long-term drying in structural elements. Compared to the layered approach, the present pointwise THM model eliminates the need for pre-analysis of hygrothermal effects in the material behaviour, as the material model is evaluated directly during mechanical analysis rather than being provided by the user. The pointwise THM model comprehensively considers the influence of local temperature and relative humidity values in a straightforward manner and eases the performance of multi-parametric studies of the environment and boundary conditions, which would be highly resource-consuming when employing the layered approach.

4.4.5 INVESTIGATION OF THE REINFORCEMENT DESIGN AND DEGREE OF RESTRAINT ON LONG-TERM CRACK WIDTHS

4.4.5.1 Minimum reinforcement design according to Eurocode 2

In the design of reinforced concrete structures, the required reinforcement quantities are often conditioned by cracking criteria. Design standards such as Eurocode 2 [51] define methods for design reinforcement to control cracking, assuming a limit stress in the reinforcement corresponding to the tensile forces in the concrete immediately before it cracks. The minimum reinforcement is calculated according to the following equation:

$$A_{s,min} \sigma_s = k k_h f_{ctm} A_c \quad (4.16)$$

where $A_{s,min}$ is the minimum reinforcement, σ_s is the steel stress, k is a parameter that depends on the loading, k_h is a parameter that depends on the element thickness, f_{ctm} is the mean tensile strength of concrete and A_c is the cross-section area of concrete.

The formulation presented is of quick application, as it significantly simplifies the physical behaviour of structural elements with the use of the parameters k and k_h . In pure tensile situations, the k parameter can be considered equal to 1. The parameter k_h depends on the thickness of the RC element. Recently, the new version of EC2 (prEN1992-1-1:2023) presented differences in calculating the minimum reinforcement. For concrete elements subjected to pure tension, the differences are restricted to the values adopted for the k_h parameter. Fig. 163 shows the differences in the parameter k_h determined according to EN1992-1-1:2010 and prEN1992-1-1:2023.

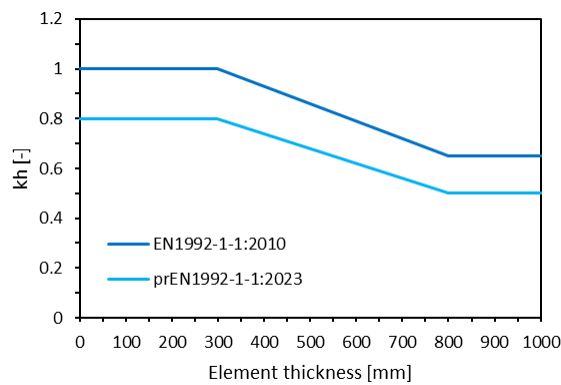


Fig. 163 – Evolution of parameter k_h according to EN1992-1-1:2010 and prEN1992-1-1:2023.

In EN1992-1-1:2010, this parameter varies linearly between 1.0, for elements up to 300 mm thick, and 0.65, for elements with a thickness of 800 mm. In prEN1992-1-1:2023, the k_h parameter varies between 0.8, for elements with a thickness of 300 mm, and 0.5, for elements with a thickness of 800 mm. These changes result in a proportional reduction in reinforcement to control cracking of 20% to 23% compared to the values recommended in EN1992-1-1:2010.

This chapter investigates the limitations of simplification in designing minimum reinforcement to control cracking due to restrained deformations. To this end, the pointwise THM model is used to perform a parametric investigation of the long-term behaviour of a reinforced concrete tie constrained from the early ages with different reinforcement solutions. The material models, hygrothermal properties, boundary conditions and geometry modelling are the same as those employed in Chapter 4.4.1. Only temperature strains and shrinkage are applied to the element based on the temperature and relative humidity in Fig. 157, with no additional external loading.

The RC tie investigated represents the behaviour of an infinite slab or wall with a thickness of 0.50 m. According to the value of k_h in Equation (4.16) and Fig. 163, the considered thickness is within the mid-range values of the linear transition between the upper and lower limits. The reinforcement was designed according to EN1992-1-1:2010 and prEN1992-1-1:2023 for the criterion to avoid yielding of the reinforcement. The reinforcement was installed and divided in an analogous way near the top and bottom faces, resulting in configurations of bars of $\phi 12/0.091$ in the first case and $\phi 12/0.115$ in the second. These reinforcement solutions fulfil Equation (4.16) for EN1992-1-1:2010 and prEN1992-1-1:2023, respectively. Two degrees of restraint are considered: $R = 2/3$ and $R = 1$, modelled by springs according to Equation (4.15). Table 33 summarises the numerical analyses considered in this parametric study.

Table 33 – Summary of the numerical analysis: reinforcement and degree of restraint.

Analysis	Label	Reinforcement	Spacing	Degree of Restraint
EN1992-1-1:2010 $R=2/3$	EC2:2010 $R=2/3$	$\phi 12$ mm	90.7 mm	2/3
EN1992-1-1:2010 $R=1$	EC2:2010 $R=1$	$\phi 12$ mm	90.7 mm	1
prEN1992-1-1:2023 $R=2/3$	EC2:2023 $R=2/3$	$\phi 12$ mm	114.7 mm	2/3
prEN1992-1-1:2023 $R=1$	EC2:2023 $R=1$	$\phi 12$ mm	114.7 mm	1

4.4.5.2 Results and discussion

The differences in the evolution of the temperature and relative humidity over the cross-section of the element may lead to different local stresses. Fig. 164 shows the concrete stress evolution in the early ages at the core and surface of the element and the tensile strength evolution for the analysis considering $R = 2/3$ and $R = 1$.

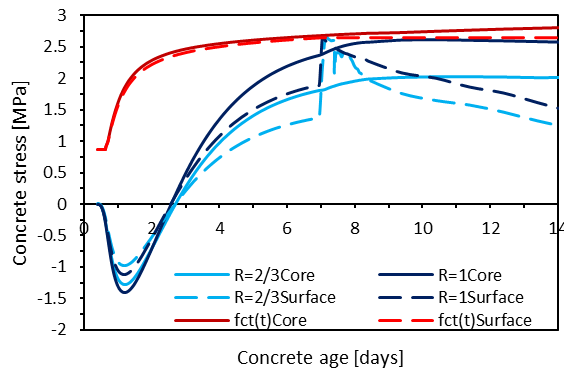


Fig. 164 – Tensile strength evolution and stress in the early ages for analysis with $R = 2/3$ and $R = 1$.

The results show that restraint conditions in the RC tie generate compressive stresses in the early ages, around 1.0 to 1.5MPa, which turn into tensile stresses after cooling. This effect is related to the maturity of the concrete, where compressive stresses appear during the heating phase, while tensile stresses arise after cooling occurs, which occurs in a much stiffer stage (as shown experimentally and numerically in Chapter 4.2). In the analyses that consider the degree of restraint equal to 1, the higher degree of restraint leads to an increase in the initial compressive stresses during the temperature rise and an increase in the residual tensile stresses after cooling down. The residual tensile stresses in the core are higher than those observed on the element's surface due to the differences in temperature history resulting from the thermal analysis. At 7 days, the formwork removal exposes the surface finite elements to the outside environment, resulting in the loss of relative humidity and a subsequent increase in the stress for the surface elements of all analyses reaching the tensile strength value. At this stage, the surface elements experience surface microcracking, which softens the stress evolution over the following days. Despite those, the tensile strength in the core continues to evolve due to high relative humidity values, in contrast to the tensile strength in the surface elements, which remains constant over the remaining analysis time.

Fig. 165 shows the results of the deformed FE mesh for the EN1992-1-1:2010 $R = 2/3$ analysis for different times (considering the symmetry plane at half of the thickness of the element).

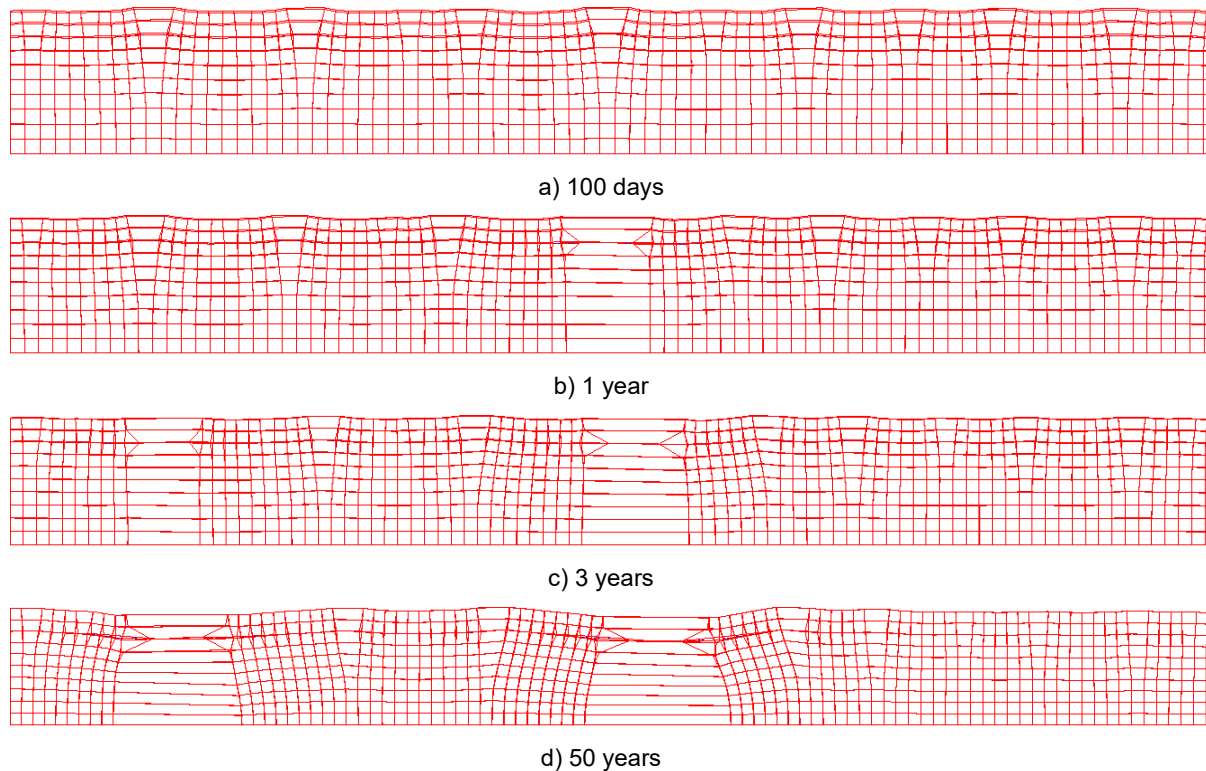


Fig. 165 – Deformed mesh for the analysis EN1992-1-1:2010, with $R=2/3$ for: a) 100 days; b) 1 year; c) 3 years; d) 50 years;

The deformed mesh shown in Fig. 165 is similar to that in Fig. 161 b). However, Fig. 161 b) presents the full thickness of the element without symmetry conditions, while Fig. 165 shows only the top half of the RC tie due to symmetry. The differences between the two analyses are due to minor variations in the reinforcement configuration, which result in slight changes in the locations of the drying cracks. This variability is common when the crack locations are not imposed in the numerical simulations of crack patterns of RC elements that include multiple cracks. Even minor parameter changes, negligible from an engineering standpoint, can lead to variations in crack location. Nevertheless, these differences do not affect the overall results, provided the crack pattern remains realistic, for example, by avoiding crack localisation in finite elements adjacent to supports or nodes where the imposed deformation is applied (notice that in the simulations of the present chapter, there are no imposed deformations).

The cracking process begins with localised cracks on the element's surface, which progress slowly and almost synchronously towards the core, driven by the drying progression. When cracking reaches the core of the RC tie, the first through-crack occurs, penetrating the entire thickness of the element. Consequently, the restraining forces are resisted by the reinforcement at the through-crack. These forces are transferred to the concrete, along the reinforcement length, through the steel-concrete bond. As drying continues, new through-cracks can form, while at the same time, there is an increase in the opening of existing through-cracks. In the long term, the crack opening in the first-formed through-crack tends to be larger in the core of the element than on the surface. This effect is due to strain compatibility resulting in strain distribution over a greater number of drying cracks at the reinforcement level than the smaller number of through-cracks responsible for the same strain in the element core (see Chapter 4.3).

Fig. 166 shows the steel stress and the crack width calculated at the element's surface.

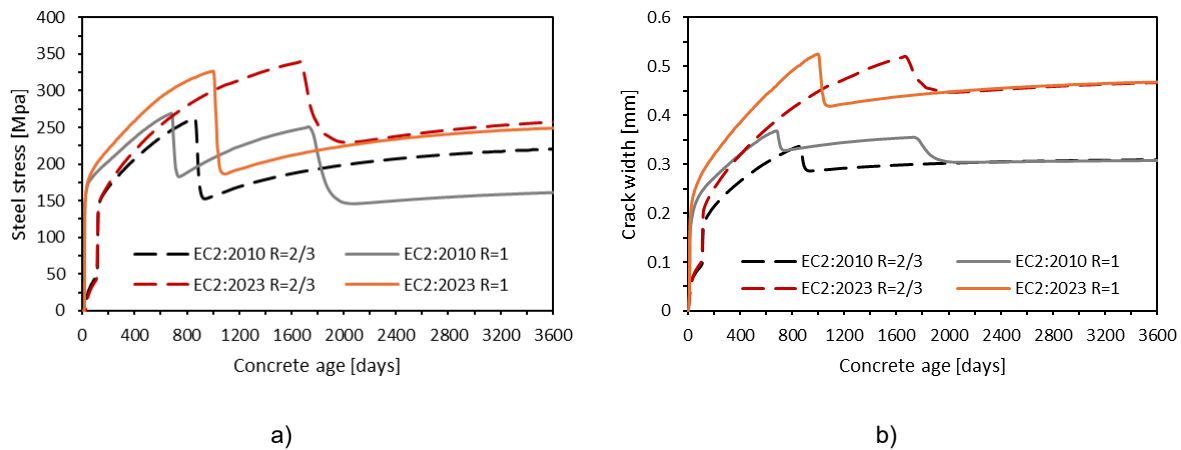


Fig. 166 – Evolution over time for: a) reinforcement stress; b) crack widths.

The stresses in the reinforcement are significantly lower than the yielding limit of the steel ($\sigma = 500$ MPa) that was considered in the design stage. The maximum stress value in the reinforcement is generally observed when the second through-crack is generated, corresponding to a noticeable drop in the stresses in the reinforcement. In analyses with reinforcement according to EN1992-1-1:2010 (EC2:2010 R=2/3 and EC2:2010 R=1), maximum reinforcement stresses of 250-275 MPa are observed, while in analyses with reinforcement according to prEN1992-1-1:2023 (EC2:2023 R=2/3 and EC2:2023 R=1), the maximum reinforcement stresses are in the order of 325-350 MPa. The degree of restraint seems to have almost negligible influence on the stress peaks. However, it influences the time of occurrence of cracking, where a higher degree of restraint leads to early cracking, while a lower degree of restraint leads to later cracking.

Fig. 166 b) shows the evolution of crack opening over time in the crack with the largest opening in each analysis (first-formed through-crack). In the analyses corresponding to EN1992-1-1:2010 (EC2:2010 R=2/3 and EC2:2010 R=1), the maximum crack opening varies between 0.30 and 0.35 mm. In the analyses for prEN1992-1-1:2023 (EC2:2023 R=2/3 and EC2:2023 R=1), the maximum crack opening varies between 0.45 and 0.55 mm. Noticed that reinforcement was not designed for the crack width control, but to avoid yielding in the reinforcement (500 MPa). After forming a new through-crack, the crack opening tends to decrease, in line with the reduction of the restraint force. It is important to note that crack opening is strongly influenced by the bond-slip conditions between the concrete and the reinforcement and by the contact perimeter of the reinforcement, which is a function of its diameter, adopted in the design phase. The degree of restraint seems to have a negligible effect on the maximum crack width values, with similar values of the long-term crack widths for the same analysis with different degrees of restraint. Nevertheless, a higher degree of restraint leads to the acceleration of cracking occurrence.

Fig. 167 shows the evolution of steel stress, shear slip and shear stresses over the reinforcement length for the time before opening the second through-crack, corresponding to the maximum steel stress in the numerical analyses.

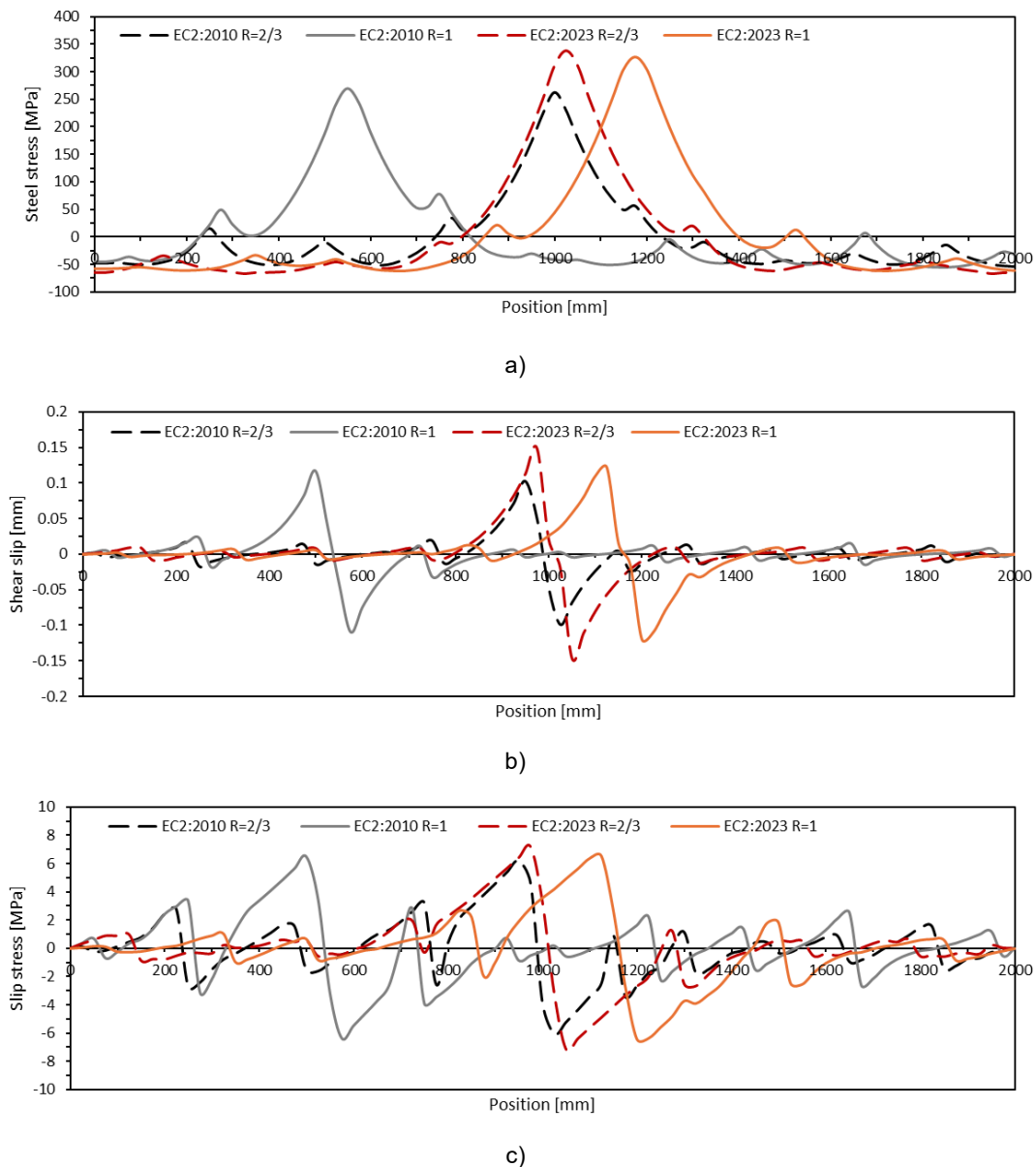


Fig. 167 – a) Stress evolution; b) slip; c) bond stress for the time before the maximum stress is reached in the reinforcement.

Along the length of the reinforcement, it is possible to identify the maximum stress peak corresponding to the location of the first through-crack. Small stress peaks, which develop periodically along the reinforcement, are visible and correspond to the other drying crack zones. The shear slip results show that the maximum slip occurs close to the location of the through-crack, suggesting that this is the region with the largest crack opening. This observation is consistent with the analysis of the bond stresses. The bond stresses reach maximum values around 8 MPa in the same region.

In the reinforcement configurations analysed, the stresses observed in the steel are relatively lower than the design assumptions. The EN1992-1-1:2010 formulation is more conservative than the prEN1992-1-1:2023 version. prEN1992-1-1:2023 allows the amount of reinforcement used in the minimum

reinforcement design to be reduced. For this case study, the results lead to an optimised use of reinforcement while still satisfying the assumed design criteria. However, the conclusions drawn should be considered specific to this case. It is important to note that Equation (4.16) was formulated to address multiple design conditions that differ from those considered in the present investigation. The present case study using the pointwise THM model shows that the structure response, considering the influence of local temperature and relative humidity values and local material properties, significantly differs from the behaviour considering averaged temperature, relative humidity values and material properties. The present findings show that the pointwise THM model can be used to analyse this realistic behaviour and the effectiveness of the design assumptions for any particular case of interest.

5

CONCLUSIONS

This chapter presents the conclusions of the PhD thesis, addressing the main objectives and applications of the research conducted. The discussion focuses primarily on the key developments presented in Chapters 3 and 4, which comprise the core contributions of this PhD work. The conclusions are organised by topic, with final remarks at the chapter's end. Each section also outlines potential future research directions that could build upon and enhance the findings of this thesis.

5.1 THERMO-HYGR0-MECHANICAL FRAMEWORK

The research presented in Chapter 3 led to the development of an advanced pointwise thermo-hygro-mechanical model tailored to simulate modern concrete behaviour under coupled physical processes. The following key contributions and insights were achieved:

- extension of the thermo-hygral model to include basic shrinkage as a self-desiccation model incorporating temperature and relative humidity function in the basic shrinkage. This enhancement provides a more realistic representation of the relative humidity results, accounting for the effects of ongoing drying in the slowdown of hydration and, consequently, effects on basic shrinkage. The provided relative humidity variations due to self-desiccation influence other hygral-dependent models like the transient creep model. The transient creep in the absence of drying remains close to the basic creep due to the small relative humidity drop of the analysed concrete mixtures, but may be an important feature when dealing with concretes with huge basic shrinkage values subjected to restrained conditions since the early ages;
- the single particle hydration model was reviewed to incorporate hydration into the macroscale simulations. However, it was found that the model's complexity, accuracy, and high number of empirical parameters make it less practical than the transformed times approach for current macroscale analysis. Future work should explore possible correlations between empirical parameters in the transformed time and single-particle hydration approaches to enable more unified formulations;
- multiple shrinkage models were implemented in the pointwise THM model, allowing for better representations of shrinkage development for different concrete mixtures. The Kwak shrinkage model, dependent on relative humidity, was reformulated as a rate-based law labelled the dKwak model. This new strategy allows the shrinkage simulation to be more straightforward, maintaining the advances of the original Kwak formulation. Additionally, the model allows the

definition of the equivalent shrinkage coefficient based on the ultimate shrinkage value. The rate-law function also gives flexibility to the numerical simulations since the equivalent shrinkage only needs to be calibrated to the relative humidity histories that are expected to occur in the experiment, in contrast with the previous approach that would require the entire description of the shrinkage behaviour, even if lower relative humidities were not achieved in the experiment. This approach means that the shrinkage model is kept accurate for the numerical simulation of the entire drying process, like the original Kwak shrinkage model. However, it may also be used to simulate shrinkage in the presence of small relative humidity drops, for example, in the numerical simulation of basic shrinkage through the self-desiccation model;

- basic creep was modelled using the solidifying Kelvin chain theory and calibrated through a modified version of the Post-Widder formula that incorporates additional empirical parameters to achieve a better curve fit. A configuration of 10 Kelvin-Voigt elements reliably reproduces ageing and non-ageing creep compliance up to 250 years, showing the long-term modelling capacities of the creep model. To improve usability, the calibration process of the solidifying Kelvin chain was embedded within the pointwise THM model itself, eliminating the need to externally provide the modulus of elasticity of the Kelvin Voigt element in the Kelvin Chain. This feature contributes to easing the model accessibility. The microprestress theory was implemented to simulate transient creep effects, enabling the exploration of time-dependent relaxation behaviour under varying hygrothermal effects. The model's formulation regarding the microprestress variable offers flexibility for calibrating diverse new relaxation laws and future investigations. These creep modelling advancements contribute to a more physically representative and computationally efficient simulation framework for concrete creep under hygrothermal effects;
- the total strain models with rotating and fixed crack orientations and a single-crack model based on strain decomposition were integrated into the pointwise THM model. A novel algorithm was proposed to incorporate maturity effects into the total strain approach, enhancing its applicability to serviceability assessments and delayed cracking analysis. These cracking models were subjected to a comprehensive validation process through numerical simulations involving multiple loading, unloading, and reloading scenarios. The results were benchmarked against equivalent models implemented in DIANA FEA, demonstrating good agreement between those. This comparative validation confirms the reliability of the implemented models and supports their use in research and practice, while also providing the added flexibility to combine those crack models with other implemented material models. The combination of rotating and fixed crack concepts represents an important characteristic for the pointwise THM model in the numerical simulation of complex crack patterns, since the microcracking initiation towards the macrocrack propagation.

While the pointwise THM model developed in this thesis offers a comprehensive framework for simulating the coupled thermo-hygro-mechanical behaviour of concrete, several areas remain open for further refinement and exploration. Addressing these aspects would enhance both the physical realism and computational robustness of the model, and could significantly expand its range of applicability:

- the hygral and shrinkage model was developed with a focus on drying processes. This confines the use of the present THM framework to structures subjected only to static environmental conditions (e.g. interior structural elements of a building). Most structures are subjected to complex dynamic environments, including drying and wetting cycles. The sorption curves show hysteresis behaviour between drying and wetting cycles, affecting the moisture transport and shrinkage equations. The pointwise THM model needs to be updated to include this hysteresis behaviour to allow numerical simulations of drying and wetting. Although slow moisture transport reduces the effect of a short-lived dynamic environment on the element's surface, future investigations should include the development, implementation, investigation and validation of moisture transport and shrinkage coefficient evolution under wetting and drying cycles;
- the current cracking framework primarily relies on the Rankine failure criterion, which includes the hydrostatic stress effects in the crack initiation. While Rankine's failure criterion is popular for the numerical simulation of cracking in concrete structures, it may not be adequate in the numerical simulation of complex multiaxial loading conditions, particularly in regions where confinement or triaxial stress states are relevant. Future work should explore the new formulations of the total strain models, considering the decomposition of strain and stress into deviatoric and hydrostatic values and formulating the respective stress-strain laws;
- the implemented single-crack model based on strain decomposition shows potential but remains limited in handling multiple crack orientations. Extending this formulation to a multi-fixed crack model would improve its ability to simulate distributed cracking and damage accumulation in complex loading scenarios;
- shear behaviour in the crack plane was modelled using a constant shear retention approach, which is widely used in numerical simulations of cracking. However, the literature presents a range of alternative shear models that may be more accurate in reproducing shear behaviour under specific conditions beyond the scope of the field applications considered in this PhD work. The shear behaviour should be investigated in detail in future developments, and new models may be implemented. Also, other tension-softening laws beyond MC2010 and Hordijk tension softening models may be implemented to enhance the model's versatility and applicability. A particular research topic consists of investigating the bilinear ascending part of the MC2010 tension softening model and extending this prior to cracking behaviour to other tension softening models;
- the implemented cracking models remain sensitive to numerical issues associated with strain localisation, particularly in large finite element meshes, which can adversely affect convergence. While careful time step discretisation can partially mitigate these issues, a more robust solution would incorporate regularised continuum models (non-local or gradient-enriched damage formulations). These approaches offer improved stability and convergence behaviour by reducing mesh sensitivity and more accurately capturing the spatial distribution of damage in regions prone to crack localisation;

- although the model performs efficiently on small meshes, simulations involving medium to large meshes (i.e., $> 10\,000$ elements) reveal a significant increase in computational time, especially when using cracking models. The present numerical model code was developed carefully to keep the code readable and direct. Nevertheless, little time was spent improving the runtime and optimising the code. Future research could include optimising the model computation to improve the analysis runtime;
- while the current implementation of the pointwise THM model was developed in a 3D solid finite element context to address general structural problems, it is recognised that in many practical cases, 3D analysis can be efficiently replaced by reduced-dimensional models or simplified formulations using alternative element types. Future work may focus on reformulating the present 3D model to accommodate these alternative analysis types, thereby enhancing computational efficiency and broadening its applicability to a larger range of engineering problems without compromising its core capabilities. It may also be necessary to support alternative iterative methods that require access to the tangent stiffness matrix, which was not computed in the pointwise THM model, since the iterative method selected for the numerical analysis performed in this PhD thesis was the BFGS iterative method (secant method). These improvements would allow flexibility in applying the pointwise THM model and exploring new numerical approaches to improve convergence in nonlinear problems.

5.2 NUMERICAL SIMULATION OF THE RELATIVE HUMIDITY AND SHRINKAGE TESTS

The application of the pointwise THM model to the simulation of drying and shrinkage in IntegraCrete concrete elements led to the following key findings and contributions:

- the numerical simulations demonstrated good agreement between the predicted and experimentally measured relative humidity, validating the hygral model's parameters and capability to reproduce hygral profiles across different concrete element thicknesses (10 cm and 15 cm);
- the shrinkage behaviour simulated using the previously calibrated hygral parameters, combined with the dKwak shrinkage model, showed close correspondence with experimental shrinkage measurements. This validation confirms that the model can accurately simulate the shrinkage of modern concrete mixtures incorporating additives. The present investigations show that modern concretes exhibit nonlinear sorption behaviour, affecting the evolution of shrinkage. In contrast, traditional concretes (e.g., constituted by CEM I, water, and aggregates, with no additives) can often be assumed to exhibit linear sorption and constant shrinkage coefficients. These findings highlight the need for more sophisticated shrinkage and sorption models when simulating the behaviour of modern concrete materials.

The findings show the importance of flexibility within the pointwise THM framework, particularly the ability to accommodate different shrinkage laws and moisture transport formulations. Future applications should continue exploring and calibrating these models for diverse concrete compositions to ensure accurate long-term performance predictions in structural and durability assessments.

5.3 NUMERICAL SIMULATION OF THE SHRINKAGE AND CREEP TESTS FROM BRYANT AND VADHANAVIKKIT

The application of the pointwise THM model to the simulation of shrinkage and creep tests from Bryant and Vadhanavikkit led to the following key findings and contributions:

- an algorithm was introduced to calibrate the hygral and shrinkage parameters by establishing boundary limits and quantifying the influence of each parameter on the moisture distribution across the cross-section. This approach enabled a structured calibration process for different specimen geometries and exposure conditions when there is no relative humidity data available for the numerical calibration of the hygral model;
- the calibrated model accurately captured both the size effect and variations in drying conditions, confirming that a single set of parameters can be applied as long as the concrete mixture remains unchanged. This underscores the model's versatility in handling different structural configurations without requiring recalibration of the material parameters;
- as previously observed by other authors, the original microprestress theory (MPS) was inadequate in capturing the size-dependent behaviour of drying creep observed in the experimental campaign. To address this, a refined microprestress theory (RMPS) was proposed, which retains the hygral coupling of MPS while introducing an additional parameter to account for extra drying creep due to transient effects. The RMPS model agreed well with experimental creep data across varying specimen sizes and drying conditions. These findings improve the numerical simulation of drying creep for different elements with the same concrete mixture. Default parameters were proposed for the RMPS model in this study. However, further research is needed to test the RMPS under different thermo-hygral histories. Future modifications may affect the microprestress relaxation function and the newly introduced parameters. Future validation work should involve dedicated creep experiments, ideally incorporating internal relative humidity measurements to validate the present numerical dependence of the drying creep on the relative humidity history;
- the comparison of slabs and prisms' shrinkage and creep numerical results and experimental measurements revealed the need to introduce a shape factor to establish a consistent relationship between notional size for different drying conditions. Based on experimental results, preliminary values for this shape factor were proposed for slabs and prisms. These findings highlight the importance of drying configuration in analysing the experimental data. The findings also show the importance of using numerical tools like the pointwise THM model to investigate and assess differences in the concrete behaviour due to physical changes affecting the moisture content evolution.

5.4 NUMERICAL SIMULATION OF THE UNRESTRAINED RING TEST

The application of the pointwise THM model to the simulation of drying shrinkage in prisms and in the unrestrained ring test led to the following key findings and contributions:

- the study revealed notable differences in shrinkage between prisms and rings, even when both specimens shared the same notional size. This finding suggests that geometry and boundary conditions have a measurable effect on shrinkage behaviour and that a direct comparison requires the introduction of a shape factor to account for these differences;
- the initial numerical simulations of the unrestrained ring test underestimated shrinkage compared to the experimental results. Improved agreement was achieved by accounting for slow drying through surfaces that were previously considered to be sealed. These findings raise two important questions: Whether the sealing used in the experimental ring tests was fully effective or whether the pointwise THM model requires further calibration to accurately simulate shrinkage in shotcrete mixtures. Future works may include experimental and numerical studies involving sealed and unsealed ring tests to clarify whether the discrepancies observed are due to the experimental boundary condition uncertainties or limitations of the current modelling approach for this type of material.

This case study shows the sensitivity of shrinkage simulations to the boundary conditions and sealing techniques, highlighting the importance of accurately defining element exposure surfaces in both experimental and numerical settings. Even small variations in moisture transport can significantly affect the global structural response. The results also demonstrate the capability of the pointwise THM model to identify potential moisture-related discrepancies not initially accounted for, like possible moisture transport occurring through the polystyrene formwork. Additionally, shotcrete mixtures may exhibit distinctly different hygral-dependent behaviour that may be associated with substantial microstructure changes occurring over larger periods than conventional concrete mixtures.

5.5 NUMERICAL SIMULATION OF THE RING TEST

The application of the pointwise THM model to the simulation of the restrained shrinkage ring tests under top and bottom, as well as radial drying, led to the following key findings and contributions:

- using a THM simulation approach for concrete restrained members enables an adequate consideration of the relevant complex phenomena required to predict the behaviour of restrained concrete elements throughout their service life. This was demonstrated by the ample agreement between experimental and numerical results for a concrete ring under top and bottom drying;
- temperature development in 70 mm × 70 mm concrete rings (and therefore, in even smaller cross-sections) of the particular concrete investigated, cured under standard conditions, can be disregarded. While a generalisation may not be claimed, similar behaviour is expected in concrete rings with similar geometries, mix proportions, and characteristics of those investigated in this study;
- drying shrinkage develops faster on the concrete ring under top and bottom drying than under circumferential drying. Consequently, moisture equilibrium is attained much earlier for the concrete ring under top and bottom drying;

- cracking generally occurs earlier under top and bottom drying conditions and is initiated at the inner circumference of the concrete ring. Although cracking was not detected in the test duration of 120 days, it is predicted in the numerical simulation at ~110 days;
- in the case of radial drying, microcracking occurs first at the outer circumference of the concrete ring due to the self-restraining effect which arises from moisture gradients. Drying progression leads to microcracking at the steel-concrete interface and eventually to the generation of a macrocrack;
- further understanding of the concrete ring behaviour can be reached in an experiment if the strain is measured in various positions along the steel inner circumference.

While several insights regarding restrained ring behaviour are obtained from the present study, it should be recognised that these pertain particularly to the ring geometries, drying conditions, and mix composition investigated. Different behaviours are expected for other ring geometries, drying conditions, and mix compositions, motivating the numerical simulation of different ring test geometries as performed in Chapter 4.1.5.

5.6 NUMERICAL SIMULATION OF THE DIFFERENT RING TEST GEOMETRIES

The application of the pointwise THM model to the simulation of the restrained shrinkage in different ring test geometries under top and bottom, as well as radial drying, led to the following key findings and contributions:

- the numerical results demonstrated the influence of ring geometry on the degree of restraint. The ASTM and ExpConf1 configurations exhibited higher restraint levels, while AASHTO and ExpConf2 showed significantly lower restraint. This variation directly influenced stress development and cracking behaviour;
- inner steel strains were more pronounced in configurations with lower restraint (AASHTO and ExpConf2), while configurations with higher restraint (ASTM and ExpConf1) produced lower inner steel strains. The average concrete stresses from the numerical simulations were compared with analytically derived stresses based on steel strains. A correction factor, linked to the degree of restraint, was proposed to enhance the accuracy of analytical stress estimations in ring test analyses;
- drying and shrinkage developed quickly in the ASTM and ExpConf1 configurations, particularly under radial drying conditions, leading to earlier crack formation. In contrast, the AASHTO and ExpConf2 geometries exhibited slower drying rates and delayed cracking, even after extended durations;
- these findings suggest that ring-test geometry plays a critical role in evaluating the cracking risk of concrete mixtures. In particular, ASTM and ExpConf1 configurations, with higher restraint and accelerated drying, may be more suitable for comparing normal concrete mixtures subjected to drying-induced cracking, due to rapid shrinkage evolution in those tests; AASHTO and ExpConf2 may be more appropriate for high-shrinkage concretes (e.g. those with elevated basic

shrinkage or drying shrinkage). Compared to the other test geometries, the AASHTO ring test geometry also shows higher temperature histories due to cement hydration;

While the present study provides a consistent framework for comparing ring-test geometries under different drying regimes, further validation is needed. Future work should extend the analyses to other concrete mixtures with different shrinkage properties and investigate combined drying conditions, e.g., simultaneous top, bottom, and radial drying.

5.7 NUMERICAL SIMULATION OF THE ARF TESTS

The application of the pointwise THM model to the simulation of the tests made in the adjustable restraining frames led to the following key findings and contributions:

- the model successfully reproduced the main behavioural trends observed in the experiments using a material formulation based on published concrete creep models, without requiring additional numerical calibration. Compressive stresses were developed during the heating phase, while tensile stresses were generated during the cooling phase. Good agreement between numerical and experimental results demonstrates the robustness of the pointwise THM framework for practical applications involving restraint from early ages;
- the numerical simulations captured the combined influence of early-age restraint due to thermal and shrinkage effects and long-term imposed deformations. This validates the model's ability to handle different stress sources over time in a unified formulation;
- the simulations revealed that crack widths vary significantly across the cross-section, depending on the location and nature of restraint. The crack widths near the reinforcement level are considerably smaller than the crack widths at the surface of the element. Nevertheless, using truss elements to model reinforcement in 3D analyses results in the concentration of the reinforcement volume in a single point of the element cross-section, which may not sufficiently capture the spatial variation of crack development. This issue limits the analysis of results associated with the bond law between reinforcement and concrete. Future work should explore more detailed representations of reinforcement and bond-slip between reinforcement and concrete.

5.8 NUMERICAL SIMULATION OF THE MODIFIED FRAME TEST

The application of the pointwise THM model to the simulation of the test made in the modified frame led to the following key findings and contributions:

- the numerical simulations successfully reproduced the experimentally observed crack pattern, consisting of a primary crack extending through the full thickness of the element, and secondary cracks that rotate in depth towards the primary crack. The total strain model with rotating cracks is essential for the secondary cracks to rotate towards the primary cracks, while the fixed crack concept provides a more realistic simulation of the shear stress transfers at the crack location.

Combining rotating and fixed crack concepts allows the pointwise THM model to simulate complex crack patterns typically observed in restrained concrete elements;

- the development of secondary cracks was found to reduce or stabilise the crack width of the primary crack over time. This phenomenon was consistently observed in the experimental and numerical results, highlighting the importance of primary and secondary crack interaction;
- the bond-slip law influences the crack width development and secondary crack formations. Therefore, an accurate representation of the bond between reinforcement and concrete is essential for reliable crack width predictions;
- the core crack width equals the sum of the crack widths at the surface in the numerical model and the experimental test, confirming the strain compatibility in the numerical model and experimental campaign.

5.9 NUMERICAL SIMULATION OF THE 0.50 m RC TIE RESTRAINED SINCE EARLY AGES

The application of the pointwise THM model to the simulation of the 0.50 m RC tie restrained since early ages led to the following key findings and contributions:

- the results highlighted the importance of using a pointwise THM formulation for structures sensitive to moisture and temperature effects. Compared with the average and layered approaches, the pointwise model delivered comparable or improved accuracy in predicting load-displacement behaviour, crack width development, and delayed thermo-hygral effects, while maintaining greater efficiency and independence from geometric constraints;
- the simulations confirmed that drying cracks initiate at the surface due to strain localisation and gradually propagate towards the core, eventually forming a through-crack. Stress transfer between the steel and concrete occurs through the bond interface, and both the viscoelastic behaviour and tensile strength of concrete vary across the cross-section in response to local temperature and humidity conditions;
- the pointwise THM model enables a more rigorous representation of material behaviour than traditional uniform-property modelling techniques, particularly in the presence of hygrothermal effects;
- minimum reinforcement configurations calculated using EN1992-1-1:2010 and prEN1992-1-1:2023 were compared for two levels of restraint. The prEN1992-1-1:2023 version was found to be less conservative yet complying with the design assumptions, allowing for a reduction in required reinforcement. For the concrete mixture and case studied, this corresponds to material savings while still adhering to the design criteria outlined in the code;
- while the degree of restraint had minimal influence on final crack widths and maximum steel stresses, it significantly affected the timing of crack initiation. Higher restraint levels led to earlier cracking, whereas lower restraint levels delayed the onset of cracking;
- this case confirms the value of the pointwise THM model in simulating the interplay between material properties, restraint conditions, and time-dependent environmental effects. It also

illustrates the model's usefulness in validating and investigating code-based reinforcement design, particularly under early-age and drying-induced cracking scenarios.

The reinforcement configurations assessed in this study were based on minimum reinforcement to avoid yielding. Future research should investigate crack width control based on other analytical formulations or empirical models proposed in the literature, explore a broader range of restraint conditions and concrete mixtures, particularly those with modern admixtures or high shrinkage potential, consider the combined effects between external restraint and loading, analyse different thermohygral conditions and investigate other reinforcement design procedures.

5.10 FINAL REMARKS

This PhD thesis presented and validated a comprehensive numerical tool capable of simulating the hygrothermal behaviour of concrete, addressing the coupled effects of moisture, temperature, and mechanical response. The developed pointwise thermo-hygro-mechanical model was successfully applied across a diverse range of numerical case studies, enabling the investigation of several key phenomena:

- drying effects in elements of varying size and geometry, and the influence of notional size on shrinkage and creep;
- improved understanding of ring test behaviour, highlighting the strengths and limitations of various ring-test geometries;
- simulation of early-age stress development and the long-term effects of imposed deformations in restrained concrete;
- accurate reproduction of complex crack patterns, including through-thickness cracking and delayed cracking in restrained reinforced concrete elements;
- assessment and comparison of analytical design approaches for reinforcement, especially concerning minimum reinforcement calculation using standard code formulations.

Across these applications, the pointwise THM model demonstrated its capacity to serve as an analytical tool for fundamental understanding and practical support of experimental campaigns. Its ability to simulate hygrothermal effects spatially and temporally in detail makes it particularly suitable for research and advanced structural design where moisture-related behaviour plays an important role.

Looking forward, the author recognises that the model, while robust, is not static. As the scientific understanding of concrete evolves and new constitutive models emerge, the pointwise THM framework should be updated and refined to incorporate these advancements. The current implementation is computationally intensive, especially for large-scale meshes. However, ongoing improvements in computational hardware and cloud-based computing will make such sophisticated simulations increasingly feasible in routine practice.

Moreover, integrating this modelling framework with emerging technologies (like artificial intelligence techniques) could enhance future prediction capabilities, support data-driven optimisation of concrete

mixtures, and contribute to sustainable construction practices by reducing overdesign and material waste.

In this context, the present work also serves as an invitation to other researchers to continue exploring and advancing the objectives of this PhD project. May the insights gathered here serve as proof of concept and a foundation for the next generation of researchers in concrete behaviour and other related topics.

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