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Fracture in fibre-reinforced thermoplastics across the scales

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Abstract

Failure in Unidirectional (UD) fibre Reinforced Polymers (FRPs) is a complex, multi-scale phenomenon where various damage mechanisms such as matrix cracking, fibre-matrix decohesion, and delamination interact and evolve. At the micro-scale, localized events like plasticity and interface failure initiate damage, which later coalesce into larger meso-scale cracks that can compromise the entire laminate structure. Understanding these failure mechanisms across scales is crucial for designing more resilient composites. Micro-mechanical analysis using finite element methods has become a powerful approach for investigating these phenomena by explicitly modelling the fibre, matrix, and fibre-matrix interface.

This work reviews the state-of-the-art numerical methods for studying micro-scale failure in UD FRPs, emphasizing the evolution of modelling techniques from single fibre-matrix systems under various boundary conditions to, later, more advanced methodologies such as representative volume elements (RVEs) and embedded cell models. Special focus is given to the Phase-Field (PF) approach for fracture, which has emerged as a robust tool for simulating crack initiation and propagation. The document examines the assumptions, constitutive models, boundary conditions, and material parameters used in PF-based studies, and explores its application in advanced thermoset and towards thermoplastic UD FRPs. Additionally, this thesis incorporates an evaluation of PF implementation strategies in finite element software and provides an initial analysis of the predictive capabilities of PF formulations.

The review reveals significant variability and contradictions in current methodologies, particularly regarding fibre distribution, RVE size, boundary conditions, and material parameters. These discrepancies complicate the validation and comparison of numerical results. Numerical simulations conducted in this work highlight the influence of PF parameters, cohesive interface properties, and geometric configurations on fracture predictions. While traditional PF formulations can effectively model tensile failure, their applicability under compressive, shear, and multi-axial loading is less certain. Furthermore, the analysis underscores a lack of reliable experimental data for validating numerical models, emphasizing the need for more systematic approaches. It was demonstrated that traditional PF formulations impose a variety of restrictions to effectively predict transverse fracture in RVEs and failure in cross-ply laminates. Nonetheless, this methodology can still offer valuable insights in still open questions, such as the origin and evolution of oblique cracks in cross-ply laminates. However, the findings also reveal significant gaps in experimental validation and numerical consistency. This thesis advocates for further investigation into the refinement of experimental methodologies and the development of advanced PF formulations to address the identified limitations, ultimately contributing to the improved design and analysis of UD FRPs in general, and fibre-reinforced thermoplastics (FRTPs) in particular.

Keywords: Failure, Composites, Micro-mechanics, Phase-Field.

Resumo

A falha em Polímeros Reforçados com Fibras Unidirecionais (UD FRPs) é um fenômeno complexo e multiescala, no qual vários mecanismos de dano, como fissuração da matriz, descoesão fibra-matriz e delaminação, interagem e evoluem. À escala microscópica, eventos localizados, como a plasticidade da matriz e falhas na interface, iniciam os danos que, posteriormente, coalescem em fissuras de maior escala capazes de comprometer a integridade estrutural de todo o laminado. Compreender esses mecanismos de falha ao longo das escalas é crucial para o desenvolvimento de compósitos mais resistentes. A análise micromecânica utilizando o método dos elementos finitos tornou-se uma abordagem poderosa para investigar estes fenômenos, modelando explicitamente as fibras, a matriz e a interface fibra-matriz. Este trabalho apresenta uma revisão dos métodos numéricos de última geração para o estudo da falha em UD FRPs à microescala, destacando a evolução das técnicas de modelação desde sistemas de fibra-matriz simples sob diferentes condições de fronteira até metodologias mais avançadas, como elementos de volume representativos (RVE) e modelos de células embutidas. É dado especial enfoque à abordagem de Phase-Field (PF) para fratura, que emergiu como uma ferramenta robusta para simular a iniciação e a propagação de fissuras. O documento examina as suposições, modelos constitutivos, condições de fronteira e parâmetros materiais utilizados em estudos baseados no método PF, explorando a sua aplicação em UD FRPs avançados, começando pelos termoendurecíveis de modo a melhor compreender os termoplásticos. Além disso, esta tese incorpora uma avaliação das estratégias de implementação do PF em software de elementos finitos e fornece uma análise inicial das capacidades preditivas das formulações de PF. A revisão revela uma variabilidade significativa e contradições nas metodologias atuais, particularmente no que diz respeito à distribuição de fibras, ao tamanho dos RVEs, às condições de fronteira e aos parâmetros materiais. Estas discrepâncias dificultam a validação e a comparação dos resultados numéricos. As simulações numéricas realizadas neste trabalho destacam a influência dos parâmetros do PF, das propriedades das interfaces coesivas e das configurações geométricas nas previsões de fratura. Embora as formulações tradicionais de PF consigam modelar eficazmente a falha em tração, a sua aplicabilidade em condições de compressão, corte e carregamentos multiaxiais apresenta-se menos clara. Adicionalmente, a análise sublinha a falta de dados experimentais fiáveis para validar modelos numéricos à escala micromecânica, reforçando a necessidade de abordagens mais sistemáticas. Demonstrou-se que as formulações tradicionais do PF impõem várias restrições para prever eficazmente a fratura transversal em RVEs e a falha em laminados cruzados. Contudo, esta metodologia ainda pode fornecer informações valiosas sobre questões em aberto, como a origem e a evolução de fissuras oblíquas em laminados cruzados. No entanto, os resultados também revelam lacunas significativas na validação experimental e na consistência numérica. Esta tese defende a necessidade de investigações adicionais para aperfeiçoar as metodologias experimentais e desenvolver formulações de PF mais avançadas, abordando as limitações identificadas e contribuindo para a melhoria da

conceção e análise de UFRP, incl. compósitos de matriz termoplástica.

Keywords: Falha, Compósitos, Micromecânica, Phase-Field.

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Chapter 1

Introduction

1.1 Micro-mechanics with Phase-Field

The Phase-Field (PF) method as a variational approach to fracture has received notable attention, especially during the last decade [23, 24, 25]. This is due to its inherent advantages when compared to more traditional methods to model fracture nucleation and propagation. Particularly, PF unlike cohesive zone models (CZM) does not require predefining paths for crack initiation or propagation, and it does not suffer a strong mesh dependency like traditional Continuum Damage Mechanics (CDM) models. In addition, the PF method is based on a strong physical foundation established by the thermodynamic balance of Griffith [23, chap. 1], unlike traditional CDM which are not strictly derived for fracture propagation phenomena. Also, PF does not require any ad-hoc propagation criteria to predict crack propagation direction such as the kind required by XFEM models [26, 1]. Moreover, it can easily cope with crack branching and merging, which is by no means a trivial task in computational fracture mechanics [23, 24]. Due to its advantages and ease of implementation into finite element codes, there has been an increasing number of PF models in different applications, such as micro [11, 14, 27, 28, 29, 30, 31] and meso [30, 32, 33, 34, 35, 36, 37] -scale analysis of composite laminates, functionally graded materials [38, 39], and ceramic materials [40]. It has been used as a stand-alone tool and in conjunction with cohesive surface damage [40, 41, 42].

The use of PF on single fibre analysis is limited to linear elastic material formulations, infinitesimal deformations and no account for residual stresses. Crack kinking is always studied under the plane-strain assumption. 3D effects such as crack tunnelling have only been addressed in the 3D model of Song et al. [43]. Only the work of Guillén-Hernández et al. [27] and Song et al. [43] consider realistic micro-scale dimensions; the work of Zang et al. [11, 32] is limited to fibre diameters of 0.5 mm, which are not representative of the micro-scale. Experimental validation was done only for the study of Song et al. [43]; the other studies are purely numerical. The publications [11, 32, 43] use a geometric and a damage PF variable to define the interface and fracture within both the bulk matrix and the diffuse interface, while Guillén-Hernández et al. [27] use PF damage only in the matrix, while cohesive damage is considered at the interface. The fibre

is always considered linear elastic. As a final remark, it is necessary to mention that while the work of Song et. al [43] and Guillén-Hernández et al. [27] use the formulation without damage threshold called AT2, which implies a non-linear behaviour from the beginning of the straining of the material, other authors, such as Espadas-Escalante et al. [29] resort to formulations where the elastic threshold is defined according to the length scale parameter; this formulation is called AT1. There are also formulations such as the one of Zhang et. al [11, 32] where a modification of the Phase-Field cohesive zone model (PF-CZM) developed by Wu and Nguyen [44] is used to reduce the length scale to micro-scale dimensions while defining an elastic threshold based on energy criteria instead of the length scale parameter.¹

The work on Representative Volume Element analysis (RVE) of composite micro-structures using PF fracture is very limited if compared to the studies using CDM. The first author that performed micro-mechanical analysis of fracture using PF was Espadas-Escalante et al. [29] in 2019. In this publication a 2D plane-strain model was used with an AT1 formulation and compared the performance of Amor and Miehe energy splits² in the predictive capabilities of fracture under pure tension and pure compression. In this work, fibre-matrix interaction was assumed as perfectly bonded, and validation was performed by comparing transverse tensile strength with the value obtained from the experimental results in [45] and the transverse compressive stress-strain curve in [45]. Later, Yin and Zhang [30] used a 3D model with an AT2 formulation to evaluate the influence of fibre orientation on the transverse strength of a composite material. In this case, fibre-matrix interface damage was also ignored. The results were not validated because the specimen and fibre dimensions were not representative of micro-scale dimensions. More recently, Li et al. [31] and Zhang et al. [11] considered a diffuse fibre-matrix interface using a geometric PF variable. Li et al. [31] uses a 2D Von Mises plasticity model coupled with an AT2 formulation, but neither the material properties nor the fibre dimensions are representative of the micro-scale in a polymer-based composite.

On the other hand, the RVE analysis of Zhang et al. [11] uses a 3D model with different volume fractions and fibre distributions to study transverse tension. The formulation in this work is a modification of the Phase-Field cohesive zone model developed by Wu and Nguyen [44], again driven by the need to reduce the length scale to fractions of the fibre diameter. So far, there have not been studies of the capabilities of PF for the prediction of failure envelopes, nor the influence of the Boundary Conditions (BCs) and RVE size on the accuracy of this tool. Also, up to this moment, PF with elastic and Von Mises plasticity formulations have been used always to account for fracture in the matrix or within the diffuse interface, because in transverse loading the fibre is not expected to damage. But, there has not been micro-mechanical analysis using pressure-dependent plasticity models, which are considered of primal importance in the study of polymer matrices [46].

Within the work that has been found and revised, the use of Phase-Field models for fracture is limited to the analysis of the in-situ effect [14] and R-curve in fracture of pre-notched specimens

¹A detailed explanation of the different formulations is given in the next chapter.

²A detailed explanation of the different energy splits is given in the next chapter.

[28, 47]. The study of the in-situ effect of Guillén-Hernández et al. [14] uses a standard AT2 linear elastic formulation for damage in the matrix and cohesive elements in the fibre-matrix interface. This work was based on and compared with the experimental results of Saito et al. [48]. Regarding the studies of the R-curve in fracture of pre-notched specimen under three-point bending of Tan and Martínez-Pañeda [28, 47], the AT1 linear elastic formulation is used to capture matrix fracture and cohesive surface interactions to model fibre-matrix decohesion. The studies are validated by comparison with the experimental results of Canal et al. [49]. In addition, the only study that considers 3D effects and fibre fracture in micro-mechanical studies of Unidirectional (UD) Fiber Reinforced Polymers (FRPs) is the work of Tan and Martínez-Pañeda [47], one of the first steps in modelling more realistic composite geometries, which can potentially be extended to the study of crack tunnelling and other more complex load scenarios.

After a rather extensive review, it was found that for the micro-mechanical analysis of UD FRPs using PF fracture and even using traditional CDM, there is no general trend in the methodologies and assumptions that should be considered. These tend to deviate from each other and sometimes they can be diametrically opposed. In addition, there is no qualitative comparison of the accuracy of each methodology. Thus, there is still the need to understand better the capabilities and limitations of the different methodologies and assumptions for the analysis of the micro-mechanical behaviour of UD FRPs with a more rigorous approach. It should be pointed out that inconsistencies and strong disagreements are commonly found in the general framework of the numerical micro-scale analysis. The review section focuses precisely on highlighting the most conflicting situations and the need for more accurate means of validation, which can help to evaluate how realistic are such assumptions and models.

PF has been implemented in Finite Element Analysis (FEA) tools such as FEniCS [50, 51, 52] and COMSOL [53]. However, this document is focused on the implementation using the general purpose FEA software Abaqus, where extensive work exists, mainly in the form of user element subroutines [11, 14, 32, 54, 55, 56, 57, 58]; in particular, a very recent and important contribution is the work of Navidtehrani et al. [59, 60], who implemented PF damage in a user material subroutine (UMAT) using a heat transfer analogy. Within this work, the main different Abaqus implementation methodologies are explained and compared in detail.

The PF method can be classified within the continuum damage models [61]; more specifically, it can be regarded as a non-local damage model. But, unlike other methods such as the gradient enhanced damage model of Geers et al. [62] or the gradient damage model of Frémond et al. [63] that is also conceived to trigger brittle fracture, the PF method has a strong mathematical foundation in the variational approach to fracture as described by Bourdin in [1, 2]. The underlying principle of this method consists of regularising the discrete crack geometry by means of a diffuse damaged zone of finite dimensions constrained by a length scale parameter; such damaged zone is defined by a scalar damage-like variable called PF variable, which discriminates between the pristine and fully damaged material state.

1.2 Research questions

Based on this introduction, the following research questions arise:

1. What are the main reasons for the large differences in the available values of material properties and how can one sort realist values out of such disperse pool of information?
2. Is the current experimental data reliable to perform calibration/validation of material models used to approximate local micro-scale fields?
3. How accurate are the current PF formulations to predict micro-scale fracture phenomena on UD FRPs, incl. thermoplastic-based composites, if realistic geometric dimensions and material properties are taken into account?
4. What are the dimensions and boundary conditions in an RVE analysis necessary to accurately capture micro-scale fracture phenomena using PF?

1.3 Objectives

Based on these research questions, the following objectives were defined:

1. Understand the current state-of-the-art, regarding numerical and experimental techniques used to study micro-scale fracture in UD FRPs, incl. FRTPs.
2. Understand the capabilities and limitations of current Phase-Field formulations for the micro-scale analysis of UD FRPs, incl. FRTPs, using RVE analysis and embedded cell models.

The work starts with the bibliographic review that aims to understand and give a first partial response to the first objective. Then, micro-mechanical models of a single fibre, RVE and embedded cell models are defined using traditional PF formulations and compared to current numerical approaches using other methodologies and, when possible, to experimental data. The purpose of this second part is to give a preliminary response to the second objective. Within the RVE and embedded cell studies, there is particular emphasis on the variation of results with boundary conditions, RVE/embedded zone size and fibre distribution; these provide a more detailed answer to the second objective.

1.4 Thesis outline

After this introduction, Chapters 2, 3 and 4 provide a review of the traditional PF formulations based on brittle fracture and their extensions to elasto-plastic materials. The review also presents the main numerical and experimental methodologies for the study of thermoset and thermoplastic-based UD FRPs at the micro-scale; it aims to highlight the main knowledge gaps, disagreements

between numerical approaches, and contradictions with respect to experimental evidence. In addition, the bibliographic revision tries to answer the question: *to which extent PF fracture has been successfully used to model failure in UD FRPs at the micro-scale?*

Chapter 5 assesses the PF implementation into Abaqus, comparing the advantages and limitations of using an Abaqus user element (UEL) versus an Abaqus user material (UMAT) for Phase-Field modeling. It explores the performance of various combinations of formulations and energy splits under different loading scenarios, providing a detailed comparison of these implementation strategies in terms of computational cost, convergence behaviour, and overall accuracy for fracture predictions.

Once PF as a numerical material model is understood, additional variables are systematically introduced to refine the micro-scale model. This refinement process begins with the inclusion of a single fibre and its interface within a polymer matrix, examining the cohesive interaction effects as a stand-alone damage mechanism as well as in conjunction with PF-based matrix damage in Chapter 6. This dual approach provides insights into the relative contributions of interfacial and matrix damage and how they collectively influence the predictive accuracy of the model.

Further model refinement is achieved by expanding the microstructural representation to include multiple fibres within a representative volume element (RVE) in Chapter 7. Allowing the model to capture more complex scenarios, such as the simultaneous fibre-to-fibre and fibre-matrix interactions. Variations in fibre arrangement and RVE size are systematically studied to assess their influence on load distribution, crack initiation, and propagation. These investigations reveal great influence of the variability in the RVE configuration and material parameters in the subsequent volatility of fracture predictions. There is an emphasis in critical factors such as, fibre distribution and RVE dimensions, which are considered of paramount importance if one attempts to mimic realistic composite behaviour.

Chapter 8 concludes with an analysis of advanced modelling scenarios that incorporate the study of oblique cracks in cross ply laminates, assessing the PF model adaptability to complex, non-homogeneous loading. These simulations aim to assess the robustness of the PF method under diverse conditions, inspiring new model validation efforts against experimental data and contributing to a more comprehensive evaluation of the PF effectiveness in capturing micro-scale failure mechanisms in UD FRPs, inc. fibre-reinforced thermoplastics (FRTPs). Finally, this chapter outlines prospective directions for enhancing the PF capabilities in fracture prediction, particularly for multi-axial applications and composite structures with varied interface properties.

Finally, Chapter 9 presents the main conclusions and directions of future work.

Chapter 2

Phase-Field method

This chapter presents the theory of Phase-Field (PF) brittle fracture.

The derivation of the PF constitutive equations is presented in a general fashion and then, the particularities of the most common PF formulations (i.e. AT1, AT2, and PF-CZM) are detailed.

2.1 Griffith thermodynamic balance

The PF method for fracture is based on the thermodynamical analysis made by Griffith et al. [64], where, according to the first law of thermodynamics, crack growth can only occur if such a process implies that the total energy of the system either decreases or remains constant with an increase in the crack area. In this context, a critical condition for crack propagation is defined (under equilibrium conditions) as the scenario where there is no change in total energy [60]. Thus, the Griffith principle is a local (differential) minimum for the total energy Π , based on the variation of Π with respect to the increment of the crack area dA as expressed in equation 2.1.

$$\frac{d\Pi}{dA} = \frac{d\Psi_0}{dA} + \frac{dW_c}{dA} - \frac{dW_{ext}}{dA} \quad (2.1)$$

Where Ψ_0 is the internal strain energy, W_{ext} is the work done by the external forces, and W_c is the energy required to create new surfaces, whose variation with respect to the incremental crack area is known as the critical energy release rate $G_c = dW_c/dA$.

2.2 Variational form of the Griffith thermodynamic balance

The differential expression in equation 2.1 can be expressed in a variational form as explained by Bourdin et al. [1, 2], according to equation 2.2.

$$\Pi(\mathbf{u}) = \int_{\Omega} \Psi_0(\mathbf{u}) d\Omega + \int_{\Gamma} G_c dS - W_{ext}(\mathbf{u}) \quad (2.2)$$

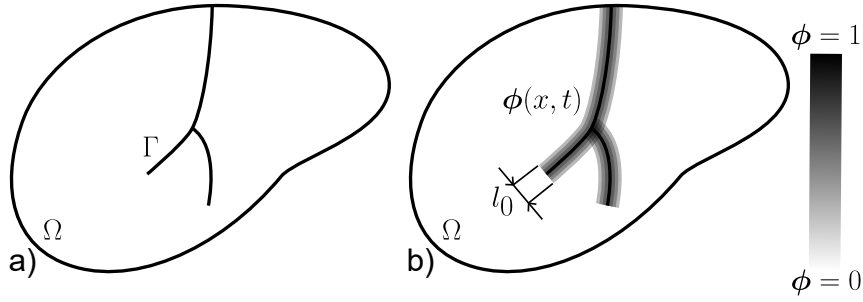


Figure 2.1: Schematic representation of a solid body with (a) an internal discrete discontinuity, and (b) a Phase-Field approximation of the same discontinuity [1, 2].

This equation is given within the domain defined by the pre-cracked body $\Omega \subset \mathbb{R}^n$, ($n \in [1, 2, 3]$) where the internal discontinuity contour is defined by Γ and the displacement is defined by the vector $\mathbf{u}$, see Fig. 2.1 a).

Within the framework of the calculus of variations, the displacement field should be found by minimizing the total energy described in equation (2.2), but as the crack path is also an unknown, the solution to the variational problem posed by equation (2.2) can become extremely complex [23]. To reduce the difficulty of tracking the actual crack path, Bourdin et al. [1, 2] proposed a regularised version of the crack surface using an auxiliary damage-like variable ϕ . Thus, the sharp crack topology is replaced by a diffuse damaged zone of finite dimensions, controlled by a length scale parameter l_0 . Then, according to Refs. [1, 2], the total energy $\Pi(\mathbf{u})$ in equation (2.2) can be approximated by $\Pi(\mathbf{u}, \phi)$ defined in equation (2.3).

$$\Pi(\mathbf{u}) \approx \Pi(\mathbf{u}, \phi) = \int_{\Omega} \Psi(\mathbf{u}, \phi) d\Omega + \int_{\Omega} \frac{G_c}{4C_w} \gamma(\phi; \nabla \phi) d\Omega - W_{ext}(\mathbf{u}) \quad (2.3)$$

Where $\Psi(\mathbf{u}, \phi)$ is the degraded internal energy and $\frac{G_c}{4C_w} \gamma(\phi; \nabla \phi)$ is the regularized fracture energy; these are explained in detail in the following subsections.

2.3 Crack surface density function

The surface energy in equation 2.2, initially computed in the specific crack path is now approximated in a damaged zone of finite width (see Fig. 2.1 b)) according to equation 2.4.

$$\begin{aligned} \int_{\Gamma} G_c dS &\approx \int_{\Omega} \frac{G_c}{4C_w} \gamma(\phi; \nabla \phi) d\Omega \\ \gamma(\phi; \nabla \phi) &= \left(\frac{\alpha(\phi)}{l_0} + l_0 |\nabla \phi|^2 \right) \end{aligned} \quad (2.4)$$

Where $\gamma(\phi; \nabla \phi)$ is known as the crack surface density function given in terms of the PF variable ϕ , its gradient $\nabla \phi$ and the length scale parameter l_0 . The integral term is also called the dissipated energy, because in the balance equation (2.2), the external work $W_{ext}(\mathbf{u})$ exerted on the

body can either be stored as accumulated strain energy $\int_{\Omega} \Psi_0(\mathbf{u})d\Omega$ or dissipated in the form of surface energy due to fracture $\int_{\Gamma} G_c dS$.

2.4 Geometric crack function

The total dissipated (or fracture) energy described in equation (2.4) can also be given in terms of regularised damage models as explained in Ref. [51]. Hence, the regularised term $\int_{\Omega} G_c \gamma(\phi; \nabla \phi) d\Omega$ is divided into local (depending on ϕ) and non-local (depending on $\nabla \phi$) contributions as shown in equation (2.5).

$$\int_{\Omega} G_c \gamma(\phi; \nabla \phi) d\Omega = \frac{G_c}{4C_w} \int_{\Omega} \left(\frac{\alpha(\phi)}{l_0} + l_0 |\nabla \phi|^2 \right) d\Omega \quad (2.5)$$

Where $\alpha(\phi)$ is known as the geometric crack function, which defines the spatial distribution of the damage variable $\phi = \phi(x, y, z)$ in the domain Ω , and C_w is a normalization parameter that guarantees the same energy dissipation regardless of the PF formulation (see equation (2.6)).

$$C_w = \int_0^1 \sqrt{\alpha(\xi)} d\xi \quad (2.6)$$

If the material has not been damaged $\phi = 0$, there is no dissipated energy $\alpha(0) = 0$, and when damage reaches its maximum value $\phi = 1$, the local dissipation also reaches its maximum $\alpha(1) = 1$. Additionally, it is required that $\frac{\partial \alpha(\phi)}{\partial \phi}$ must be non-negative to ensure an always increasing fracture energy dissipation; $\frac{\partial \alpha(\phi)}{\partial \phi} < 0$ would imply healing of the crack, which is thermodynamically inconsistent.

2.5 Energy degradation function

According to the formulation of continuum mechanics models, the strain energy should be degraded with the evolution of the damage variable. Hence, the strain energy term $\int_{\Omega} \Psi(\mathbf{u}) d\Omega$ must be modified accordingly to yield equation (2.7):

$$\begin{aligned} \int_{\Omega} \Psi_0(\mathbf{u}) d\Omega &\approx \int_{\Omega} \Psi(\mathbf{u}, \phi) d\Omega \\ \int_{\Omega} \Psi(\mathbf{u}, \phi) d\Omega &= \int_{\Omega} [g(\phi) \Psi^+(\mathbf{u}) + \Psi^-(\mathbf{u})] d\Omega \end{aligned} \quad (2.7)$$

Where $g(\phi)$ is called the energetic degradation function, and $\Psi^+(\mathbf{u})$ and $\Psi^-(\mathbf{u})$ are the positive and negative contributions to the strain energy. The energy split is performed in order to avoid fracture under dominant compressive stresses.

For an undamaged material ($\phi = 0$) all the external work is stored as strain energy; thus, $g(0) = 1$. On the other hand, when the material is completely damaged ($\phi = 1$) it loses all its

load-carrying capacity $g(1) = 0$; besides, this function should be a decreasing function, $\frac{\partial g(\phi)}{\partial \phi} \leq 0$, such that the evolution of damage can only decrease the internal energy.

2.6 Euler equations (strong form)

Considering that the work of external forces can be expressed as the sum of surface tractions $\mathbf{t}^*$ on the part of the boundary $\partial\Omega_t$, and body forces $\mathbf{b}^*$ over the volume of the body Ω , the external work can be rewritten as equation 2.8.

$$W_{ext}(\mathbf{u}) = \int_{\partial\Omega} (\mathbf{t}^* \cdot \mathbf{u}) d\partial\Omega + \int_{\Omega} (\mathbf{b}^* \cdot \mathbf{u}) d\Omega \quad (2.8)$$

Thus, by using equations 2.4, 2.5, 2.7, and 2.8; the total energy functional in equation 2.2 can be rewritten as equation 2.9.

$$\Pi(\mathbf{u}, \phi) = \int_{\Omega} \Psi(\mathbf{u}, \phi) d\Omega + \frac{G_c}{4C_w} \int_{\Omega} \left(\frac{\alpha(\phi)}{l_0} + l_0 |\nabla \phi|^2 \right) d\Omega - \int_{\partial\Omega} (\mathbf{t}^* \cdot \mathbf{u}) d\partial\Omega - \int_{\Omega} (\mathbf{b}^* \cdot \mathbf{u}) d\Omega \quad (2.9)$$

According to the calculus of variations, the actual displacement $\mathbf{u} = \mathbf{u}(x, y, z)$ and PF variable $\phi = \phi(x, y, z)$ fields are the stationary functions of the total energy functional in equation (2.9), which can be found by setting the variation of $\Pi(\mathbf{u}, \phi)$ with respect to $\mathbf{u}$ and ϕ equal to zero and then applying the divergence theorem to obtain equations (2.10).

$$\begin{aligned} \delta\Pi(\mathbf{u}, \phi) = & - \int_{\Omega} \left[\nabla \cdot \left(\frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \epsilon(\mathbf{u})} \right) + \mathbf{b}^* \right] \cdot \delta \mathbf{u} d\Omega + \int_{\partial\Omega_t} (\boldsymbol{\sigma} \cdot \mathbf{n} - \mathbf{t}^*) \cdot \delta \mathbf{u} d\partial\Omega \\ & + \int_{\Omega} \left[\frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \phi} + \frac{G_c}{4C_w} \left(\frac{\partial \gamma}{\partial \phi} - \nabla \cdot \left(\frac{\partial \gamma}{\partial \nabla \phi} \right) \right) \right] \cdot \delta \phi d\Omega + \int_{\partial\Omega} \frac{G_c}{4C_w} \left(\frac{\partial \gamma}{\partial \nabla \phi} \cdot \mathbf{n} \right) \delta \phi d\partial\Omega \end{aligned} \quad (2.10)$$

Where $\mathbf{n}$ is the outward normal vector.

From equation 2.10, the Euler equations or strong form can be extracted as a coupled system of differential equations 2.11.

$$\begin{aligned} \nabla \cdot \left(\frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \epsilon(\mathbf{u})} \right) + \mathbf{b}^* &= \mathbf{0} \quad \text{in } \Omega \\ \frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \phi} + \frac{G_c}{4C_w} \left(\frac{\partial \gamma}{\partial \phi} - \nabla \cdot \left(\frac{\partial \gamma}{\partial \nabla \phi} \right) \right) &= 0 \quad \text{in } \Omega \end{aligned} \quad (2.11)$$

With the boundary conditions in equation 2.12:

$$\begin{aligned} \boldsymbol{\sigma} \cdot \mathbf{n} &= \mathbf{t}^* \quad \text{on } \partial\Omega \\ \nabla \phi \cdot \mathbf{n} &= 0 \quad \text{on } \partial\Omega \end{aligned} \quad (2.12)$$

The term $\frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \phi}$ is called the energetic crack driving force, and it can be expressed as equation 2.13.

$$\frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \phi} = \frac{\partial \Psi(\mathbf{u}, \phi)}{\partial g(\phi)} \frac{\partial g(\phi)}{\partial \phi} = \Psi^+(\mathbf{u}) \frac{\partial g(\phi)}{\partial \phi} \quad (2.13)$$

Also, the terms $\frac{\partial \gamma}{\partial \nabla \phi}$ and $\frac{\partial \gamma}{\partial \phi}$ can be simplified as shown in equation (2.14).

$$\begin{aligned} \frac{\partial \gamma}{\partial \nabla \phi} &= \frac{l_0}{2C_w} |\nabla \phi| \\ \frac{\partial \gamma}{\partial \phi} &= \frac{1}{4C_w l_0} \frac{\partial \alpha(\phi)}{\partial \phi} \end{aligned} \quad (2.14)$$

2.7 Phase-Field formulations

The particular forms of the normalization parameter C_w , degradation function $g(\phi)$ and geometric functions $\alpha(\phi)$ define the specific PF formulations. The most popular are: (i) the AT1 model which uses a quadratic degradation function and a linear geometric function, (ii) the AT2 model which uses quadratic functions for both geometric and degradation functions (the main difference between these two models resides in the geometric crack function) and (iii) the Phase-Field Cohesive zone model (PF-CZM) which uses a quadratic geometric function and a rational degradation function [23, chap. 3], see Table 2.1. AT1 and PF-CZM present linear-elastic behaviour up to the maximum stress while AT2 has the particularity $\frac{\partial \alpha}{\partial \phi}(\phi = 0) = 0$ which enforces non-linear behaviour prior to the predefined strength is reached, see Fig. 2.2. In the AT1 and AT2 models, the PF length scale parameter is used to control the material strength (σ_c) and can be related to the material properties according to the 1D analytical solution of the PF differential equations (weak form) described in equations (2.11). Conversely, in the PF-CZM model the strength is explicitly defined and it does not depend on the length scale parameter.

Throughout the progressive loading, the PF variable approaches one, and the degradation function tends to zero. This imposes a zero stiffness in the material that can create numerical instabilities and an ill-posed tangent matrix. This is why some authors [60, 65, 59] recommend using a modified version of the degradation function for AT1 and AT2 models, see equation (2.15), where κ is a very small positive number.

$$g(\phi) = (1 - \phi)^2 + \kappa \quad (2.15)$$

2.8 Strain energy split

As mentioned before, fracture under dominated compressive stresses is precluded by means of a decomposition of the strain energy into active $\Psi^+(\mathbf{u})$ and inactive $\Psi^-(\mathbf{u})$ contributions (see

Table 2.1: Geometric and degradation functions for AT1, AT2 and PF-CZM models [23].

Model	$\alpha(\phi)$	$g(\phi)$	C_w	l_0
AT1	ϕ	$(1 - \phi)^2$	$2/3$	$\frac{8G_c E}{3\sigma_c^2}$
AT2	ϕ^2	$(1 - \phi)^2$	$1/2$	$\frac{27G_c E}{256\sigma_c^2}$
PF-CZM	$2\phi - \phi^2$	$\frac{(1-\phi)^p}{(1-\phi)^p + Q(\phi)}$	$\pi/4$	$[-]$

equation (2.7)). The most common decomposition methods for infinitesimal elasticity formulations are: the volumetric-deviatoric split of Amor et al. [66] (see equation (2.16)) and the spectral decomposition of Miehe et al. [67] (see equation (2.17)). These decompositions apply only to the AT1 and AT2 formulations. The default decomposition used in PF-CZM is the one shown in equation (2.18).

$$\begin{aligned}\Psi^-(\epsilon(\mathbf{u})) &= \frac{K}{2} \text{tr}^-(\epsilon(\mathbf{u})) \\ \Psi^+(\epsilon(\mathbf{u})) &= \frac{K}{2} \text{tr}^+(\epsilon(\mathbf{u})) + \mu \epsilon_D(\mathbf{u}) : \epsilon_D(\mathbf{u})\end{aligned}\tag{2.16}$$

$$\begin{aligned}\Psi^\pm(\epsilon(\mathbf{u})) &= \frac{K}{2} \langle \epsilon_1(\mathbf{u}) + \epsilon_2(\mathbf{u}) + \epsilon_3(\mathbf{u}) \rangle_\pm^2 + \\ &\quad \mu (\langle \epsilon_1(\mathbf{u}) \rangle_\pm^2 + \langle \epsilon_2(\mathbf{u}) \rangle_\pm^2 + \langle \epsilon_3(\mathbf{u}) \rangle_\pm^2)\end{aligned}\tag{2.17}$$

$$\begin{aligned}\Psi^+(\sigma(\mathbf{u})) &= \frac{\langle \sigma_1(\mathbf{u}) \rangle_+^2}{2E} \\ \Psi^-(\sigma(\mathbf{u})) &= \frac{1}{2E} [\sigma_1(\mathbf{u}) \langle \sigma_1(\mathbf{u}) \rangle_- + \\ &\quad \sigma_2(\mathbf{u})^2 + \sigma_3(\mathbf{u})^2 - \\ &\quad 2\nu (\sigma_2(\mathbf{u})\sigma_3(\mathbf{u}) + \sigma_1(\mathbf{u})\sigma_3(\mathbf{u}) + \sigma_1(\mathbf{u})\sigma_2(\mathbf{u}))]\end{aligned}\tag{2.18}$$

Here, K and μ are the elastic Lamé parameters, E is the Young's modulus, ν is the Poisson's ratio, $\epsilon(\mathbf{u})$ is the infinitesimal strain tensor, ϵ_D is the deviatoric part of the infinitesimal strain tensor, $\sigma(\mathbf{u})$ is the Cauchy stress, $\sigma_i(\mathbf{u})$ are the principal stresses and $\langle \cdot \rangle$ is the Macaulay operator.

Any particular form of the energy split applied in the balance of linear momentum as well as the PF balance (equations (2.11)) leads to the so-called "anisotropic" PF formulation, because when damage progresses, the material response under compression and tension is different, and the material is no longer isotropic. The use of the energy split in the PF balance only renders the so-called "hybrid" formulation.

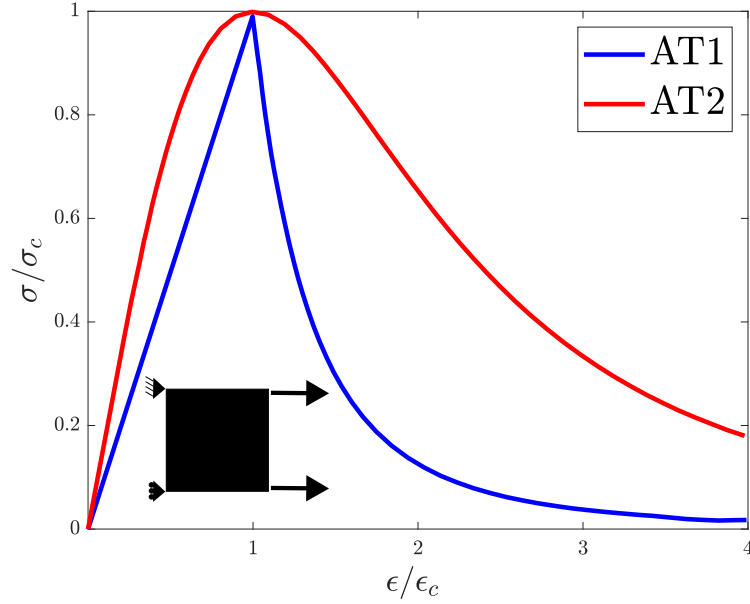


Figure 2.2: Stress-strain behaviour for AT1 and AT2 models in a single finite element under tension [3], where σ_c is the strength and ϵ_c is the strain when the stress reaches σ_c .

2.9 Damage irreversibility

The damage irreversibility condition ($\dot{\phi} \geq 0$) is ensured by using a local history variable H that satisfies the fracture Karush-Kuhn-Tucker conditions in equation (2.19). H is defined in equation (2.20).

$$\Psi^+ - H \leq 0, \dot{H} \geq 0, \dot{H}(\Psi^+ - H) = 0 \quad (2.19)$$

$$H = \max_{\tau \in [0, t]} \Psi^+(\tau) \quad (2.20)$$

2.10 Phase-Field balance equations

The strong form in equation (2.11) is rewritten using the definition of the energetic crack driving force in equation (2.13) and the history variable defined in equation (2.20), to define the balance equations of the PF method in equation (2.21), under the same boundary conditions defined in equation (2.12).

$$\begin{aligned} \nabla \cdot \left(\frac{\partial \Psi(\mathbf{u}, \phi)}{\partial \epsilon(\mathbf{u})} \right) + \mathbf{b}^* &= \mathbf{0} \quad \text{in } \Omega \\ H \frac{\partial g(\phi)}{\partial \phi} + \frac{G_c}{2c_w} \left(\frac{1}{2l_0} \frac{\partial \alpha(\phi)}{\partial \phi} - l_0 \nabla \cdot |\nabla \phi| \right) &= 0 \quad \text{in } \Omega \end{aligned} \quad (2.21)$$

2.11 Solution Scheme

In the coupled system of equations (2.21) the displacements and PF variable are both unknown. When this system is discretized and linearized using the Newton-Raphson method, it can be solved using two different approaches. If the displacements and PF variable are solved simultaneously, the solution method is called "*monolithic*", a method that does not depend on the size of the time step increment, but the solution is non-convex, which may lead to convergence issues [58]. In the "*monolithic*" scheme, convergence can be improved by using quasi-Newton methods, as was shown by Wu and Nguyen [58] using the PF-CZM formulation and by Kristensen and Martínez-Pañeda [68] using AT1 and AT2 formulations. On the other hand, the system of equations (2.21) can be solved by iteratively freezing displacements and solving for the PF variable, then freezing the PF variable and solving for displacements, this solution method is called *staggered*, in this case, the solution depends on the size of the time increment, therefore it requires convergence studies on the time step. When the system of equations (2.21) is decoupled, both PF and displacement problems become convex with respect to each variable; this is why convergence in the *staggered* scheme is often ensured [58].

Chapter 3

Phase-Field fracture coupled with plasticity

This Chapter presents a review of the general trends for coupling PF fracture with plasticity models. This review is based on the work of Alessi et al. [69]. It shows from a general perspective the most relevant approaches to gradient damage and gradient plasticity, which is a generalization of elasto-plastic fracture using PF from a variational perspective. The extension of Phase-Field fracture to account for plasticity has been done in several ways, the diversity of approaches comes from the fact that, unlike brittle fracture, there is no unique energy functional that accounts for an additional dissipation term due to plastic deformation. Then, the work of most authors focuses on suggesting possible forms the elastic-plastic-fracture functional can be expressed. The general form of this functional is an extension of the functional shown in equation (2.3) to account for the plastic dissipation.

The general expression for the elastic-plastic-fracture functional is shown in equation (3.1), where $\Psi^e(\boldsymbol{\varepsilon}^e(\mathbf{u}), \phi, \gamma)$ is the elastic strain energy that depends on the elastic strain tensor ($\boldsymbol{\varepsilon}^e(\mathbf{u})$), the PF variable (ϕ) and the plastic multiplier (γ). $\Psi^p(\phi, \gamma, \nabla\gamma)$ is the plastic work, it depends on the plastic multiplier, and it may depend on the PF variable or the gradient of the plastic multiplier ($\nabla\gamma$) for gradient plasticity models. The specific form of these two defines the expression for the driving force $H(\boldsymbol{\varepsilon}^e(\mathbf{u}), \gamma)$ previously defined in equation (2.20), which may now depend on the elastic and plastic strains. $G_c(\gamma)$ is the fracture energy that may also depend on the plastic strains.

$$\Pi(\mathbf{u}, \phi, \gamma) = \int_{\Omega} \Psi^e(\boldsymbol{\varepsilon}^e(\mathbf{u}), \phi, \gamma) d\Omega + \int_{\Omega} \Psi^p(\phi, \gamma, \nabla\gamma) d\Omega + \int_{\Omega} G_c(\gamma) \gamma(\phi; \nabla\phi) d\Omega - W_{ext}(\mathbf{u}) \quad (3.1)$$

In addition to the fracture KKT in equation (2.19), plasticity requires the definition of a plastic threshold ($f^p(\boldsymbol{\varepsilon}^e(\mathbf{u}), \phi, \gamma)$) and a flow rule ($\boldsymbol{\varepsilon}^p = \dot{\gamma} \mathbf{N}$ where $\mathbf{N}$ is the flow vector) in order to establish the plasticity KKT conditions in equations (3.2). The flow vector and plastic threshold forms depend on the energy functional and the specific plasticity model.

$$\begin{aligned}
\dot{\gamma} &\geq 0 \\
f^p(\boldsymbol{\varepsilon}^e(\mathbf{u}), \phi, \gamma) &\leq 0 \\
f^p(\boldsymbol{\varepsilon}^e(\mathbf{u}), \phi, \gamma) \dot{\gamma} &= 0
\end{aligned} \tag{3.2}$$

Some of the most common modelling approaches are summarized in Table 3.1, using the notation defined by equations (3.1) and (3.2); this review is not meant to be exhaustive; it aims at point out the main methodologies using specific examples.

The connection between PF and plasticity evolution is done mainly in three different ways:

- The first way, which is the most common one is by defining a degradation function that affects both the elastic and plastic components of the energy [4, 54, 70, 71], this way the driving force for PF initiation and evolution includes both elastic energy and plastic work, using this methodology the return mapping algorithm is defined with effective or undamaged quantities, thus the procedure is not modified by the PF evolution. This is an advantage when it comes to implementation because no extra derivations need to be done, but it is a strong limitation in the sense that if effective quantities are used, the plastic return mapping is computed even for areas highly distorted and highly damaged, where the convergence of the return mapping may become extremely difficult.
- The second way, which is the methodology used by Ambati et al. [72], uses a degradation function that is affected by both PF and plasticity, but such degradation is applied only on the elastic energy and not on the plastic work; thus the driving force is only elastic strain energy. In this case, the plastic return mapping is affected by the PF variable, which brings additional efforts to the derivation and implementation, but in this case, when damage has increased enough the stresses will not be able to reach the plastic threshold and plastic evolution will stop for large deformations.
- Finally, the third methodology is the one of Yin and Kaliske [73], where again the degradation function affects only the elastic part of the energy, but in this case, the plastic evolution decreases the fracture toughness of the material, this approach posses similar advantages and disadvantages of Ambati et al. [72] regarding implementation and convergence.

Several models require additional parameters. Some of them, like one of Ambati et al. [72] need a critical equivalent plastic strain ($\epsilon_{eq,crit}^p$) and a parameter to control the influence of plasticity on the stiffness degradation (m); and also the model of Yin and Kaliske [73], where the initial fracture toughness G_{c0} is degraded according to the evolution of plastic strains $\boldsymbol{\varepsilon}^p(\gamma)$. The decreasing fracture toughness function is $f(\gamma)$ gradually diminishes with increasing values of γ or $\boldsymbol{\varepsilon}^p$; variables that could be very difficult to measured in practice. In these cases, the parameters can be easily related to the physics of the problem, while on the other hand models such as the one of Borden et al. [71] require the parameter k to increase or reduce the degradation, which is more a numerical parameter lacking a clear physical meaning.

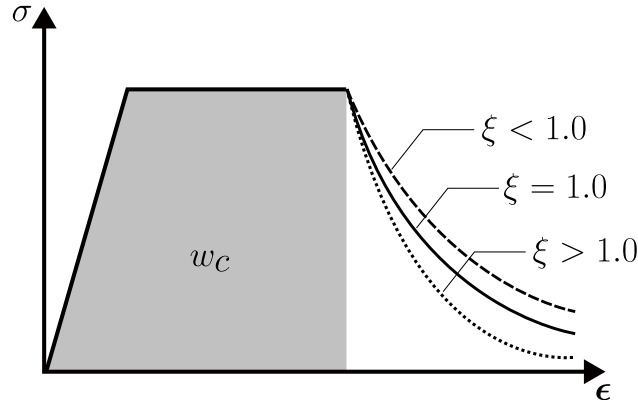


Figure 3.1: Graphical representation of w_c and ξ parameters in the PF formulation of Miehe et al. [4].

It is necessary to mention that in the approach of Miehe et al. [4], the fracture dissipated energy integral $\int_{\Omega} G_c(\gamma) \gamma(\phi; \nabla \phi) d\Omega$ (see Table 3.1) is replaced by equation (3.3) where w_c is an energy threshold parameter and ξ is a softening parameter; which are also additional properties that require calibration, see Fig. 3.1. Miehe's methodology shows, as it is normal in gradient plasticity formulations, that the plastic work depends on the plastic multiplier γ and its gradient $\nabla \gamma$. The specific form of the gradient component of the plastic work, expressed here as the function $h(\gamma, \nabla \gamma)$ is also assumed differently by different authors. However, such function always requires an additional plastic length scale parameter.

$$\int_{\Omega} G_c d\Omega = (1 - (1 - \phi)^2) w_c + \frac{w_c}{\xi} l_0 \left(\frac{\phi^2}{l_0} + l_0 |\nabla \phi|^2 \right) \quad (3.3)$$

The methodology of Fang et al. [54], previously explained as the first method to connect PF and plasticity evolution (see Table 3.1), is one of the easiest to implement. This modification can be done to other plasticity models in a rather straightforward manner. In addition, it does not require additional parameters from the ones needed in the plasticity and PF models, and this is why this is the most straight forward methodology to implement PF fracture coupled with plasticity inside the UEL/UMAT of Abaqus.

Table 3.1: Comparison of most common gradient plasticity-damage models.

Author & Plasticity model	$\Psi^e(\varepsilon^e(\mathbf{u}), \phi, \gamma)$	$\Psi^p(\phi, \gamma, \nabla \gamma)$	$G_c(\gamma)$	$H(\varepsilon^e(\mathbf{u}), \gamma)$
Ambati et al. [72]	$(1 - \phi)^{2p(\gamma)^m} \Psi^{e+}(\varepsilon^e(\mathbf{u})) + \Psi^{e-}(\varepsilon^e(\mathbf{u}))$	$\frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma$	G_c	$\max_{\tau \in [0, \hat{\mu}]} \Psi^{e+}(\tau)$
Von Mises	$p(\gamma) = \frac{\varepsilon_{eq}^p(\gamma)}{\varepsilon_{eq, crit}^p(\gamma)}$			
Fang et al. [54]	$(1 - \phi)^2 (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma)$	$(1 - \phi)^2 (\frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma)$	G_c	$\max_{\tau \in [0, \hat{\mu}]} (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma) + \frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma$
Von Mises				
Fang et al. [70]	$(1 - \phi)^2 (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma)$	$(1 - \phi)^2 (\frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma)$	G_c	$\max_{\tau \in [0, \hat{\mu}]} (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma) + \frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma$
Multi-surface plasticity				
Yin and Kaliske [73]	$(1 - \phi)^2 \Psi^{e+}(\varepsilon^e(\mathbf{u})) + \Psi^{e-}(\varepsilon^e(\mathbf{u}))$	$\frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma$	$G_c f(\gamma)$	$\max_{\tau \in [0, \hat{\mu}]} \Psi^{e+}(\tau)$
Von Mises				
Borden et al. [71]	$g(\phi) (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma)$	$g(\phi) (\frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma)$	G_c	$\max_{\tau \in [0, \hat{\mu}]} (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma) + \frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma$
Von Mises	$g(\phi) = (1 - \phi)^2 (1 + \phi(2 + k))$ Where $k > 0$			
Miehe et al. [4]	$(1 - \phi)^2 (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma)$	$(1 - \phi)^2 (\frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma + h(\gamma, \nabla \gamma))$	G_c	$\max_{\tau \in [0, \hat{\mu}]} (\frac{1}{2} \varepsilon^e(\mathbf{u}) : \sigma) + \frac{1}{2} \hat{H} \gamma^2 + \sigma_\gamma \gamma + h(\gamma, \nabla \gamma)$
Von Mises				

Chapter 4

Micro-mechanical analysis of composite materials

4.1 Introduction

There has been an extensive study of the mechanical performance of UD FRPs using experimental (see left side of Fig. 4.1) and numerical approaches using the Finite Element Method (see right side of Fig. 4.1). This Chapter presents an extensive review of the most relevant work performed in the micromechanical context of UD FRPs. This revision considers numerical studies in the light of what the experimental work can corroborate or question. This review tries to set a context before going into deeper details. However, it is meant to be concise.

Experimental as well as numerical modelling of the mechanical behaviour of UD FRPs can be done at different scales, depending on the purpose of the analysis. Usually, structural analysis and design are performed at the macro-scale level [74, 75], where the entire volume of the laminate is assumed as a homogeneous continuum material with orthotropic mechanical properties; see Fig. 4.1. On the other hand, meso-scale models are used for the determination of macro-scale models or properties, and the study of design allowables [76, 77, 78, 79]; in this scale, the analysis is performed considering each ply and its interaction with the others through interface models such as cohesive elements [76]. Thus, at this level, each lamina is still assumed as a homogeneous continuum material with orthotropic mechanical properties, but the interaction between laminae is taken into account [76, 77, 78, 79]; see Fig. 4.1. The highest level of detail is achieved in a micro-mechanical analysis, which refers to the study of materials composed of different phases or constituents, where the different phases, in this case, matrix, fibres, and their interfaces are considered explicitly; see Fig. 4.1. Sometimes even defects such as voids or inclusion can be included; see Tan and Martínez-Pañeda [28]. Thus, no assumptions such as homogeneity, specific geometric distributions, lack of defects or perfect interface bonding need to be considered. This work is focused on the analysis of the last case, with special emphasis on the study of fracture initiation and propagation.

The idea of micro-mechanical analysis is to be able to understand and predict the detailed

interaction of the constituents (fibre, matrix and interface) and the parameters that govern such interaction (matrix and fibre stiffness/strength, interface strength and fracture toughness). This allows to identify several important features of the design and analysis of UFERP such as:

- The increased global stiffness due to the inclusion of a stiff fibre in a soft medium (matrix) [80, Chapter 4].
- The most basic damage mechanisms and failure sequences in a very controlled and isolated system in the analysis of single embedded fibre models or Representative Volume Elements (RVEs) [7, 81].
- The equivalent bulk or meso-scale properties obtained from the analysis of either a Representative Volume Element (RVE) [46], or an embedded cell model [28].

A model with a single embedded fibre is the first and probably the oldest approach in micro-mechanics studies. It consists of a perfectly circular fibre, perfectly centred inside a square volume constituted by the matrix; see Fig. 4.2. This volume can be stretched or compressed to study the influence of the inclusion on the overall stiffness and strength improvement or reduction with respect to the reference bulk or monolithic matrix properties.

The addition of more fibres in this volume is the way a Representative Volume Element (RVE) is created, this is the name that is most commonly given used in this context, but it has also been used for single fibre models [82] and embedded cell sections [83]. The most general agreement says that an RVE is a fixed volume that contains an arrangement of different phases. Such volume is assumed to contain a representative sample of the specific geometric distribution, characteristic strength and stiffness of the composite material. The most appealing characteristic of the micro-mechanics modelling approach is related to the fact that, while accounting for the geometric arrangement of an RVE, specific and homogeneous deformation states can be imposed without much effort, avoiding the difficulty or impossibility of testing in states such as pure shear, pure compression or controlled mixed modes [18].

On the other hand, an embedded cell model is a combination of meso- and micro-scale features inside the same analysis. The micro-scale features are limited to the zone where a meso-scale approach could not yield accurate results, or could simply not capture the desired phenomena. The micro-scale features, which are usually the ones that require a more refined mesh and more expensive computation (detailed interaction between phases, plasticity or damage calculations), are contained in the regions where these phenomena are expected to happen, while the meso-scale characteristics are used mainly to minimise the computational cost of the model. Thus, the latter are used in the regions where the behaviour is expected to remain homogeneous and with low gradients on the main fields [84]; see Fig. 4.3.

Micro-scale analyses have been particularly appealing for the study of UD FRPs. Due to their inherent anisotropy and the characteristics of their manufacturing procedure, constitutive models for FRPs at the meso- and macro-scale are of phenomenological nature. It means the material parameters are obtained mainly by testing different configurations of the fibre-matrix combination,

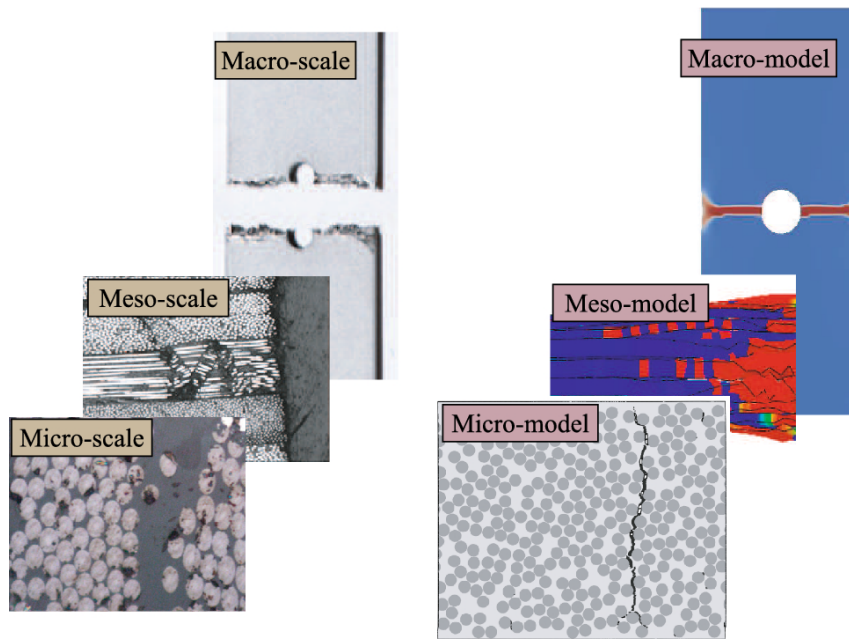


Figure 4.1: Modelling damage in composite materials at different scales [5]. *Reprinted by permission from Springer Nature: Archives of Computational Methods in Engineering, Simulation of the Mechanical Response of Thin-Ply Composites: From Computational Micro-Mechanics to Structural Analysis, Albertino Arteiro et al, Copyright (2019).*

considering the different ways the material can be oriented during loading, the different volume fractions, and the degree of curing due to different manufacturing conditions [85]. This makes the physical characterization process very demanding because standard test campaigns can be extremely complex by the amount of material that needs to be used and the load configurations that need to be imposed [75, 86, 87]. Micro-scale analysis was thought initially to alleviate this process; by replacing some of the physical tests with micro-mechanical analysis, where equivalent meso-scale stiffness [80, Chapter 4], non-linear behaviour [46] and even meso-scale strength [18] can be obtained.

4.2 Micro-scale analysis of UD FRPs

This section presents a summary of the most relevant work done on micro-scale analysis of UD FRPs; the main numerical and experimental approaches, basic assumptions, contradictions and disagreements between authors are highlighted. The idea is to give a broad perspective from the initial studies on a single fibre embedded in a matrix, to the progress to RVE models that consider the interaction between fibres in the matrix. Then, the evolution of RVEs was incorporated in multi-scale analysis and embedded cell models, which consider the interaction of the fibre bundle with the other laminae within the laminate.

The work on single fibre models and RVE analyse is extensive. It covers from soil and ceramic materials to nano-reinforced polymers and metals, from uniform and non-uniform particles,

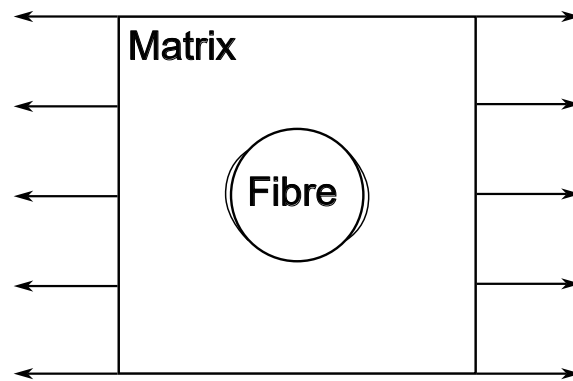


Figure 4.2: Single fibre modelling approach.

whiskers, long and short fibres, and woven and unidirectional fabrics. This review is focused on polymer composite materials with unidirectional fabrics, where the fibre is mainly carbon and glass, and the matrix is a thermoset or thermoplastic polymer. The work on thermoplastic matrices is relevant within this review; however, the information that has been found is very limited, especially if compared to what has been done in thermoset resins.

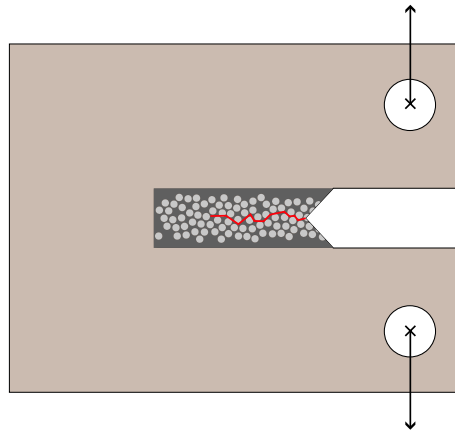


Figure 4.3: Schematic of an embedded cell simulation of fracture.

4.3 Single fibre analysis

Micro-mechanical analysis has its roots in the analysis of a single fibre embedded in a matrix mainly under transverse tensile loading; see Fig. 4.2. This problem has been extensively studied; initially using analytical models [88, 89, 90, 91, 92], experimental studies at the micro-scale [6, 93, 94, 95, 96, 97] and meso-scale [98, 99]; and later on using numerical tools such as the Finite Element Method [7, 82, 95, 99, 9, 10, 11, 27, 43, 100, 101]; peridynamics [102]; and the Boundary Element Method [81, 103]. There are studies that consider a single fibre under transverse compression [27, 104] and fatigue [105]; longitudinal tension [100] and compression [82], but these are rather uncommon and the experimental validation is in most cases not existent. The analysis of single fibre in transversal tension follows the inclusion of a secondary fibre to study the redistribution of stresses that lead to the distort both debonding angle and the direction of fracture kinking [98, 101, 103], but most work has focused on a single fibre.

The main objective of the experimental work on single fibres in a matrix under transverse tension is usually to measure or estimate interface mechanical properties (not all studies reach deformation high enough to create kinking), this was done initially in a combined numerical and experimental approach [95, 96, 97, 99], where the deformation was measured experimentally and then a numerical model was used to estimate the interface stresses before fracture; the problem comes from the fact that the material behaviour in the area close to the interface may be highly non-linear due to localized plasticity under large volumetric stresses [106]. Thus, linear elastic material assumptions in [96, 97, 99] and even the Von Mises plasticity model in [95] may fall short to predict realistic strength values. Evidence of this is the huge difference in the interface strength reported in single fibre studies such as one of Meurs et al. [95] compared with another type of studies such as the work of Chan and Piggott [107], where there is a difference of even an order of magnitude for the same material system (carbon/epoxy). Other purely experimental methods estimate the interface strength from in-situ measurements of the crack opening displacements at the interface, using a variety of other assumptions on the material behaviour [6, 94, 98]. On the other hand, numerical and analytical approaches can not be as conclusive or give as much information as the experimental work. Thus, numerics has focused on understanding the most basic failure mechanisms, the order in which they take place and the way they are influenced by the material parameters.

According to the experimental results in [6, 93], fibre debonding due to transverse tensile load is a 3D phenomenon that starts at the free surfaces in the locations of maximum normal tensile stress, see Fig 4.4 a). Increasing deformation causes the debonding to evolve both in the longitudinal (fibre axis direction) and angular direction around the fibre perimeter. The debonding angle is always larger close to the free surfaces; see Fig 4.4 b). Then, when the debonding angle reaches a critical value, the interface crack kinks inside the matrix (see Fig 4.4 b)) and debonding progress inside the specimen (tunnelling), see Fig 4.4 c). Martyniuk in [6] states that interface debonding and crack kinking both start at the free surface and then progress into the specimen's volume; this is why the work of Zhang et al. [93] uses fragmented fibres and the work of Gundel et al.

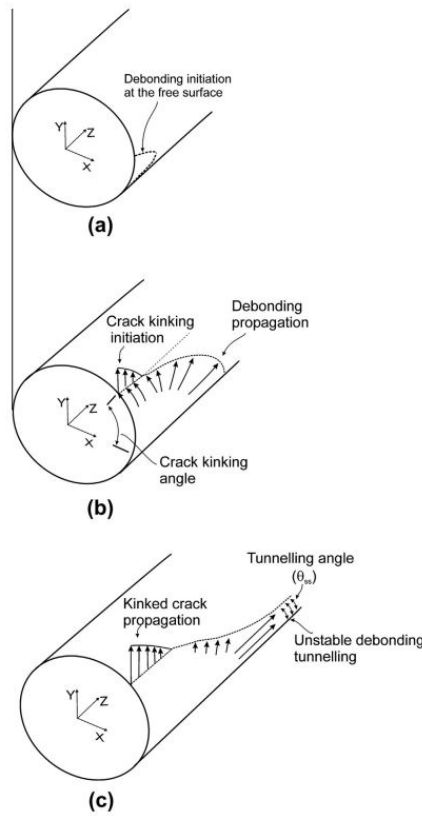


Figure 4.4: Failure sequence in a single embedded fibre: a) Debonding initiation, b) interface fracture propagation and kinking, and c) kinking propagation and tunnelling [6]. *Reprinted from 3D in situ observations of glass fibre/matrix interfacial debonding, Karolina Martyniuka, Bent F. Sørensen, Peter Modregger, Erik M. Lauridsen, Pages No. 71, Copyright (2013), with permission from Elsevier.*

[108] uses single-fibre cruciform-shaped specimens in order to study interfacial debonding while avoiding free edge effects. Other approaches, based on DIC measurements study the initiation and evolution of debonding and kinking as a 2D phenomenon [94, 98]. However, all of them agree on the sequence of damage events and the fact that both debonding and kinking changes through the thickness of the specimen.

Within the work of Martyniuk et al. [6] there were two sets of experimental campaigns both on transverse tension of single fibre specimens. The first set was called "*pre-test*", it was done in-situ using a Scanning Electron Microscope (SEM) to visualize fracture on one side of the specimens (2D view of the fracture process); the second one was called "*test*", it was done inside a synchrotron to get a full 3D view of the damage process. Both sets gave completely different results in terms of load for debonding initiation and kinking, debonding progression and even fracture patterns. Even though both sets of experiments were done using the same materials and dimensions, the specimen response was completely different (see Table 4.1 for a detailed comparison), indicating that the radiation in the synchrotron or the electric current and heat from the SEM, or

Table 4.1: Differences in the tests performed inside the SEM and synchrotron for the same EGlass/Epoxy system [6].

Test inside SEM	Test inside synchrotron
Debonding initiation: 5 MPa	Debonding initiation: 17.8 MPa
Debonding angle of 35 degrees: 6.2 MPa	Debonding angle is 9 degrees: 17.8 MPa
Crack kinking: 15 MPa	Crack kinking: 42.5 MPa
Crack kink towards the centre of the specimen	Crack kink way from the centre of the specimen

both may indeed change the material response. In the specimen tested inside the SEM, the crack kink was close to 45 degrees, then crack kinking was not fully transversal but rather tilted towards the centre of the specimen. For the specimen in the synchrotron, a larger debonding and a crack more prone to be perpendicular to the load direction was found, something similar to what was found in [94, 97, 98]. These results raise an alert because if experimental results from the in-situ measurement were to be used to determine material properties, it is necessary to account for the fact that the material may change its behaviour due to the radiation, temperature rise or electric current necessary for the method of visualization.

In contrast to the main conclusions in [6, 93], the trend in numerical and analytical studies on a single fibre embedded in a matrix is to use a 2D plane-strain assumption [7, 81, 88, 89, 90, 91, 92, 97, 9, 11, 27, 100, 101, 102, 103, 104, 105, 8]. The main contradiction comes from the fact that most studies that consider plane strain always compare the results with in-situ observations in SEM, which are observations on the free surface where the stress state is closer to plane-stress. Only a few authors consider the 3D effects of interface damage under transverse loads [95, 96, 99, 43]; and so far only one publication was found to study the 3D initiation of kinking using numerical tools; this was done using PF [43]. However, the propagation of kinking has not been analysed, apparently because of the computational resources required for this type of simulation.

The three-dimensional propagation of the initial interface crack is one of the main knowledge gaps within this type of analysis; there is not a deep understanding of the role of the stress concentration of the free surface on the debonding and kinking and the way this could affect the measurement and approximation of interface strength, interface fracture toughness, potential gradient plasticity in the matrix and micro-scale strength of the matrix. In addition, residual stresses due to thermal shrinking are known to play an important role in the failure mechanics of single embedded fibres, a factor often ignored by the traditional approaches in single fibre model. So far, it was found to be considered only in the work of Meurs et al. [95] and Totten et al. [96]. Further discussion on these topics is given at the end of this chapter.

For the numerical analysis of the fracture nucleation in single fibre models, several approaches have been followed. In this context, the "*nucleation process*" refers to the initiation of interface damage, the posterior progression of the interface crack, and final fracture kinking into the matrix. Some of the most significant methodologies to study this damage process are described next:

- Interface cohesive damage between the fibre and the matrix to capture fibre-matrix decohesion, and cohesive interfaces between all the elements inside the matrix to capture fracture inside the matrix [7, 9], see Fig. 4.5.
- Interface cohesive damage between the fibre and the matrix to capture fibre-matrix decohesion, and a kinematically enriched constitutive model for strain localization (Continuum Damage Model) [10, 82] or Phase-Field damage model (Gradient Enhanced Continuum Damage Model) [27] to capture fracture inside the matrix.
- The geometric interface and its properties are regularized using an interface Phase-Field variable; fracture inside the matrix and in the diffuse interface is captured using another Phase-Field variable [8, 11, 43]; see Fig. 4.6. This methodology requires two potentially different length scales.
- Boundary elements are used at the interface, a pre-debond is assumed; then, the virtual crack closure technique is used to estimate debonding growth and a stress criterion is employed to estimate crack kinking [81, 103, 104, 105].

From the publications that were found, it can be said that the work using the cohesive interface and bulk damage, BEM, PF damage, and some CDM are limited to linear elastic material models. Only the work of Vajari et al. [101] and Meur et al. [95] account for plasticity effects in the debonding process using a Von Mises plasticity model, and the work of Naya et al. [82] accounts for plasticity effects in debonding and matrix damage using a Drucker-Prager plasticity model coupled with CDM. However, this contradicts what was highlighted in [89], where it is mentioned that linear elastic formulations can be inaccurate in predicting material behaviour close to the interface region where debonding and kinking occur.

From the work of Guillén-Hernández et al. [27], there is an assessment of the influence of the fibre diameter on the failure process, demonstrating that there is a size effect associated with this particular problem. This size effect has been acknowledged by most of the authors, and it sets a valid argument to recognise that the macro-scale experimental [6, 98, 99] and numerical [43, 81, 95, 96, 97, 82, 103] studies where fibres ranking from 50 microns to 1 mm may not be truly representative of standard composite materials, where fibre diameters rank from around 5 microns for carbon fibres to 20 microns for glass fibres. Thus, such studies need to be carefully analysed if realistic material properties want to be extracted from there.

Validation in terms of comparing experimental and numerical or analytical results has been done mainly in qualitative rather than quantitative terms. Indeed, most of the aforementioned studies using different formulations and different material properties are able to capture the general trend of debonding initiation, debonding progression and matrix kinking. The results are a rather similar-looking damage scenario. But similar-looking patterns do not necessarily imply physically correct models, as the material properties can be easily tuned to get the desired failure pattern (this discussion is resumed at the end of the chapter). There are still reasons to doubt. Some of the most significant are: (i) inconsistency between 3D phenomena and 2D plane strain assumption, (ii)

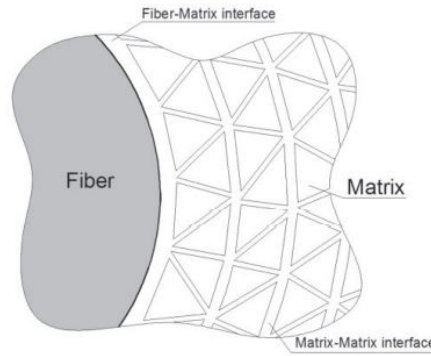


Figure 4.5: Cohesive damage modelling for interface and matrix cracking [7]. *No permission is required for the reprint of this figure.*

linear elastic material models to analyse regions where non-linear material behaviour is expected, (iii) inconsistency between scales, (iv) modification of material properties due to the measuring procedure done in-situ, (v) potential need to account for residual thermal stresses.

From what was found in the literature review, the only objective and qualitative analysis was done between numerical approaches, all of them using a single fibre of 0.5 mm diameter inside a 1 mm square matrix (not a realistic scale for composite materials), a 2D plane-strain condition and the material properties shown in Table 4.2. The comparison was made between the approaches in [7, 9] (cohesive matrix and interface damage); see Fig. 4.7 a), b); the CDM of [10]; see Fig. 4.7 c) and the PF implementation of [11]; see Fig. 4.7 d), e), f).

In all cases, interface damage is similar, the main difference is in the matrix crack pattern:

- The cohesive damage in the matrix does not create a single crack kink, but rather a network of cracks transversal to the load direction in the area of larger normal stresses, this is because, in the randomness of the mesh, the elements whose sides are aligned transversally to the load are more prone to fail, this effect is more pronounced in [9] (Fig. 4.7 b)) than in [7] (Fig. 4.7 a)).
- The CDM approach of [10] creates a damaged band whose width is close to the element size and is oriented transversally to the load direction.
- The PF implementation of [11] uses a variation of PF-CZM to compare different energy splits. These define a crack kink that either runs transversally to the load (Fig. 4.7 e), f)) or deviates towards the centre (Fig. 4.7 d)), similar to the in-situ observations using SEM in [6].

For the properties of this example (Table 4.2), traditional PF approaches such as AT1 and AT2 would yield a length scale parameter (L_0) of 0.496 mm for AT1 and 0.14 mm for AT2. The problem when the length scale is similar to the fibre diameter is that the crack cannot localize; thus, failure looks like a diffuse damage pattern rather than an approximation of a sharp crack. This is one

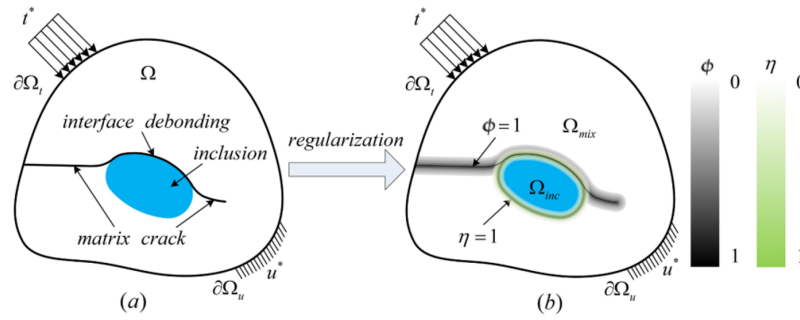


Figure 4.6: a) Sharp representation, b) diffuse interface (η) and damage (ϕ) representation [8]. Reprinted from *Modelling progressive failure in multi-phase materials using a phase field method*, PengZhang, Xiaofei Hu, Shangtong Yang, Weian Yao, Pages No. 107, Copyright (2019), with permission from Elsevier.

of the typical issues in micro-mechanical analysis using PF with traditional approaches, because the length scale is related to the matrix properties it does not account for the fibre or specimen dimensions, creating limitations to specific scales of the model, where the specimen and geometric details must be larger than the length scale.

4.3.1 Thermoplastic based composites in single fibre analysis

It is necessary to mention that according to the publications that have been found, single fibre models have been studied exclusively using thermoset matrices.

4.3.2 PF in single fibre analysis

The use of PF on single fibre analysis is limited to linear elastic material formulations, infinitesimal deformations and no account for residual stresses. Crack kinking is always studied under the plane-strain assumption; 3D effects such as crack tunnelling and kinking initiation have only been addressed in the 3D model of Song et al. [43]. Only the work of Guillén-Hernández et al. [27] and Song et al. [43] consider realistic micro-scale dimensions; the work of Zang et al. [8, 11] is limited to fibre diameters of 0.5 mm, which are not representative of the micro-scale. Experimental validation was done only for the study of Song et al. [43]; the other studies are purely numerical. The publications [8, 11, 43] use a geometric and a damage PF variable to define the interface and fracture with both the bulk matrix and the diffuse interface, while [27] uses PF damage only in the matrix, while cohesive damage is considered at the interface. The fibre is always considered linear elastic. As a final remark, it is necessary to mention that the work of [27, 43] use the AT2 formulation while [8, 11] use a modification of the Phase-Field cohesive zone model (PF-CZM) developed by Wu and Nguyen [109] in order to reduce the length scale to micro-scale dimensions. So far, there is no work on plasticity models, large deformations or proper validation of crack kinking in a 3D scenario. This last comment is made due to inconsistencies found in [43] where tunnelling is compared with the results of synchrotron while crack kinking is compared

Table 4.2: Mechanical properties used in single fibre analysis under transverse load [9].

Elastic properties					
E_{matrix}	ν_{matrix}	E_{fibre}	ν_{fibre}		
4 GPa	0.4	40 GPa	0.33		
Fracture toughness					
Matrix					
G_{Ic}	G_{IIc}	σ_t	σ_s	μ	K
0.25 N/mm	0.25 N/mm	30 MPa	30 MPa	2.0	10^6 N/mm
Interface					
G_{Ic}	G_{IIc}	σ_t	σ_s	μ	K
0.05 N/mm	0.05 N/mm	10 MPa	10 MPa	2.0	10^6 N/mm

with results from SEM in [6], this is inconsistent given the differences found in the results from both experimental observations; see Table 4.1.

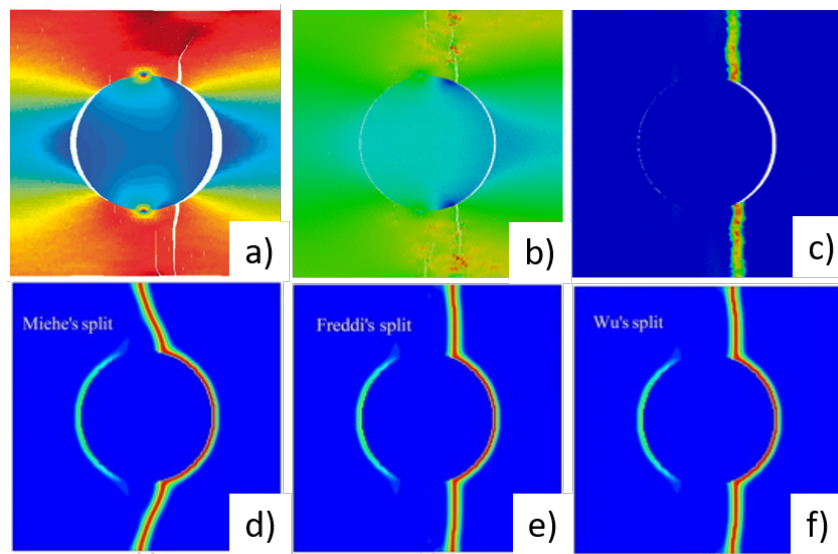


Figure 4.7: a) Cohesive matrix and interface damage modelling approach of [7], b) Cohesive matrix and interface damage modelling approach of [9]. *Reprinted from Discontinuous Galerkin/extrinsic cohesive zone modeling: Implementation caveats and applications in computational fracture mechanics, Vinh PhuNguyen, Pages No. 58, Copyright (2014), with permission from Elsevier.* c) CDM approach of [10], and Phase-Field approach of Zhang et al. [11] using d) Miehe's energy split, e) Freddi's energy split and f) Wu's energy split. *Reprinted from 3D micromechanical progressive failure simulation for fiber-reinforced composites, Peng Zhangab, Weian Yaoab, Xiaofei Huab, Tinh Quoc Bui, Pages No. 8, Copyright (2020), with permission from Elsevier.*

4.4 RVE analysis of composite materials

From the analysis of single fibres embedded in a matrix; the next step is the inclusion of more fibres to imitate the actual micro-structure of a composite material. The initial mechanical definition of an RVE is given by Hill in [110], one of the first publications on RVE analysis, and it defines RVE as: *'a sample that (a) is structurally entirely typical of the whole mixture on average, and (b) contains a sufficient number of inclusions for the apparent overall moduli to be effectively independent of the surface values of traction and displacement, so long as these values are "macroscopically uniform". That is, they fluctuate about a mean with a wavelength small compared with the dimensions of the sample, and the effects of such fluctuations become insignificant within a few wavelengths of the surface. The contributions of this surface layer to any average can be made negligible by taking the sample large enough.'* This goes in line with the analysis of Trias et al. [111]; in this publication, there is a special emphasis on the need to define the minimum finite size of the RVE to be considered representative in the mechanical sense. Trias concludes that for a mechanical definition, the minimum RVE size depends on the specific analysis to be performed and the metric to be analysed; namely, the analysis of effective elastic properties requires a larger RVE than the analysis of stresses or strains.

However, in the analysis of stresses and strains, the minimum RVE size varies if the conclusions are based on metrics such as the mean value, coefficient of correlation or percentual difference. In addition to the mechanical definition, there is a statistical definition related to the analysis of *'point pattern formed by the distribution of fibres or inclusions centres in the matrix, that is to focus on the representativeness of the random geometry'* [111]. This is the focus of the work of Melro et al. [112] and Li et al. [113] where different statistical-based criteria are used for the definition of the RVE and then, these criteria are assessed by studying the error when approximating elastic mechanical properties; namely, verifying that the "mechanical definition" is met.

Even though there have been considerable efforts in determining the mechanical and statistical definitions of the RVE, there is no general agreement and the terminology is still used rather ambiguously, e.g:

- In the work of Naya et al. [82] one of the analysis is performed on a single fibre model that is called *"single-fibre RVE"*, which is incompatible to the statistical definition of RVE given in the work of Melro et al. [112] and Li et al. [113].
- In the work of Nguyen et al. [114] the term RVE is replaced by *"statistical microstructural volume elements"* (SMVE). Where an SMVE is equivalent to the statistical definition of RVE but the fibre arrangement definition is not restricted by the periodic arrangement assumption (see Fig. 4.8 b)); in contrast to the work of Melro et al. [112] where the RVE is also specified based on the statistical definition but a periodic fibre arrangement is enforced (see Fig. 4.8 c)).

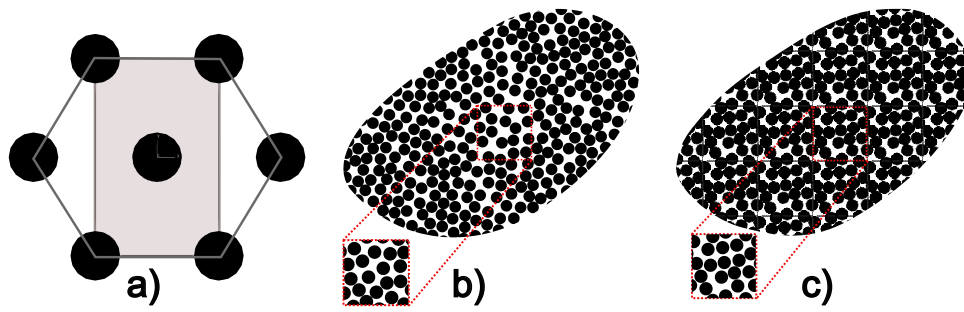


Figure 4.8: a) RVE with a hexagonal fibre distribution [12], b) non-periodic RVE with a random fibre distribution [13], and c) periodic RVE with a random fibre distribution.

- In the work of Wu et al. [44] the term RVE is replaced by the terminology "*Stochastic Volume Elements*" (SVEs), where SVE can be seen as a statistical definition of RVE in stochastic multiscale analysis.
- The work of Pulungan et al. [115] refers to RVEs of random, square and hexagonal fibre patterns (see Fig. 4.8 a)); in this case, the RVE concept is defined in a way closer to the mechanical definition. In Pulungan et al. [115], an RVE with square and hexagonal fibre patterns completely contradicts the statistical requirements mentioned in [112, 113].
- In the work of Arteiro et al. [83] the term RVE refers to sections of an embedded cell model for a cross-ply laminate analysis, where periodicity is assumed in the longitudinal direction.
- The work of Bai et al. [116] mentions Statistical Volume Elements (SVEs) and RVEs. In [116], the definitions are linked to the size of the unit cell, as explained "*If the size of the unit cell is not large enough then the randomness of the fibers position significantly affects the response of the composite and the unit cells are called Statistical Volume Elements (SVEs). However, if a sufficiently large domain is considered, then the homogenized response is virtually independent of the randomization of the microstructure and the unit cell is denominated as a Representative Volume Element (RVE)*". Thus, the RVE definition of Bai et al. [116] is closer to the statistical concept. However the word "*statistical*" in the rather new concept of SVE can just add more confusion.

The use of RVE models for the analysis of UD FRPs is extensive. This is because it can be approached from different perspectives and with different objectives; some of the most relevant goals in RVE analysis are:

- The use of mechanically loaded RVEs to study or predict the failure initiation and progression of composites under different loading scenarios [11, 29, 30, 31, 44, 46, 117, 82, 106, 118, 116, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 114, 134, 135, 136, 137].

- Study the influence of mechanical properties of the constituents (fibre, matrix, interface) on the meso-scale strength and stiffness of composites [46, 117, 106, 118, 116, 119, 120, 121, 122, 123, 124, 125, 126, 129, 134].
- Examine the influence of residual thermal or hygroscopic loads and environmental conditions on the mechanical response of the composites [117, 119, 120, 126].
- Study the influence of geometric parameters such as RVE size, boundary conditions, fibre orientation/misalignment and initial defects in the predicted meso-scale strength of the composite [44, 46, 82, 111, 126, 127, 128, 129, 133, 114, 135, 136].
- Validate and verify the suitability of the use of novel material, damage or interface interaction models for the micro-scale analysis of composite materials [7, 11, 12, 29, 30, 31, 46, 106, 130, 132, 114, 134, 138].
- Assess the suitability of experimental approaches such as micro-DIC for the analysis of micro-scale deformation of composite materials [135, 139, 140].

To carry out any of the aforementioned analysis types, a general procedure must be defined, containing: (i) the definition of the fibre distribution algorithm, (ii) the selection of the size of the RVE and boundary conditions, (iii) modelling approach (main assumptions, material and interaction models) and (iv) verification and validation approaches. In this section, there is a description of the main methodologies that have been used to approach each of these steps.

4.4.1 Definition of the fibre distribution

As mentioned earlier, there are different ways in which the transversal pattern of fibres can be staked; the more simplistic approach is the assumption of a specific geometric distribution of fibres. The hexagonal fibre pattern, which is one of the most commonly used [12, 30, 122, 128, 132] requires no more than two fibres and symmetric boundary conditions to obtain an equivalent periodic arrangement; see Fig. 4.8 a). The fact that this method requires less amount of fibres within the RVE makes it ideal for 3D analysis. All the publications that were found using a hexagonal distribution are in fact 3D models.

This is particularly relevant for capturing phenomena such as buckling due to longitudinal compression [128]. But it may look oversimplified if transverse failure is considered and the thickness of the RVE is lower than the fibre diameter [12, 132] because no actual 3D effects are captured. This arrangement method, even though is the most computationally efficient due to the small mesh, it does not represent realistic composite micro-structures which are intrinsically random [111]; besides, according to Pulungan et al. [115], hexagonal fibre patterns can heavily overestimate the meso-scale transversal strength.

Approximations to random fibre distributions are artificially generated using mainly two methods: the random sequential adsorption [29, 120]; which in a 2D transverse perspective consists of randomly placing circles inside an area, where there are restrictions on the maximum number of

fibres to define a specific volume fraction and a minimum distance between fibres; and the nearest neighbour method developed by Vaughan and McCarthy [141] that uses experimentally measured statistical parameters to define the arrangement of fibres. This allows the artificially created distributions to approximate the interactions between fibres [141]. This method was validated by matching effective elastic properties, which is not a very strong argument because even the most simplistic analytical micro-mechanical models can be very accurate in the elastic predictions [80, Chapter 4].

These two methods have been extensively used, in fact, they are the most used methods for micro-mechanical analysis. But the most accurate approach for the definition of fibre distributions in the RVE is by replicating micro-graph pictures from transversal cuts on unidirectional laminates [135, 139]. This method, even though is more realistic, it may require tuning if periodic boundary conditions for periodic arrangements are expected to be used [135]. According to Hernandez et al. [142] the fibre distribution has been shown to *"significantly impact the transverse cracks formation and pattern"*, while most of the artificial algorithms to generate fibre distributions have been validated only in terms of stiffness there is still the need to evaluate the overall performance of these algorithms with more objective metrics that include non-linear behaviour and fracture.

4.4.2 Boundary conditions and RVE size

From the mechanical definition of RVE, one of the main concerns is the need to "eliminate" the stress concentration or inhomogeneous effects generated by the RVE edges. The most common strategy to do it is by using periodic Boundary Conditions (BC) [143]. The way periodic BC are applied implies a kinematic coupling between all the nodes located on opposite faces, edges, and vertices, and these are at the same time linked to the far field strains. The procedure is explained in detail in [144, Chapter 6]. Periodicity is imposed in such a way that the randomness is limited to what is contained inside the RVE; thus, assuming that such randomness is indeed periodic [13, 145], see Fig. 4.8 c).

The periodic BC assume that the structure is periodic and also every phenomenon that happens inside; then, any sort of damage becomes periodic [143]. As a consequence, the macro-scale perception is not like a single crack that runs through the material, but rather a material that is fragmented into pieces, where the dimension of each piece is proportional to the size of the RVE. Then, after damage onset, there is no sudden load drop but rather a gradual softening. Smaller RVEs show a more pronounced delay of crack propagation (this has already been mentioned by Nguyen et al. [114]). The reason for this softening is that the smaller the RVE, the larger the virtual interaction between cracks in the meso-scale response; when the RVE size is increased the interaction diminishes and failure becomes more brittle. This is one of the observations from the results and it will be further discussed later.

Even though periodic BC are widely used, these are not the only type. If the size of the RVE is large enough *linear BC*, which consist of imposed displacements on the edges, give similar or equivalent results to periodic BC according to some authors [7, 30, 31, 127, 128, 134, 136]. *Linear BC* are particularly useful when explicit analysis is performed because it avoids spurious

oscillations [127, 134]. The main issue with this approach is related to the fact that the edges of the RVE act as stress concentrators, this is why, if fibres are cut on the edges, fracture starts from those areas [127, 134], and the results may under-estimate the strength. Some authors avoid this issue by generating a resin reach region around the RVE border [7, 30, 31, 136] or by placing the RVE inside a homogeneous material with equivalent properties (Embedded cell) [111]. Creating a resin-rich region can alleviate the stress concentration on the edges, but reduces the volume fraction; this reduction is proportional to the RVE size. Thus larger RVEs are required to maintain a specific volume fraction if a spread fibre distribution is required.

These last two types of BC are much easier to implement and they do not suffer from spurious softening effects even for small RVEs. Other traditional BC conditions are uniform traction or minimal BC [143], which compel the borders to remain straight. These can heavily underestimate the meso-scale strength while overestimating the stiffness. This is why they are rarely used. Novel BC such as the ones developed by Coenen et al. [143] are equivalent to periodic BC and they can localize damage. However, the implementation is highly complex; that is why they are not extensively used.

One of the most detailed analyses on the effect of the RVE size on the predicted meso-scale strength is the work of Trias et al. [111] (previously mentioned) and the one of Van Der Meer [133]. This last publication relates the mean values and variation of meso-scale tensile stresses to the size of the RVE while using periodic BC. One important conclusion from Trias et al. [111] and Van Der Meer [133] is the fact that smaller RVEs provide a higher scatter, but such scatter is gradually diminished in the limit of an RVE of infinite dimensions. From [133], it is important to learn that one cannot draw conclusions from a single RVE model, and even the mean value can be misleading if the size of the RVE is too small. Even though this is an important contribution, studies that compare fracture from RVEs with different sizes [46, 114, 136], do not follow a similarly rigorous analysis which can allow getting estimates of appropriate RVE size for specific loading and material behaviour. Thus, there is not a deep understanding of the role of RVE size on the accuracy and variation of results for fracture prediction and potential dependency on the direction of loading and BC.

4.4.3 Modelling approach: Assumptions and boundary conditions

As mentioned earlier, one of the most appealing aspects of RVE analysis is the fact that arbitrary complex stress states can be imposed. However, depending on the purpose of the analysis, some assumptions can be made. The study of pure transverse loading is usually done using 2D plane-strain models or quasi-3D models [129]. Quasi-3D refers to models using a 3D mesh but where the thickness of the RVE is much smaller than the fibre diameter; with usually less than five elements. Thus, quasi-3D and 2D plane-strain models focus on transverse tension and compression loading [7, 29, 31, 119, 120, 130, 131, 114, 136, 139, 140], shear loading is studied mainly as an example [118, 123, 124, 138]; but it is considered less relevant because results for this scenario cannot be validated.

For quasi-3D models when used to study transverse failure, due to the periodic BC on the thickness direction, these impose out-of-plane constraining that is not as strong as plane strain but is more restrictive than plane stress [12, 46, 126, 129, 132, 133, 134, 135, 137]. These differences have a key relevance in the fact that some of the quasi-3D models use pressure-dependent plasticity models. Thus the effect of the thickness and lateral constraining can have important repercussions on the meso-scale response. So far, there was not a comparison between both approaches, nor a study of the influence of the RVE thickness and lateral constraint on the predicted stiffness, strength, or plasticity effects.

Sometimes quasi-3D models are used for out-of-plane loading analysis, specifically where shear is applied [12, 46, 117, 125, 126, 129, 132, 133, 134, 135, 146], but also for longitudinal compression and tension [132]. There is not a comparison or analysis of the effect of RVE thickness on the prediction of out-of-plane failure, but there are considerable differences in the literature; some authors study out-of-plane shear using an RVE thickness as low as 8% of the fibre diameter [146] and some others reach 100% of the fibre diameter [134]. 3D models where the thickness dimension is close to the RVE size or larger are mainly used to study longitudinal buckling [82, 116, 127, 128] or longitudinal tension [122]. Studies using the Phase-Field method have been employed only to study transverse fracture in 3D geometries [11, 30], but no characteristic 3D effect such as tunnelling or surface crack kinking has been captured.

4.4.4 Modelling approach: Material and interaction models

The extensive work on micro-mechanical analysis has come with a large variety of material and interaction models. The material models used in the fibre are always linear elastic isotropic models in the case of glass fibre and linear elastic orthotropic in the case of carbon fibre. Only a very few publications account for fracture in the fibre and they do so by placing layers of cohesive elements perpendicular to the fibre axis [122] or using CDM [132]. So far these methodologies do not account for the distribution and size effect of the fibre strength reported in the experimental results of Wisnom and Atkinson [147]. The only micro-mechanical work that accounts for the dynamic effect and fibre strength distribution is the work of Tavares et al. [148].

On the other hand, the assumptions and material models used in the matrix are far from reaching a common agreement. Publications can be found assuming small and large deformations for the same type of material. There are authors that consider for epoxy resin, linear elastic formulations that account for damage using cohesive interaction between each element [7] (see Fig. 4.5), CDM [136], XFEM [131], and PF fracture [11, 29, 30]. For the same type of epoxy, there are also elasto-plastic models where areas high plastic deformation are considered as fractured but without accounting for an explicit damage or fracture model [118, 119, 120, 121, 122, 124, 125]. Or elasto-plastic models coupled with damage, using the model of Melro et al. [149] (see [46, 116, 126, 127, 129, 133, 134]) and the build-in Drucker-Prager/damage of Abaqus (see [117, 106, 126, 131, 132, 135]). Some more advanced models account for viscoelastic/plastic with entropy damage [130], elasto-plastic gradient enhanced damage models [44] and hyper-elastic viscoelastic-viscoplastic-damage [114]. The trend has been to use a plasticity model, initially Von

Mises plasticity [31, 128], but then they evolved to plasticity models that account for the volumetric part of the deformation; most of the literature is limited to Melro's model [149], Drucker-Prager and Mohr-Coulomb.

Regarding the interaction models, even though the main trend is to use cohesive models or cohesive surface interaction [7, 46, 117, 82, 106, 118, 119, 120, 121, 122, 123, 124, 125, 126, 129, 131, 132, 133, 134, 135, 137], there are authors that assume the interaction is a perfect union [12, 30, 116, 128, 130, 114, 136, 138, 146] or, on the contrary, some authors assume the interface region is a transition zone of finite thickness, where the strength and stiffness vary from the values on the fibre to the values of the matrix. This transition zone is given as a thin section with homogeneous properties and attached to the fibre through cohesive interaction [134] or the fibre-matrix boundary is a smooth diffuse transition represented with a PF geometric parameter that controls the gradual change in the properties over a small region (see Fig. 4.6 b)) [11, 30, 31]. The main limitation of this last assumption is the fact that there is no experimental evidence that can support the existence of such a transition zone, and as explained by Canal et al. [139] the deformation measurements that can be done in the transition area (using DIC for example) are not accurate because its characteristic high gradient due to the difference in the stiffness of the fibre and the matrix.

4.4.5 Verification and validation

When the analysis is elastic, validation is performed most of the time. However, if failure is taken into account, validation is usually not conducted. Instead, sometimes, verification is done using standard meso-scale failure criteria [11, 123, 124, 126]. On the other hand, standard meso-scale tests on unidirectional laminates are mainly used for back-calibration of mechanical properties and in fewer cases for validation. According to Nguyen et al. [114], a modelling approach that has been calibrated from meso-scale results cannot be called "*predictive*"; in this work, there is a clear emphasis that for a model to be called "*predictive*", it needs to account for input material properties that have to be extracted from the individual material tests and not reverse calibrated from testing the composite itself. In contradiction to this idea, other authors back-calibrate mechanical properties using experiments on standard composite laminates and then highlight predictive capabilities by comparing numerical results with the same results that were used for calibration [132, 134, 135].

According to the publications that were revised, most authors that perform validation, do so by comparing stress-vs-strain curves extracted from the standard tests on laminates [12, 29, 131, 132] or by comparing specific strength and stiffness values extracted from manufacture's data-sheets. On the other hand, there are authors that are very rigorous in the validation methodology, such as Chevalier et al. [106] and Mehdikhani et al. [140], that perform validation using micro-DIC measurements to compare strain distributions measured directly at the fibre scale, the problem with such a measurement, according to [139], is that the strain fields cannot be accurately captured by DIC in the area close to the fibre-matrix interfaces, which is precisely the most critical region.

Due to the limitations on testing setup, validation is usually performed in pure transversal tension and compression, shear in the 12, and some off-axis tests. Results on shear 23 or a combination of shear 23 and transversal compression/tension predictions have not been validated due to experimental limitations.

Moreover, many authors do not perform either calibration or verification but rather focus on the analysis of the influence of different parameters within the specific modelling approach [7, 11, 30, 31, 46, 118, 129, 130, 133, 136, 138, 146].

4.4.6 Thermoplastic based composites in RVE analysis

Within the work on RVE analysis of long fibre-reinforced polymers, most of the work that has been revised is dedicated to epoxy matrices. The only publications that were found to study thermoplastics are:

- The work of Hsu et al. [150] is one of the first publications on RVE analysis of thermoplastic composites using AS4/PEEK; it studies transverse compressive failure and in-plane shear using a Drucker-Prager model that includes viscous effects and damage to model failure in the matrix but disregarding the effect of interface damage. It is not mentioned if the finite or small deformation assumption was considered. Conclusions are given based on a single RVE with a hexagonal fibre pattern.
- The work of Totry et al. [125] studies failure initiation on carbon/PEEK under transverse shear/compressive loading, where the material is assumed as rate independent. Plastic deformation was modelled using the Mohr-Coulomb criterion, assuming infinitesimal deformations theory. Besides, interface damage was accounted for using cohesive interaction, but no damage or fracture model was employed in the matrix. The areas of higher plastic strains were assumed as fractured. Conclusions are given according to the results of six different RVE under periodic BC.
- The work of Pulungan et al. [115], which studies failure on glass/polypropylene under transverse tension loading. In this case, they do not account for rate dependent effects explicitly but rather assume homogeneous strain rates throughout the RVE and calibrate quasi-static material response to match kinetic stress-strain curves at the given average strain rate that is expected in the RVE. Plasticity and damage were included using the built-in Drucker-Prager model of Abaqus, but it is not mentioned if the finite or small deformation assumption was considered. Besides, interface damage was accounted for using cohesive interaction. Conclusions are given according to the results of five different RVE under periodic BC.

The material models and assumptions used in the case of thermoplastic matrices do not differ significantly from what is found in the case of epoxy matrices. The methodologies so far can be considered equivalent.

4.4.7 Phase Field fracture in RVE analysis

The work on RVE analysis using PF fracture is also very limited and dedicated exclusively to epoxy resins. The first author that performed micro-mechanical analysis of fracture using PF was Espadas-Escalante et al. [29] in 2019. They used a 2D plane-strain model with an AT1 formulation and compared the performance of Amor and Miehe splits in the predictive capabilities of fracture under pure tension and pure compression. In this work, fibre-matrix interaction was ignored (even though it has been proven to play a major role in compressive failure [126, 135]), and calibration of the mechanical properties was performed by comparing tensile transversal strength with the value obtained from the experimental results in [45] and the transversal compressive curve in [45]. The calibrated results were compared to the experimental data; however, these are not considered as a way of performing validation given the arguments of Nguyen et al. [114].

The next was the work of Yin and Zhang [30], where a 3D model using an AT2 formulation was used to evaluate the influence of fibre orientation on the transverse strength of a composite material. In this case, fibre-matrix interface damage was also ignored. The results were not validated because the specimen and fibre dimensions were not representative of micro-scale dimensions.

The most recent is the work of Li et al [31] and Zhang et al [11] which consider diffuse interface using a geometric PF variable. Li et al [31] uses a 2D Von Mises plasticity model coupled with an AT2 PF formulation, but neither the material properties nor the fibre dimensions are representative of the micro-scale in a polymer composite. Zhang et al [11], on the other hand, performed an analysis limited to transverse tension and considered a 3D mesh with different volume fractions and fibre distributions. It uses a modified PF-CZM formulation; in this work there is no comparison with experimental data.

So far there has not been a study of the capabilities of PF for the prediction of failure envelopes, nor the influence of the BC and RVE size on prediction capabilities using this tool. Also, up to this moment, PF with elastic and Von Mises plasticity formulations have been used, but there has not been micro-mechanical analysis using pressure-dependent plasticity models coupled with PF.

4.5 Embedded cell models

Reinforced polymer micro-structures can be embedded as subsections in the interior of specimens to create embedded cell models; see Fig. 4.3. The most common use of this technique is for the analysis of fracture in the ply located at 90 degrees. In laminates loaded in the transverse direction, the laminate can be quasi-isotropic [151], but the majority of studies focus on cross-ply laminates [14, 152, 153, 154, 83, 155, 156, 157]. Within the micro-mechanical study of cross-ply laminates, the main focus is the study of the in-situ effect [14, 15, 83, 155, 156, 157, 158]. In addition, micro-mechanical models have been used for the analysis of fracture propagation tests, such as:

- Three-point bending on pre-notched notched [28, 47, 49] and pre-cracked specimens [159].
- Delamination migration experiments [160].
- Transverse crack tension tests [161].

Similarly to the RVE studies, the following subsections describe and discuss the methodologies and assumptions that have been used so far for embedded cell models.

4.5.1 Definition of the fibre distribution

Just like in RVE analysis, for embedded cell models, most authors use artificially generated fibre distributions [15, 28, 47, 49, 152, 153, 83, 155, 156, 157, 158, 160, 161], there is a minority that extracts such distribution from micrographs [14, 151, 154, 159].

Even though the differences and relevance of the origin of fibre distributions were discussed for RVE analysis. This topic presents additional relevance to embedded cell models. One of the reasons is that artificial fibre distribution does not usually account for the fibre clusters or resin reach areas that are common in composite laminates. Besides, the borders of the micro-mechanical zone are usually non-homogeneous resin-rich regions, which have not been accurately represented with artificial fibre generators; see for example the difference in the artificial fibre distribution of Fig. 4.9 b) and the fibre distribution extracted from micrographs in Fig. 4.9 a).

The two microstructures depicted in Fig. 4.9 a) and b) represent the horizontal view of the micro-scale structure of a 90-degree thin-ply laminate. However, the morphology is completely different, specially on the upper and lower edges, and on the resin-rich regions created in the transitions from one thin-ply to the next one.

Unlike in RVE analysis, embedded cell models do account for the edge effects when they are located either on the external surface or next to another type of material/layer; thus, an accurate representation of the micro-structure in these areas can potentially make a difference in the predictions. So far, only the work of Sharifpour et al. [152, 153] studies the effect of internal and interplay resin-rich regions, micro-voids and micro-cracks with artificially generated microstructures. They conclude that the results are highly dependent on the lateral constraining of the section; resin-rich regions are considered critical if there is a high constraint and cavitation failure is expected because these areas are more prone to yield and cavitate. Still, voids and micro-cracks are

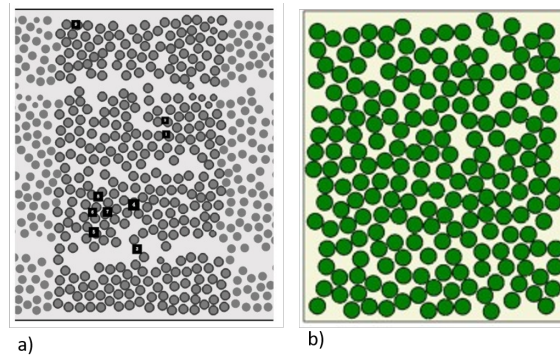


Figure 4.9: Comparison of micro-scale fibre distributions: a) generated from micro-graphs [14] (Reprinted from *Micromechanical analysis of damage mechanisms under tension of 0° – 90° thin-ply composite laminates*, M.Naderi, N.Iyyer, Pages No. 2, Copyright (2020), with permission from Elsevier), b) artificially generated [15] (Reprinted from *In-situ strength effects in long fibre reinforced composites: A micro-mechanical analysis using the phase field approach of fracture*, T.Guillén-Hernández, A.Quintana-Corominas, I.G.García, J.Reinosoc, M.Paggi, A.Turón, Pages No. 10, Copyright (2020), with permission from Elsevier).

considered more critical. From this study, even though there is no validation, the artificial fibre distributions and assumed defects are clearly different from micro-structural images; the conclusions are still relevant, and all the manufactured induced defects can potentially play a significant role in the performance of composite laminates.

4.5.2 Boundary conditions and embedded cell size

Embedded cell models inherit the same trends and contradictions found in RVE analysis regarding the out-of-plane thickness, RVE size, and boundary conditions. Regarding the size of the embedded cell section, the most straightforward comparison can be given for cross-ply analysis, comparing the relationship between the length of the section L and the 90 degree ply thickness t_{90} , see Fig. 4.10; there are authors that consider very small sections, such as the work of Guillén-Hernández et al. [14] and Naderi and Iyyer [15] where a single crack is expected, the length L is approximately equal to the 90 degree ply thickness t_{90} ; while in models such as [154, 158], can nucleate several cracks and show the interaction between them, the longitude L is around 13 times the 90-degree layer thickness t_{90} . So far there is no study of the influence of the ratio L/t_{90} on the accuracy of in-situ or transverse strength predictions.

Regarding boundary conditions, again, there are opposite opinions. Some authors impose Dirichlet BC [14, 151, 154, 156]; while others prefer to use periodic conditions on the longitudinal direction [15, 152, 153, 83, 155, 158] and the thickness direction [83, 155]. The selection of either option is not related to the length L of the section, there are examples of works with very small values of L using Dirichlet [14] and Periodic [15] BC, and very long sections with both approaches as well. It is known and acknowledged by the authors the fact that periodic BC have considerable

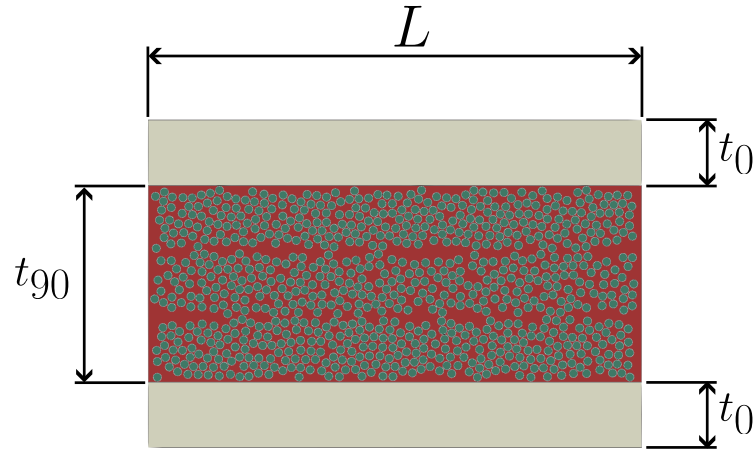


Figure 4.10: Relation between laminate length L , 0 degree ply thickness t_0 , and 90 degree ply thickness t_{90} .

influence on the post-failure behaviour of the model, but there is no study that compares or analyses the effect of BC on the predicted transverse strength or in-situ effect.

4.5.3 Modelling approach: Assumptions and boundary conditions

In the combined experimental/numerical study of the in-situ effect using quasi-isotropic laminates of Koheler et al. [151], fracture initiation is measured using in-situ observations in an optical microscope and using acoustic emission (AE). They show that the predicted in-situ strength is different if estimated based on the observations of cracks on the surface or based on acoustic events. Normally free edge cracks are visible at lower strains compared to what is perceived by AE. This goes in line with the experimental study of [6], and the conclusion is the same, surface observations can only tell part of the story. Apparently, the acoustic event is triggered not by the initial free-edge crack but by its propagation inside the specimen. Thus, performing validation of numerical or analytical approaches using only surface measurements or crack densities is potentially inaccurate into the light of a broad collection of experimental evidence.

2D plane stress analysis such as [14, 28, 47, 49, 153, 154, 156, 157, 158, 159] may fall short to capture the complete physics of the event. Likewise, 3D analysis with thin sections poses similar limitations, most of the models are thin, unconstrained, or under-constrained only with periodic BC in the out-of-plane direction. Unconstrained models are closer to plane stress, depending on the thickness of the section which can vary considerably in different publications. On the other hand, periodic BC in the out-of-plane direction are partially constrained, they are somewhere in the middle of plane stress and plane strain, which makes it difficult to assume which part of the laminate they represent if the middle or the outer surface.

The numerical work of Koheler et al. [151] shows that there are significant differences in the predicted results if the 3D model is constrained to approach the bulk (inside of the specimen) or the free edge. The conclusion of that work is that depending on the laminate thickness, the

free-edge BC (similar to plane stress) predicts higher strength compared with bulk BC (similar to plane strain). The numerical results of this work are rather unexpected or somehow contradictory, because plane-stress-like predictions (BC for free edge) are closer to AE events, while plane-strain-like predictions (BC for bulk) are closer to free edge observations. Thus, a more realistic 3D modeling approach or constraining method should be used to attempt more realistic predictions of such failure scenarios. Besides, the effect and degree of accuracy of out-of-plane BC have not been addressed so far, and neither has the effect of out-of-plane thickness of the representative section.

So far, only the approach of Canal et al. [49] accounts for large deformations on the three-point bending simulation of the notched specimens. This is ignored in the work of Tan and Martínez-Pañeda [28, 47] whose modeling approach uses PF and infinitesimal deformations to model the same experimental results in [49]. In this particular scenario, large deformations may be quite relevant because one of the variables for validation is the measure of the Crack Mouth Opening Displacement (CMOD), and such deformation can reach values close to the notch dimension. The remaining studies on the embedded cell models also assume infinitesimal deformations, even if the local strains in the matrix close to the damaged areas reach deformations higher than 5% (according to most solid mechanic books [162, 163], strains higher than 5% should be considered as finite deformations). Unlike previous studies comparing RVE results under finite and infinitesimal deformations for RVE analysis in [117], such a study has not been performed for embedded cell models; thus the influence and accuracy of the infinitesimal assumption are still unknown.

4.5.4 Modelling approach: Material and interaction models

Just like in RVE analysis, the fibre is always considered either isotropic linear elastic for glass fibre or orthotropic linear elastic in the case of carbon fibres and adjacent meso-scale layers. The variety of material models used for the matrix in embedded cell models is more limited; some of the first publications used Von Mises model coupled with CDM [156], but most of the analyses are performed using the elasto-plastic-damage model of Melro [152, 83, 155, 160, 161], or a variation of this model [154]; also, the Drucker-Prager model coupled with damage [151, 153], a variation of Drucker-Prager [49, 157, 158] or Mohr-Coloumb plasticity coupled with damage [159]; which are the most typical models used in RVE analysis. In addition, there are models based on linear elastic CDM formulations [15] and linear elastic PF damage [14, 28, 47]. The main characteristics and potential limitations of the material models are discussed in the following sections.

Regarding interaction models, there is general agreement on using cohesive damage to capture fibre-matrix debonding. Only the work of [152, 153] considers perfect bonding in the fibre-matrix interface.

4.5.5 Verification and validation

Validation in embedded cell models can be done more rigorously than in RVE analysis. In pre-notched [28, 47, 49] and pre-cracked [159] specimens a detailed quantitative comparison has been

done in terms of load vs displacement, and in the case of pre-notched even CMOD could be compared; this is all in addition to the usual comparison of crack patterns. The studies on cross-ply laminates validate results mainly by comparing crack patterns. This comparison can be qualitative if the crack density [151] or the crack length [14, 156] are used. For transverse fracture under longitudinal tension, the load-displacement curve cannot be used for comparison, because the 90-degree layer does not contribute significantly to the stiffness, and thus non-linearity due to fragmentation or fracture in this layer cannot be easily perceived.

There are still purely numerical publications that are not validated nor based on specific experimental campaigns but still provide valuable insight into the studied phenomena and find acceptance on purely qualitative comparisons with damage patterns observed in similar experimental studies. From the non-validated results, one of the most significant contributions is the work of Arteiro et al. [155], which suggests a potential in-situ effect in compression, this study is backed up by analytical predictions and brings valuable information for potential new applications of thin-ply composites.

4.5.6 Thermoplastics in embedded cell analysis

All the embedded cell studies that have been found have been dedicated exclusively to model epoxy-based composites.

4.5.7 Phase Field fracture in embedded cell analysis

Within the publications that have been found and revised, the use of Phase-Field models for fracture is limited to the analysis of the in-situ effect in thermoset composites of Guillén-Hernández et al. [14] using an standard AT2 linear elastic formulation for damage in the matrix and bilinear cohesive elements in the fibre-matrix interface. This work was based on and compared with the experimental results of Saito et al. [48]. Also, the studies of the R-curve in fracture of the pre-notched specimen under three-point bending of Tan and Martínez-Pañeda [28, 47]. These publications use the AT1 linear elastic formulation to capture matrix fracture and cohesive surface interactions to model fibre-matrix decohesion. The studies are validated by comparison with the experimental results of Canal et al. [49]. So far, the only study that considers 3D effects and fibre fracture in micro-mechanical studies of composite materials is the work of Tan and Martínez-Pañeda [47], this is one of the first steps in modeling more realistic composite geometries, which can potentially be extended to the study of crack tunnelling and other more complex load scenarios.

4.6 Constitutive models, interactions and material properties

In the micro-mechanical analysis of composite materials there are three important constituents that need to be modelled explicitly: the fibre, the matrix and the interface. In this section there is a detailed description of the most relevant material and interaction models for these three components of all micro-mechanical analysis.

4.6.1 Fibre material models

Within the micromechanical analysis of composite materials, there is a general agreement on the linear elastic behaviour of the fibres and the fact that the strength of the fibres is much higher than the matrix, thus transverse tension/compression, longitudinal compression and in-plane shear loading are dominated exclusively by interface and matrix behaviour (plasticity/damage). The only loading scenario where fibre fracture is considered as the case of longitudinal tension. In this case, so far RVE analysis considered fibre failure using cohesive and CDM models while the embedded cell model of Tan and Martínez-Pañeda [47] assessed fibre fracture using PF.

For the type of analysis that considers fibre strength distributions based on Weibull distribution and dynamics effects (which are considered to be crucial for fibre-dominated failure [148]) are models more simplistic such as the work of Tavares et al. [148]; where the fibres are considered as a collection of longitudinal springs connected to shear springs that represent the matrix; in this case, the peeling effect due to fibre-matrix debonding is not considered. Thus, within this review a methodology that combine dynamic, interface and strength distribution has not been found.

4.6.2 Matrix material models

The stress-strain behaviour of an epoxy resin measured from standard size specimens is shown in Fig. 4.11; likewise, the stress-strain response of a thermoplastic (PEEK) polymer is shown in 4.12. It can be seen that the first part of the curves is linear, then there is a highly non-linear behaviour that is more pronounced in compression and shear. Most authors attribute all the non-linear behaviour to plastic deformation [46, 117, 106, 116, 122, 123, 126, 127, 129, 131, 132, 133, 134, 164], some others say there is a non-linear elastic behaviour that is usually ignored because most of the characterization is done using monotonically increasing loading [12]. What has become a common practice is to fit the monotonic test data to well-known elasto-plastic material models.

The trend in the micro-mechanical analysis is the use of mainly three plasticity models (or modifications of these): the elasto-plastic model developed by Melro et al. [149], Drucker-Prager, and Mohr-Coulomb. These are preferred material models because they can capture the pressure dependence plasticity and different yield strengths in tension and compression, which are well known to be characteristic in polymers from standard tests [16, 165] as well as in-situ observations of the strains in the matrix around the fibre [106].

Regarding the different modelling approaches to account for plasticity and damage in the matrix. There are authors that without considering explicit damage or fracture models assume

that the areas of higher plastic strains are the ones who define the precise location of cracks [118, 119, 120, 121, 122, 124, 125, 135, 159]. The problem with such assumptions are several: (i) they don't define a threshold or admissible plastic deformation from where the material should be considered as fractured or damaged; thus, the analysis becomes highly qualitative and even ambiguous; (ii) areas with very high plastic deformation still have a considerable load carrying capacity, thus they do not represent softening mechanisms typical of damage or fracture; this cannot be overseen if the stress-strain behaviour is meant to be predicted; which is common practice in almost all of the publications that use this approach; (iii) in reality, the fracture can be initiated in areas where plastic deformation is limited or excessively constrained (which is the case on the resin in the middle of fibres that are closely packaged), such a modelling approach would not expect these areas to be a potential failure locus. To try to overcome these limitations CDM models are usually integrated into these traditional elasto-plastic models; then, the fracture is assumed in the areas of higher damage localization.

Unlike XFEM and cohesive damage models where the matrix crack is modeled explicitly; or in the PF method, where the matrix crack is regularized in a small zone defined according to the length scale, which should be smaller than the fibre diameter. In CDM the highly inhomogeneous stress distribution typical of micro-mechanical analysis most of the time leads to the localization of damage within one or very few elements. Then, paths of localized damage are assumed as cracks. But it is necessary to remember that unlike PF, CDM is not based on fracture mechanics principles [144, chapter 8], [166]. Some of the most basic literature on CDM explicitly state that CDM is not meant to model crack-like patterns and fracture propagation phenomena; because the way CDM approaches failure is by considering an average of voids and cracks much smaller than the structure's volume. Then, material degradation and failure is represented by the growth of those voids or micro-cracks but without considering the interactions, orientations and stress concentration of these lower scale defects [166].

According to Leimatr et al. [166], the volume represented by the CDM which in a finite element model corresponds to the volume of an element *"must be small enough to avoid smoothing of high gradients but large enough to represent an average of the micro-processes."* In this context CDM for the typical scales in polymers could not be used for element sizes whose volume is below 1 mm³ according to [166]. This goes in direct contradiction with all micro-mechanical analyses using CDM, where the element size is in the order of microns; damage localization and propagation are indeed treated as crack-like phenomena.

Regarding the most widely used elasto-plastic and elasto-plastic-damage models. The model developed by Melro et al. [149] is an elasto-plastic material model coupled with damage; it is formulated to work under the small deformations assumption. It is initially linear elastic with a paraboloidal yield criterion based on tensile and compressive yield curves; it follows a non-associative flow rule that accounts for a specific plastic Poisson's ratio. Damage onset is also based on a paraboloidal criterion computed in terms of the tensile and compressive strength. Damage evolution is given in terms of energy dissipation, where the so-called "fracture energy" is regularized with the element characteristic length to avoid mesh dependency. This model has been

extensively used in micro-mechanical RVE analysis [46, 116, 127, 129, 133, 134] and embedded cell models [152, 154, 83, 155, 160, 161].

However, there are authors that consider it inappropriate because even though the model was formulated based on meso-scale data, using standard compression, tension, and shear to calibrate the response in single element tests, validations such as the one performed by Morelle et al. [165] in notched meso-scale samples or any sort of fracture related test was never undertaken [126]. It was always used in micro-mechanical fracture analysis, considering mainly meso-scale properties [126]. Besides, it is a model conceived for small deformations, but the curves that were used for the initial definition [149] can reach strains up to 60% in shear and 40% in compression, which cannot be considered small. Thus, even though the meso-scale failure of the composite material (taking IM7/8552 as an example) does not go beyond 0.7% strain for transverse tension [167], it can reach 5% in compression [168] and 10% in transverse shear [169].

Locally, the deformations in the matrix can go far beyond that; there are authors such as Chevalier et al. [106] that have been able to measure micro-scale in-situ deformations using DIC. Strains in highly constrained areas can reach up to 15% on the surface. On top of that, as explained by Canal et al. [139], the strains obtained with micro-DIC can underestimate realistic strains, due to high strain gradients close to the fibre-matrix interface. Thus realistic local strains on the surface are expected to be higher than 15% which is already far from what is considered appropriate for the infinitesimal deformation assumption according to standard solid mechanics textbooks. An additional limitation of this plasticity-damage model is related to the way damage is coupled with plasticity, as plasticity is expected to stop completely once damage initiates. This model cannot predict crack blunting due to plasticity, once the first element reaches the damage threshold, the global response becomes brittle.

The Mohr-coulomb plasticity model has a pyramidal-shaped yield function whose axis is the hydrostatic line; this is what is called multisurface yield criteria where each side of the pyramid is a plane on the principal stress space [170]. "The Mohr–Coulomb criterion is based on the assumption that the phenomenon of macroscopic plastic yielding is, essentially, the result of frictional sliding between material particles" [170]. Namely, this plasticity model is inspired by the physical phenomena observed in soils, rocks, and concrete-like materials, whose behaviour is far different from the one of polymers; this is one of the main reasons such criteria is considered inappropriate to model the epoxy matrix in polymer based composites. The use of this plasticity model is limited to elasto-plastic analysis because it has not been used in conjunction with CDM for RVE analysis, only for embedded cell models. Regarding the main advantages, it is necessary to mention that it can be used for finite strains modeling and it is already built-in inside Abaqus [146], this probably one of the reasons it is the second most widely used plasticity model in RVE analyses.

On the other hand, the Drucker-Prager elasto-plastic model is considered a "smooth approximation to the Mohr-Coulomb law" [170]. Mathematically is very similar to the Von Mises model, but includes an extra term to incorporate pressure sensitivity. Unlike Melro's yield criteria which is paraboloidal, Drucker-Prager is a cone whose axis is also the hydrostatic line, the cone can be either tangent or embedded inside the pyramid defined by Mohr-Coloumb criteria. The flow rule

in Drucker-Prager is most of the time defined with non-associative models to avoid the overestimated dilatancy of the associative model [170]. Some of the most appealing characteristics of the Drucker-Prager plasticity model are:

- It can define different yield strengths in tension and compression.
- It can be easily extended to large deformations.
- It has been coupled with CDM.
- It is already integrated inside Abaqus, in small and large deformations assumption and it is already coupled with a CDM.

Drucker-Prager is by far the model that is most extensively used; but there are authors who considered it inappropriate to use Drucker-Prager or Mohr-Coulomb models for polymers [46, 116, 171, 172]; these authors are the main developers of paraboloidal plasticity models, and the main arguments against the use of Drucker-Prager plasticity model for polymers are the fact that it can overestimate the stiffness and yields unrealistic plastic Poisson's ratio under compressive loading.

All the aforementioned models are of phenomenological nature; namely, they are mathematical models that try to fit the different stress-strain curves but these are not based on the actual physics and mechanics of the internal deformation of the polymer. The type of modeling approach that considers the actual physics of polymer atomistic mechanics such as the work of Chevalier et al. [173] and Van Loock et al. [174] that account for the shear transformations zones, or the work of Gearing et al. [175] on shear-yielding and crazing phenomena of glassy polymers, have not been incorporated in single fibre, RVE or embedded cell models. Thus, more appropriate constitutive models for polymers still need to be integrated into the micro-scale analysis of composite materials.

4.6.3 Material properties

One of the main sources of disagreement between different authors is the way the material properties for the matrix are obtained. Some authors use mechanical properties obtained from meso-scale characterization, namely standard tension, compression and shear tests using specimens of proportions in the order of laminate dimensions (between 1 to 100 mm); in this work, such dimensions are called meso-scale. As an example, the work of Fiedler et al. [16] is one of the most common sources of matrix mechanical properties for micro-mechanical numerical analysis, in that work, neat resin slaps of 12 mm x 115 mm x 90 mm were cured and then machined into dog bone specimens for tension (square transverse section) and shear (circular transverse section) and cubic specimens for compression, see Fig. 4.13. The results in terms of stress-strain curves are shown in Fig. 4.11.

From this work, the first concerning fact is the variation in the failure strain in tension by reducing the specimen thickness. While on average the specimens with 1 mm thickness fractured

around 2% strain, the specimens with 0.4 mm thickness can reach up to 6% deformation before fracture. In addition, the stress-strain curves in compression follow two trends, one with a marked re-hardening (cubes of 1 cm³) and the other one closer to perfect plasticity (cubes of 0.125 cm³). In this experimental campaign, the change of dimensions is within one order of magnitude and yields a high variation of results which is already quite evident.

At the micro-scale, resin regions between two fibres are of the order of microns, thus the behaviour is expected to differ considerably from such meso-scale characterization. This hypothesis was already proved by Hobbiebrunken et al. [176], in the testing campaign on micro-scale samples of epoxy resin under tension where it is proven that when reducing the gauge volume of the specimen, the predicted strengths approaches the theoretical material strength computed based on atomic bond strength. And also the experimental campaign of Wang et al. [177] on compression of micro-pillars of epoxy resin, showed that reducing the diameter of the micro-pillar increases the measured yield stress and strength.

In accordance with these results, other authors choose to use mechanical properties obtained from micro-mechanical testing campaigns. In the work of Sharma et al. [135] the difference between the accuracy of micro and meso-scale stiffness and yield stress of the epoxy matrix is evaluated by comparing micro-mechanical RVE models with meso-scale experimental results. The results show that transverse tensile stiffness of the composite is more accurately represented using bulk properties; while transverse compressive stiffness is underestimated by bulk properties but overestimated by micro-scale properties. The modelling approach in this paper does not account for matrix fracture, thus there are unsolved questions regarding the role of matrix strength on meso-scale composite strength and fracture toughness.

Perhaps, the most important discrepancy comes from the wide range of values for the same mechanical properties of the same type of material and sometimes even the same material. In Table 4.3 there is a summary of some of the most representative examples of contradictions in the values for mechanical properties, all of them corresponding to epoxy resin. The *source* refers to the publications on micro-mechanical analysis and the *internal reference* refers to the publication where the actual mechanical properties were supposedly originally obtained. Values highlighted with the same colors are meant to guide the visualization of the wide differences.

Some of the most representative discrepancies are also discussed next:

- The tensile strength reported by Naya et al. [126] and Tan and Martínez-Pañeda [28] can reach 500% difference, but intermediate values that represent 150% difference (Labanda et al. [7]) and 365% difference (Melro et al. [46]) can also be found, see green tag in Table 4.3.
- The compressive strength reported in Melro et al. [46] and Song et al. [132] can reach 343% difference, but intermediate values can be found in the work of Vaughan and McCarthy [119] and Arteiro et al. [83].

- Observing the compressive strength reported in Melro et al. [46], Vaughan and McCarthy [119] and Arteiro et al. [83], even though all models mention having extracted the mechanical properties from Fiedler et al. [16], the compressive strength according to Melro et al. [46] is doubled in Vaughan and McCarthy [119] and almost tripled in Arteiro et al. [83]; see red tag in Table 4.3.
- The comparison of the fracture toughness reported in Pineda et al. [138] and Labanda et al. [7] yield a difference of three orders of magnitude, see blue tag in Table 4.3. But intermediate values in three different orders of magnitude can also be found, see cyan tag in Table 4.3.

There are some properties that are obtained through calibration; usually the matrix strength and fracture toughness are modified so the global strength predicted by the RVE reaches the meso-scale strength predicted in standard unidirectional tests. According to Nguyen et al. [114], such calibration would eliminate the predictive nature of such models. These scenarios usually produce material properties that are on the extremes of the differences previously highlighted [138]. As an example, the fracture toughness used by Pineda et al. [138] can be up to three orders of magnitude lower than the value found in other publications. Similarly, the compressive strength of Song et al. [132] can be up to five times higher than the values found elsewhere.

The main issue is not just the fact that there are extremely large and small values for the same property, but also there is a large variety of intermediate values that run from the lower to the upper extremes. This is the case for the tensile strength, compressive strength and fracture toughness. There are two main additional problems with such large variation of material properties. The first one is that, from a detailed review, no real conclusion can be reached regarding the expected material properties. The second one is that, given a new material model for the epoxy matrix that is meant to be defined by calibration, it can find justification for any value it may reach. It is not clear how to disregard non-physical values or define meaningful limits based on what is found in the literature nowadays.

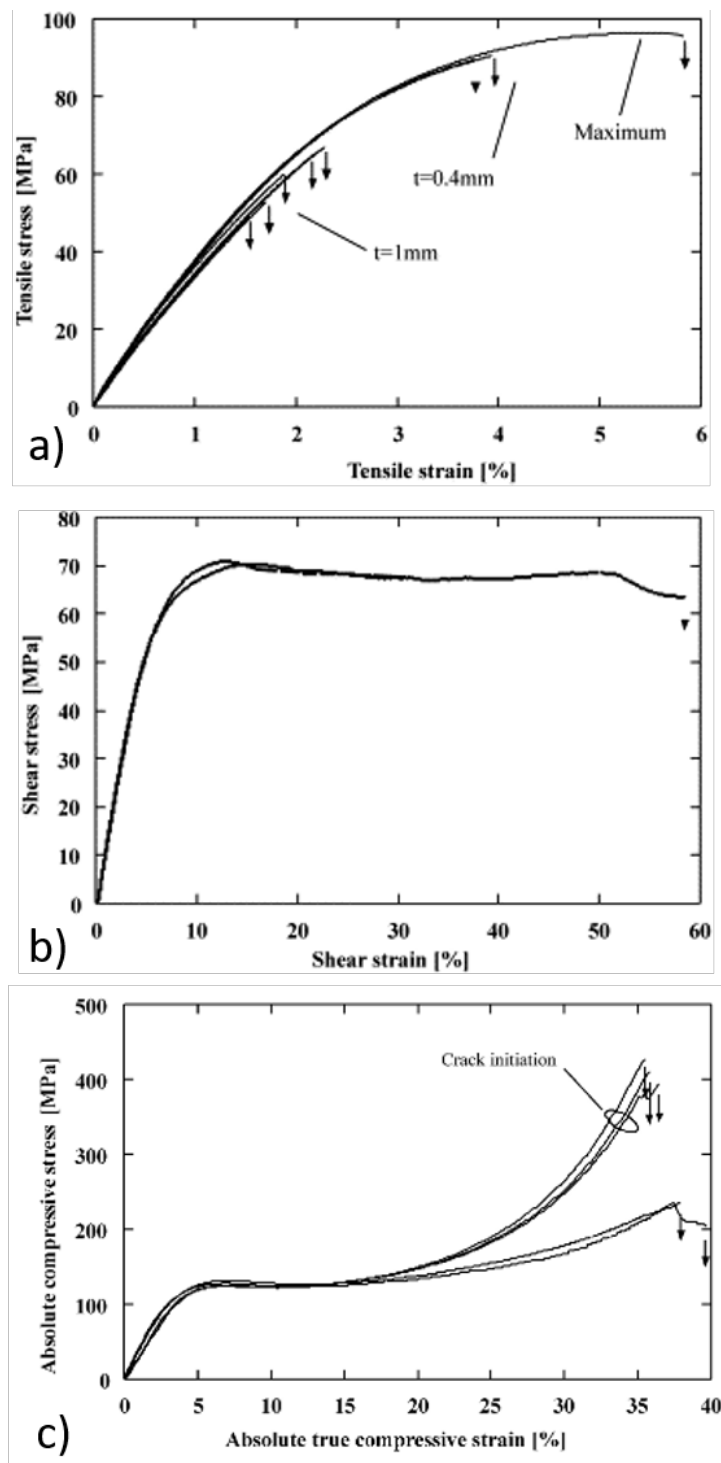


Figure 4.11: Representative stress/true strain curves for a) tensile test, b) shear test and c) compressive test [16]. Reprinted from *Failure behavior of an epoxy matrix under different kinds of static loading*, B Fiedler, M Hojo, S Ochiai, K Schulteb, M Ando, Pages No. 1617, 1618, 1619, Copyright (2001), with permission from Elsevier.

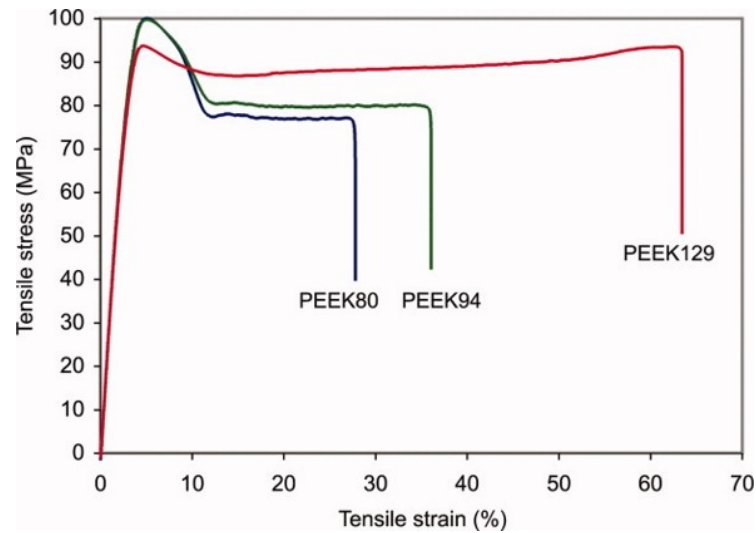


Figure 4.12: Representative stress/true strain curves for PEEK80, PEEK94 and PEEK129 thermoplastic polymer [17]. Reprinted from *Influence of molecular weight on rheological, thermal, and mechanical properties of PEEK*, Mingjun Yuan, Jeffrey A. Galloway, Richard J. Hoffman, Sanjiv Bhatt, Pages No. 101, Copyright (2010), with permission from Wiley Company.

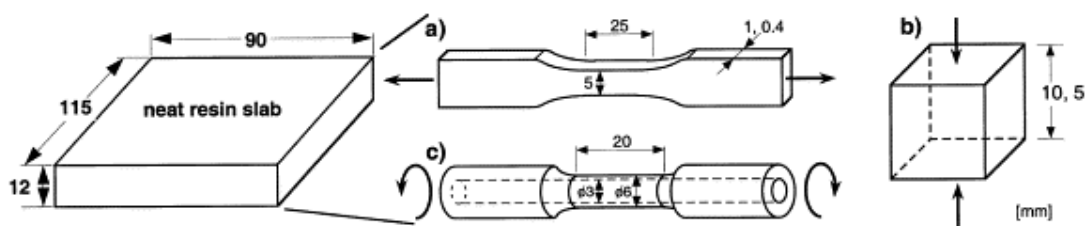


Figure 4.13: Different specimens made from resin slabs a) tension specimen, b) compression specimen, c) torsion specimen [16]. Reprinted from *Failure behavior of an epoxy matrix under different kinds of static loading*, B Fiedler, M Hojo, S Ochiai, K Schulteb, M Ando, Pages No. 1617, 1618, 1619, Copyright (2001), with permission from Elsevier.

Table 4.3: Matrix mechanical properties based on different publications.

Source/ internal reference	Material type	Tensile strength [MPa]	Compressive strength [MPa]	Fracture toughness [N/mm]
Melro et al. [46]	Hexcel 6376 (epoxy)	93	124	0.09
From Fiedler et al. [16]				
Vaughan and McCarthy [119]	Hexcel 6376 (epoxy)	103	264	—
From Fiedler et al. [16]				
Naya et al. [126]	Hexcel 8552 (epoxy)	121	176	0.1
From Herraiz et al. [158]				
Pineda et al. [138]	MY750/HY917/DY063 (epoxy)	66.5	—	0.000563
From calibration				
Chevalier et al. [106]	RTM6 (epoxy)	—	—	0.001
Morelle [165]				
Song et al. [132]	Solvalite 710-1 (epoxy)	—	550	—
From calibration				
Labanda et al. [7]	Epoxy	50	—	0.5
—				
Kohler et al. [151]	Toray TP80ep (epoxy)	—	—	0.064
Tan and Martínez-Pañeda [28]				
—	Epoxy	20	—	0.01
Arteiro et al. [83]	Toho #113 (epoxy)	93	350	0.277
From Fiedler et al. [16]				

Table 4.4: Interface mechanical properties based on different publications.

Source	Materials type	Normal strength [MPa]	Shear strength [MPa]	G_{IC} [N/mm]	G_{IIC} [N/mm]
[46]	Glass/Epoxy	50	70	0.002	0.006
[28]	Glass/Epoxy	40	60	0.125	0.15
[122]	Glass/Epoxy	10	40	0.025	0.1
[121]	Carbon/Epoxy	100	—	0.1	—
[126]	Carbon/Epoxy	42	64	0.002	0.1
[106]	Carbon/Epoxy	50	75	0.002	0.006
[158]	Carbon/Epoxy	100	75	0.01	0.01

4.6.4 Fibre-matrix interaction model

As mentioned previously, even though there are many authors that disregard the role of interface damage, the majority of the publications on micro-mechanical analysis do agree on modeling fracture initiation and propagation of the interface crack using cohesive surface interactions or cohesive elements. But, within the group that agrees on the use of cohesive damage, there are still two main sources of disagreement. The first one is the fact that once decohesion takes place, there is still some load transfer that can happen due to friction; such load transfer becomes particularly important in the case of transverse compressive loading. But, even though most authors consider the case of transverse compression as a representative example for verification and validation, only a very small minority accounts for friction effects [117, 106, 126, 135].

The other very strong source of disagreement comes from the large differences in the strength and fracture toughness values that can be found for even the same type of material combinations. In Table 4.4 there is a summary of some of the material and interface properties found in different publications. The color is used to highlight the most extreme differences found. The trend is very similar to what was found in the matrix properties, with variations on the fracture toughness of up to two orders of magnitude, while variation on the strength can be as high as 500%.

4.7 Concluding remarks

In summary, the following conclusions, knowledge gaps and main discrepancies can be identified in literature:

- In the experimental campaigns used to study micro-scale phenomena, there is evidence of potential material degradation due to the observation method, as demonstrated by Martyniuk et al. [6]. Besides, micro-DIC measurements on areas of high gradients, such as resin regions close to the fibres, cannot accurately measure strain fields and strain gradients [139]. Thus, material properties obtained (or calibrated) and constitutive models validated using these observation methods and measurement techniques may not be fully representative of composite materials. There is a lack of understanding of how to visualize and measure micro-scale phenomena while ensuring that no modifications are introduced to the material properties and that strain fields and their gradients can be accurately measured.
- There is evidence of size effect related to the fibre diameter, according to the numerical results of Guillén-Hernández et al. [27]. Besides, the experimental studies of Hobbiebrunken et al. [176] demonstrated that the micro-scale strength of epoxy is much higher than the values reported in meso-scale testing campaigns. In light of these results, numerical and experimental studies that consider fibre diameter up to two orders of magnitude higher cannot be considered representative of realistic micro-scale phenomena. In the same way, meso-scale material strength cannot be used to approximate the strength of resin regions that are several times smaller than the defects that originate failure in large specimens (bulk material testing). There is still no study on the predictive capabilities of PF for matrix fracture on composite materials when micro-scale properties and dimensions are used to study single fibre, RVE and embedded cell models.
- As demonstrated by Hobbiebrunken et al. [176] in single fibre experiments and by Kohler et al. [151] in tensile tests on cross-ply laminates, transverse cracking is a 3D phenomenon where damage starts on the surface, where a plane-stress condition dominates, and then progresses inside the specimen where a plane-strain condition dominates. Most numerical studies focus on either 2D plane-strain conditions or use quasi-3D models with periodic BC. However, there is still the need to estimate the accuracy and truthfulness of each approach to represent or at least average the progression of damage through the width of the lamina.
- According to the micro-DIC measurements of Chevalier et al. [178] and Mehdikhani et al. [140] local strains can be very high (at least higher than 15%). Thus, if validation is performed by comparing micro-strain fields instead of meso-scale results, like average stresses and strains, probably most methodologies would not be as accurate as initially stated; especially if they are founded on an infinitesimals strain assumption. Thus, there is still the need to adopt more rigorous methodologies for validation that account for both meso- as well as micro-scale accuracy, to understand the real need for more accurate material models.

- There are clear contradictions in the use of different boundary conditions and many publications do not account for the limitations exposed by other authors. One example is the incapability of periodic CB to accurately model localization phenomena such as fracture; this was explained by Coenen et al. [143]. However, most publications still employ periodic BC to study RVE fracture. Thus, there is still a lack of understanding of the way fracture predictions on RVE and cross-ply embedded cell models are affected by the imposed BC when fracture phenomena are studied.
- There is evidence of the variability of results that can be obtained from different random distributions and dimensions of the RVE, but there are many publications that expose conclusions based on the response of a single fibre model. Thus, conclusions given without following rigorous metrics to define the appropriated size of the RVE or embedded cell model may not be realistic even if they are based on accurate material and interaction models. There is no study on the influence of RVE and embedded cell model size and fibre distribution on fracture predictions using PF.
- RVE and embedded cell models using PF fracture have focused on tensile failure; only the work of Espadas-Escalante et al. [29] studied fracture of RVEs under compressive loading, without accounting for fibre-matrix interface damage. Thus, there is still the need to understand the predictive capabilities of traditional linear elastic PF formulations under compressive, shear, and mixed mode loading in composites with *weak interfaces*. A more complete study on more complex loading scenarios should bring light to the need to include elasto-plastic or hyper-elasto-plastic models and even the need to account for residual stresses due to thermal history. Besides, it should question the need for alternative PF formulations where the PF length scales can be reduced to micro-scale dimensions.
- According to Hernandez et al. [142], the fibre distribution has been shown to "*significantly impact the formation and pattern of the transverse cracks*", but the main algorithms for artificial fibre generation have been validated mainly in terms of elastic predictions and using only RVE models. There is still the need to understand the accuracy of artificial fibre distributions to predict fracture phenomena in RVE and embedded cell models. Besides, it is necessary to understand the role of the size of the resin region between plies on cross-ply embedded cell models.
- There is still the need to identify a way to properly measure the micro-scale mechanical properties of the resin and the interface. Besides, there should be a study on the source of such large disagreements on micro-scale properties, explaining the potential model-biased estimation of such properties and the consequences of such disagreements. One may argue that there has to be some authors and approaches that are just far off from realistic, and there are some others that could be more accurately approaching the analysis. However, there may be a general lack of understanding of the whole phenomena.

- There are CDM models such as [149] that have always been used at the micro-scale level, without ever been validated at the meso-scale, which, most of the time, was the scale where the initial properties were obtained. There seems to be an excessive confidence in some material models that become extensively used even if they have never been tested in the proper context.

Given the significant contradictions found in the literature review, engaging in the exercise of selecting mechanical properties, making assumptions about material behaviour, and establishing boundary conditions solely based on previous published work may become a speculative rather than investigative endeavour with a considerable margin of error. Indeed, considering the magnitude of the contradictions discovered, attempting to choose anything from this array seems more like an exercise of guessing rather than concluding. With the limited quantity of experimental studies, particularly those that can be seen as "reliable", and successful numerical validation processes being even scarcer, there appears to be no solid benchmark or certainty derived from experimental measurements to truly validate, let alone assess, a new numerical tool.

At this point, it is contemplated that perhaps the most logic way forward may involve taking a few steps back. In the author's perspective, a more exhaustive examination of micromechanical measurement procedures and experimental methodologies should precede the proposal or investment in new numerical methodologies. A proper experimental exploration could potentially help in refining or narrowing down the ranges within which properties such as fracture toughness and strength can be considered realistic. This is because in most of the numerical work, the selection of mechanical properties is the initial part of the job. As demonstrated in the preceding chapter, the act of selecting mechanical properties alone carries such a high level of uncertainty that it could entirely disqualify the credibility of numerical results, especially if they are purely grounded in deformation or fracture patterns that, in the eyes of the authors that propose them, are indeed "similar" to the ones found in micrographs.

Consequently, following a rigorous review of the state-of-the-art, the main author considers that developing a purely numerical study based on assumptions and parameters found in the literature lacks objectivity and it cannot be fully realistic. It essentially constitutes an academic exercise; with the available information it is impossible to objectively conclude how divergent or realistic the new results are. This impossibility stems from the unfeasibility of performing an objective validation.

Chapter 5

Phase-Field implementation in Abaqus

This chapter presents a summary of the first evaluation of the Phase-Field subroutines, the influence of the main parameters and formulations using an open-hole specimen under different loading conditions. The idea is to assess the response of the subroutines and the damage patterns when there is no other source of non-linearity, such as cohesive damage in single fibre models or RVE analysis.

5.1 Phase Field implementation

The implementation of the Phase-Field method into the finite element software Abaqus implies finding the displacements and PF variable from the balance equations expressed in weak form in equations (2.21). By default, Abaqus does not include a nodal damage variable. Then, apart from the displacements, an additional degree of freedom (DOF) such as temperature, rotation, warping amplitude, pore pressure, hydrostatic fluid pressure, electric potential, or connector material flow must be selected to be used as damage (PF) variable. The most intuitive approach has been to explicitly code the residual and tangent component of the PF balance in equations 2.21. But this can only be done within a User Element subroutine (UEL). The main issue with using a UEL is the fact that post-processing cannot be done easily because those elements cannot be visualized in the standard Abaqus Viewer environment. Many authors have found different ways around this issue:

- Using only a UEL to compute the residual and tangent matrix of both PF and displacements at the same time, define two layers of elements attached to the same nodes; one layer using UEL elements and the other one using standard elastic elements with an isotropic material whose stiffness is very low; the PF variable is visualized on the standard elements once the additional DOF in the UEL is defined as temperature or rotation [58].
- Using a UEL to compute the PF residual and tangent matrix, then communicate that to a User Material subroutine (UMAT) to compute the stresses, strains, and energetic driving force. This approach also requires two layers, one for the user elements and the other one

for the user material; the PF variable is visualized in the UMAT as temperature, rotation or internal variable [56].

- Using a UEL to compute the PF residual and tangent matrix, communicated to another UEL that uses the PF input to compute the displacement residual and tangent matrix; both UELs are also connected to a UMAT, the PF variable is visualized as temperature, rotation or internal variable of the UMAT. In this case, three layers of elements are needed, one for each UEL and one for the UMAT [57].
- Using a UEL to compute the residual and tangent matrix of both PF and displacements at the same time, define two layers of elements attached to the same nodes; one layer using the user elements and the other one using a UMAT with zero stiffness and stresses; the UMAT receives data from the UEL, so the PF variable is visualized as temperature, rotation or internal variable [65]. This last one is one of the approaches that is used in this work, and it is explained in the following sub-sections.

It is also possible to implement the balance equations (2.21) using only a UMAT for a thermo-mechanical analysis, where the temperature is used as PF variable. This is the only approach that avoids the use of the second layer of elements, and it will also be explained in what follows.

5.1.1 Abaqus UEL implementation

The implementation of the UEL in Abaqus is done using the reference documentation and code in the work of Martínez-Pañeda et al. [65]. The derivation for 2D analysis is as follows: to solve the system of differential equations (strong form) in equations (2.21) using the finite element method, the first step is to multiply this system by the variation of the PF $\delta\phi$ and displacement $\delta\mathbf{u}$ variables; then perform the integration over the whole domain and then use integration by parts to include the boundary conditions in a single integral equation, as shown in equation (5.1).

$$\begin{aligned} \int_{\Omega} (\boldsymbol{\sigma} \delta \boldsymbol{\epsilon} - \mathbf{b}^* \cdot \delta \mathbf{u}) d\Omega + \int_{\partial\Omega} (\mathbf{t}^* \cdot \delta \mathbf{u}) d\partial\Omega = r^{\mathbf{u}} = \mathbf{0} \\ \int_{\Omega} \left(H \frac{\partial g(\phi)}{\partial \phi} \delta \phi + \frac{G_c}{2C_w} \left(\frac{1}{2l_0} \frac{\partial \alpha(\phi)}{\partial \phi} \delta \phi + l_0 \nabla \phi \cdot \nabla \delta \phi \right) \right) d\Omega = r^{\phi} = 0 \end{aligned} \quad (5.1)$$

As usual, the domain Ω is divided into sub-domains Ω_e that correspond to the volume or area (in 2D analysis) of the elements. The integral in equation (5.1) can be obtained as the sum of integrals over each element; then, within each element or sub-domain Ω_e , the displacements $\mathbf{u}$ and PF variable ϕ are approximated from the nodal values $\mathbf{u}_i$ and ϕ_i as shown in equation (5.2).

$$\begin{aligned} \mathbf{u} &= \sum_{i=1}^m \mathbf{N}_i^{\mathbf{u}} \mathbf{u}_i \\ \phi &= \sum_{i=1}^m N_i \phi_i \end{aligned} \quad (5.2)$$

For an element with m nodes, where $\mathbf{N}_i^{\mathbf{u}}$ is defined as the matrix of shape functions shown in equation (5.3), where N_i is the shape function that corresponds to node i , $\mathbf{u}_i$ is the displacement vector at node i and ϕ_i is the PF value in node i respectively.

$$\mathbf{N}_i^u = \begin{bmatrix} N_i & 0 \\ 0 & N_i \end{bmatrix} \quad (5.3)$$

$$\begin{aligned} \epsilon &= \sum_{i=1}^m \mathbf{B}_i^u \mathbf{u}_i \\ \nabla \phi &= \sum_{i=1}^m \mathbf{B}_i^\phi \phi_i \end{aligned} \quad (5.4)$$

From the equations (5.2), the strain tensor and PF gradient can be obtained as shown in equation (5.4). Where $\mathbf{B}_i^u$ and $\mathbf{B}_i^\phi$ are defined in equation (5.5) and equation (5.6); $N_{i,x}$ and $N_{i,y}$ are the derivatives of the shape functions with respect to x and y

$$\mathbf{B}_i^u = \begin{bmatrix} N_{i,x} & 0 \\ 0 & N_{i,y} \\ N_{i,y} & N_{i,x} \end{bmatrix} \quad (5.5)$$

$$\mathbf{B}_i^\phi = \begin{bmatrix} N_{i,x} \\ N_{i,y} \end{bmatrix} \quad (5.6)$$

Following the same procedure, the virtual quantities $\delta \mathbf{u}$ and $\delta \phi$ and their derivatives are also discretized as shown in equations (5.7).

$$\begin{aligned} \delta \mathbf{u} &= \sum_{i=1}^m \mathbf{N}_i^u \delta \mathbf{u}_i, & \delta \phi &= \sum_{i=1}^m N_i \delta \phi_i \\ \delta \epsilon &= \sum_{i=1}^m \mathbf{B}_i^u \delta \mathbf{u}_i, & \delta \nabla \phi &= \sum_{i=1}^m \mathbf{B}_i^\phi \delta \phi_i \end{aligned} \quad (5.7)$$

After replacing equations (5.2), (5.3), (5.4), (5.5), (5.6) and (5.7) in the expression for the residuals in equation (5.1), and knowing that the equality must hold for any virtual variation in the displacement and PF variable. The residuals can be expressed as equation (5.8).

$$\begin{aligned} r^u &= \int_{\Omega} ((\mathbf{B}_i^u)^T \boldsymbol{\sigma} - (\mathbf{N}_i^u)^T \mathbf{b}^*) d\Omega + \int_{\partial\Omega} ((\mathbf{N}_i^u)^T \mathbf{t}^*) d\partial\Omega = \mathbf{0} \\ r^\phi &= \int_{\Omega} \left(H \frac{\partial g(\phi)}{\partial \phi} N_i + \frac{G_c}{2C_w} \left(\frac{1}{2l_0} \frac{\partial \alpha(\phi)}{\partial \phi} N_i + l_0 (\mathbf{B}_i^\phi)^T \nabla \phi \right) \right) d\Omega = 0 \end{aligned} \quad (5.8)$$

In order to solve the system in equations (5.8), Abaqus uses the Newton-Raphson method or a Quasi-Newton method. For that, it is necessary to perform a linearization procedure that allows to define an iterative search method, such as the one described in equations (5.9).

$$\begin{Bmatrix} \mathbf{u} \\ \phi \end{Bmatrix}_{t+\Delta t} = \begin{Bmatrix} \mathbf{u} \\ \phi \end{Bmatrix}_t - \begin{bmatrix} \mathbf{K}^{uu} & \mathbf{K}^{u\phi} \\ \mathbf{K}^{\phi u} & \mathbf{K}^{\phi\phi} \end{bmatrix}_t^{-1} \begin{Bmatrix} \mathbf{r}^u \\ r^\phi \end{Bmatrix}_t \quad (5.9)$$

Where the tangent matrices are defined in the following equations:

$$\begin{aligned} \mathbf{K}^{uu} &= \frac{\partial \mathbf{r}^u}{\partial \mathbf{u}} = \int_{\Omega} (\mathbf{B}_i^u)^T \frac{\partial^2 \Psi(\mathbf{u}, \phi)}{\partial \epsilon^2} \mathbf{B}_i^u d\Omega \\ \mathbf{K}^{u\phi} &= \frac{\partial \mathbf{r}^u}{\partial \phi} = \int_{\Omega} (\mathbf{B}_i^u)^T \frac{\partial \boldsymbol{\sigma}}{\partial \phi} N_i d\Omega \\ \mathbf{K}^{\phi u} &= \frac{\partial r^\phi}{\partial \mathbf{u}} = \int_{\Omega} N_i \left(\frac{\partial \boldsymbol{\sigma}}{\partial \phi} \right)^T (\mathbf{B}_i^u) d\Omega \\ \mathbf{K}^{\phi\phi} &= \frac{\partial r^\phi}{\partial \phi} = \int_{\Omega} \left(\left[H \frac{\partial^2 g(\phi)}{\partial \phi^2} + \frac{G_c}{2C_w} \frac{1}{2l_0} \frac{\partial^2 \alpha(\phi)}{\partial \phi^2} \right] N_i N_j + \frac{G_c l_0}{2C_w} (\mathbf{B}_i^\phi)^T (\mathbf{B}_j^\phi) \right) d\Omega \end{aligned} \quad (5.10)$$

5.1.2 Abaqus UMAT-Thermal implementation

The UMAT-Thermal implementation following [59, 60] is made using a heat-transfer analogy where the temperature variable is meant to work as the PF variable; this results from the similarity between equation (2.21,2) and the steady-state heat-transfer equation. To help visualize it, consider the equation (2.21,2) to be rewritten as equation (5.11).

$$k\nabla^2 T = r \rightarrow \nabla^2 \phi = \frac{2HC_w}{l_0 G_c} \frac{\partial g(\phi)}{\partial \phi} + \frac{1}{2l_0^2} \frac{\partial \alpha(\phi)}{\partial \phi} \quad (5.11)$$

Here k is the thermal conductivity, T is the temperature field and r is the heat source. The analogy is completed by defining the heat source term r as shown in equation (5.12).

$$T = \phi, k = 1, r = \frac{2HC_w}{l_0 G_c} \frac{\partial g(\phi)}{\partial \phi} + \frac{1}{2l_0^2} \frac{\partial \alpha(\phi)}{\partial \phi} \quad (5.12)$$

In Abaqus, a thermo-mechanical material model subroutine is called at every integration point inside each element. At these points, Abaqus provides the values of the PF and strain interpolated from nodal PF and displacement values which are the main input in the subroutine. It also provides the subroutine state variables, which in this case is just H . Then, as output, Abaqus requires the computation of: (i) the material Jacobian C (equation (5.13)) (ii) the Cauchy stress σ (equation (5.14)); both of them depend on the specific material model. (iii) The internal heat flux r (equation (5.11)), and (iv) its derivative with respect to the temperature field (in this case PF variable) $\frac{\partial r}{\partial T} = \frac{\partial r}{\partial \phi}$ (equation (5.15)). Additionally, the state variable H should be updated (equation (2.19)).

$$\mathbf{C} = \frac{\partial^2 \Psi(\mathbf{u}, \phi)}{\partial \epsilon^2} \quad (5.13)$$

$$\sigma = g(d) \frac{\partial \Psi(\mathbf{u}, \phi)^+}{\partial \epsilon} + \frac{\partial \Psi(\mathbf{u}, \phi)^-}{\partial \epsilon} \quad (5.14)$$

$$\frac{\partial r}{\partial \phi} = \frac{2HC_w}{l_0 G_c} \frac{\partial^2 g(\phi)}{\partial \phi^2} + \frac{1}{2l_0^2} \frac{\partial^2 \alpha(\phi)}{\partial \phi^2} \quad (5.15)$$

This scheme is equivalent to having in the global matrix of equation (5.9), the coupling or off-diagonal terms $\mathbf{K}^{u\phi}$ and $\mathbf{K}^{\phi u}$ set to zero.

5.2 Abaqus UMAT vs UEL

As mentioned previously, the implementation of PF in a UEL requires a more time-consuming pre-processing due to the need for dummy elements, which are not necessary for the UMAT-Thermal approach. However, the UMAT-Thermal approach cannot be used with a Quasi-Newton solution scheme. Besides, within the internal equilibrium loop, it can be verified that the residual computed in the UMAT-Thermal approach is different from the one in the UEL implementation.

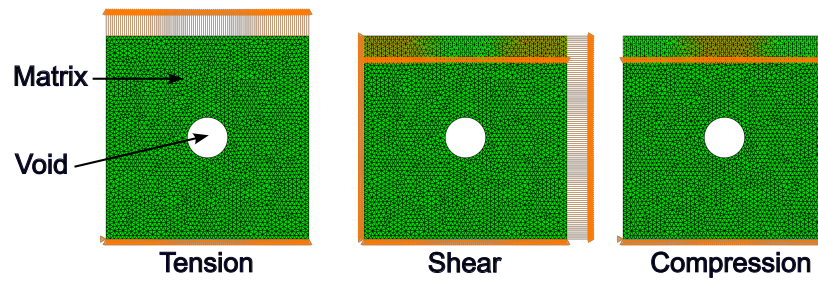


Figure 5.1: Mesh and BC for the open-hole specimen under tensile, shear and compressive loading.

The residual in the UEL is explicitly defined in the subroutine, while the residual in the UMAT-Thermal is computed internally by Abaqus, so the procedure is not very clear for the user, one can only prove that the residuals are different as they can be visualized in the solution message (.msg) file.

To compare the performance of both implementations, the open-hole specimen in Fig. 5.1 has been loaded in tension until fracture. The geometry represents a square plate of $25\ \mu\text{m}$ side length and it has a $5\ \mu\text{m}$ diameter hole in the middle. It has 20109 plane strain triangular elements and 40681 nodes. The material properties used for comparison correspond to the matrix properties and are shown in Table 5.1. The PF formulation used is AT1 in a monolithic scheme with a fixed time step of 0.01. The simulation ran on a laptop with 8 cores and 16.0 GB RAM. The crack patterns and load-displacement curves are the same in both implementation. It can be seen that the differences in the computed residuals can modify the convergence history and thus a different total number of iterations can be found depending on both the implementation and the solution method.

The most relevant results are the running time and number of iterations; see Table 5.2. The most efficient approach is the UEL using a Quasi-Newton solution method. The results demonstrate that the additional time spent in pre-processing (which can be automated) is compensated in the running time and computational effort required; this is why in the following section and remaining chapters the UEL implementation is used instead of the UMAT-Thermal implementation.

Table 5.1: Material properties for fibre, matrix and fibre-matrix interface used in linear elastic AT1 and AT2 formulations for micro-mechanical numerical tests [18].

Matrix			
E [MPa]	ν [-]	l_0 [μm]	G_c [N/mm]
3760	0.39	1.0	0.02
Fibre			
E [MPa]	ν [-]	l_0 [μm]	G_c [N/mm]
1500	0.2	[-]	[-]
Interface			
K_I [N/mm ³]	K_{II} [N/mm ³]	σ_{I0} [MPa]	σ_{II0} [MPa]
10^8	10^8	50.0	75.0
G_{Ic} [N/mm]	G_{IIc} [N/mm]	BK law [-]	
0.002	0.006	1.45	

Table 5.2: Comparison of total number of iterations and running time for the model in Fig. 5.1 (Tensile loading) using a UEL with a standard Newton-Raphson scheme, a UEL with a Quasi-Newton scheme and a UMAT-Thermal implementation.

Implementation	Total number of iterations	Running time
UEL Newton-Raphson	515	00 : 18 : 00
UEL Quasi-Newton	557	00 : 15 : 00
UMAT-Thermal	593	01 : 06 : 00

5.3 UEL performance

As an additional verification, the mesh convergence, effect of the formulation and length scale are studied using the same geometry and additional BC, such as shear and compression loading as shown in Fig. 5.1. The idea is to gradually, when it is possible, individually increase the number of parameters involved in the models. This way, the contribution of each part of the model can be assessed both separately and in conjunction with the remaining components. In this section the material properties used for comparison are shown in Table 5.1. In all cases, the UEL implementation described in the previous section is used for 2D plane strain elements and the infinitesimal deformation assumption is considered. As PF is the only source of damage, the monolithic approach can reach convergence for all loading and mesh sizes. Besides, the studies of the different energy splits were done using a "hybrid" implementation. The stress-strain curves in this chapter are computed from the reaction forces divided by the cross-sectional area of the specimen and the normalized imposed displacement. This is why they are global measurements, no local stresses or strains are depicted in the present figures.

It should be clear that, at this point, there is no rigorous qualitative comparison with experimental data, as the required data is not available. Namely, there is no source of verified micro-scale properties that come alongside similar test specimens. Thus, at this point only a qualitative evaluation can be performed between the different variables in the PF formulation. For this purpose the curves depicting specimens with a linear elastic material response are plotted alongside PF. These curves can easy visualization of the onset of non-linear response in PF damage.

5.3.1 Mesh convergence

Mesh convergence is studied for the AT1 and AT2 formulations without using an energy split and under pure tension, pure shear and pure compression imposed through displacement BC, as shown in Fig. 5.1. The crack patterns and global stress-strain curves are shown in Fig 5.2 and Fig 5.3, respectively, for tensile loading.

The plots in Fig 5.2 are shown in the undeformed state and they do not explicitly depict the mesh, however, averaging was removed in order to better visualize the gradual smoothing of the damage contours created by the PF variable. Besides, the stress-strain curves in Fig 5.3 are plotted alongside the "Linear Elastic Material" curve, which represents a model without considering PF damage and using the smallest mesh size. This curve is included in Fig 5.3 in order to better visualize the deviation from linearity due to PF damage. In case of AT1 formulation, the deviation is abrupt and it implies the fracture of the specimen, while for the AT2 formulation, deviation is gradual, there is a large softening before the main crack goes through the whole specimen.

It can be seen in Fig 5.2 that fracture occurs in the direction perpendicular to the imposed displacement and nucleating at the centre of the hole. Besides, neither the crack contour (Fig 5.2) nor the apparent strength of the specimen (Fig 5.3) is heavily disrupted by the mesh size, there is only a small difference in the mesh size of $0.75 \mu\text{m}$, where the image is not as smooth as the remaining ones. However, not even this effect implies a lower accuracy in terms of a real need for

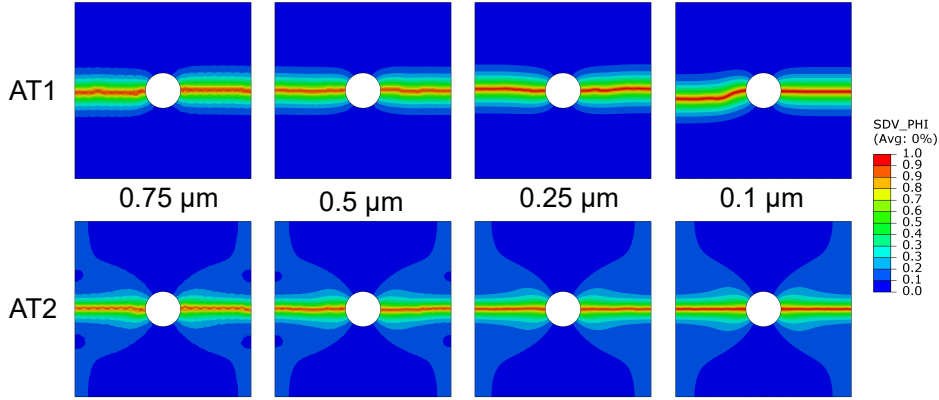


Figure 5.2: Crack patterns for AT1 and AT2 formulations under tensile loading with different mesh sizes.

further mesh refinement. In fact, as shown by the AT1 case and mesh size of $0.75 \mu\text{m}$, smaller mesh sizes are more prone to perturbations due to unsymmetrical fracture onset, in this case, the right side of the hole fractures first creating a deviation on the crack path on the left. The same effect can be observed in the other mesh sizes that use the AT1 formulation, however, it seems that the more gradual damage accumulation of the AT2 Formulations promotes more symmetric fracture patterns, and it is less sensitive to mesh distribution and size.

The crack patterns and global stress-strain curves are shown in Fig 5.4 and Fig 5.5, respectively, for shear loading. It can be seen that fracture takes place in the plane of global maximum deformation, creating a diagonal crack pattern that runs through the middle of the hole. Similar to what happened in the tensile case, there is no strong influence of the mesh size on the fracture pattern. However, as shown in Fig 5.5, smaller mesh sizes yield lower deformations at peak stress.

Finally, the crack patterns and global stress-strain curves are shown in Fig 5.6 and Fig 5.7, respectively, for compression loading. As there is no energy split, the behaviour is very similar to what happened in tensile loading, the strength is almost the same, the crack nucleates at the centre of the hole and it also runs perpendicular to the direction of the imposed deformation. However, in this case, the asymmetrical pattern is not visible in any formulation or mesh size.

In general, it can be seen that even when an open-hole specimen is used, namely, a clear area for crack nucleation is provided, the behaviour observed in single element tests or in analytical solutions (see Fig. 2.2) is still very distinctive of the AT1 and AT2 formulations. It means, while the behaviour reflected by the AT1 formulation is clearly fragile, AT2 presents gradual softening at least until the moment of accelerated fracture propagation is reached. On top of this, it should be reminded that, for the same length scale value, the strength in both formulations is different and all stress-strain plots reflect this.

Finally, it is worth to observe from Fig. 5.3, Fig. 5.5 and Fig. 5.7 that the area under the curves; thus the energy dissipated in the fracture of the specimens is highly dependent on the PF formulation. This is an enormous inconsistency that is not widely mentioned in the literature.

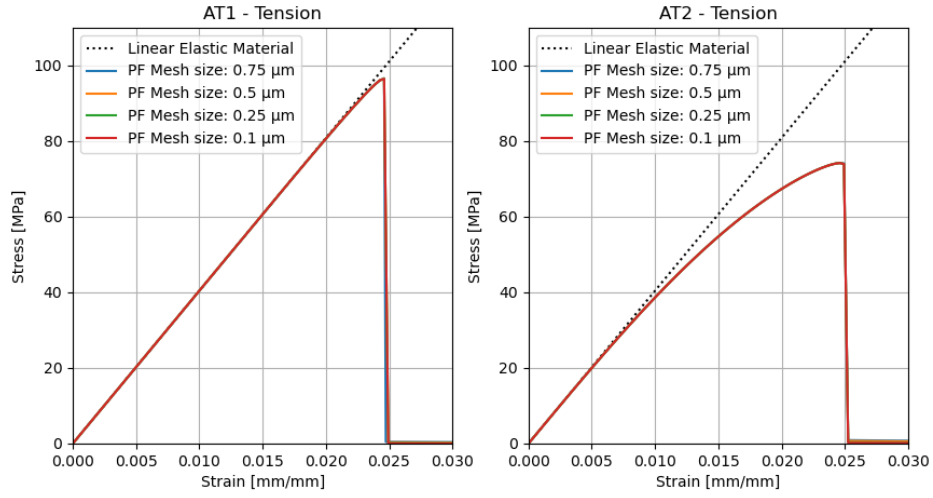


Figure 5.3: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different mesh sizes for the open-hole specimen under tensile loading in Fig. 5.1 a).

However, this inconsistency is a consequence of how close are the dimensions of the specimen with respect to the length scale parameter. For such small specimen, the damaged area is close to the specimen's size, therefore the distributed/sparse damage pattern created by the AT2 formulation and the difficulty in crack nucleation result in large underestimation of the dissipated fracture energy for AT2 with respect to AT1. As the size of the specimen increases or the length scale is reduced, both AT1 and AT2 become more alike. It means, softening of the AT2 becomes less evident and dissipated energies in AT1 and AT2 approach the same value. Such verification is known as Gamma convergence [26] and it is out of the scope of this work. However, this example provides further evidence of the numerous limitations of PF fracture for micro-scale analyses.

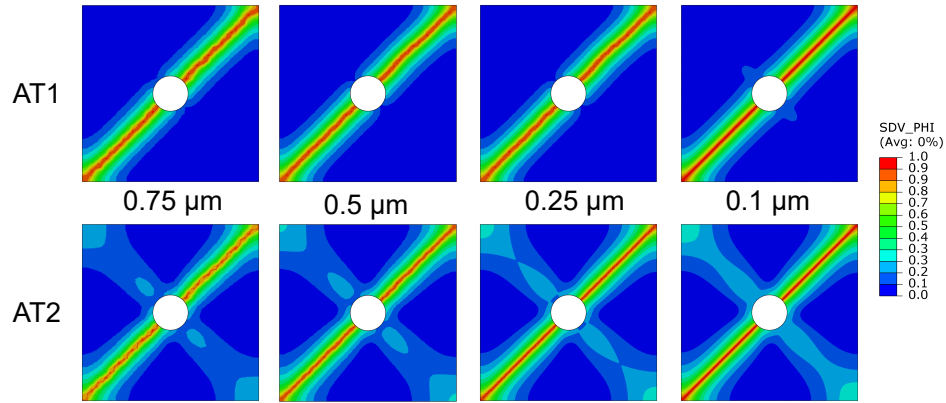


Figure 5.4: Crack patterns for AT1 and AT2 formulations under shear loading with different mesh sizes.

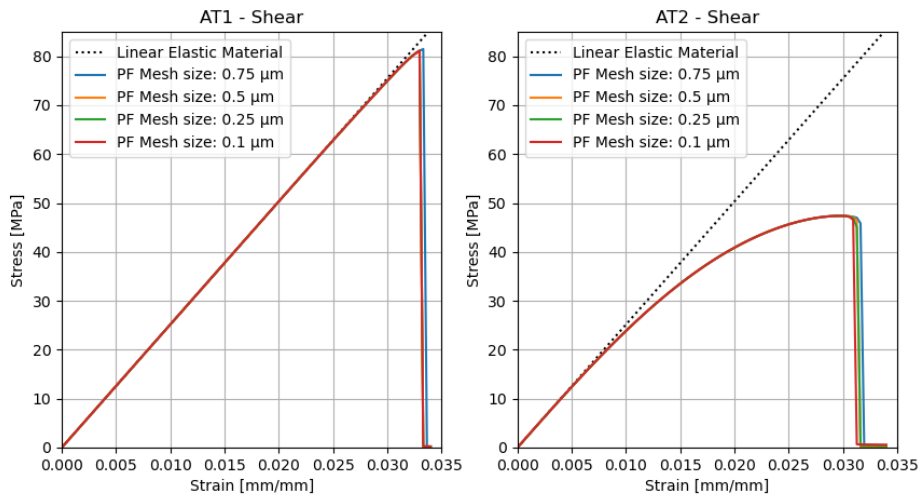


Figure 5.5: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different mesh sizes for the open-hole specimen under shear loading in Fig. 5.1 b).

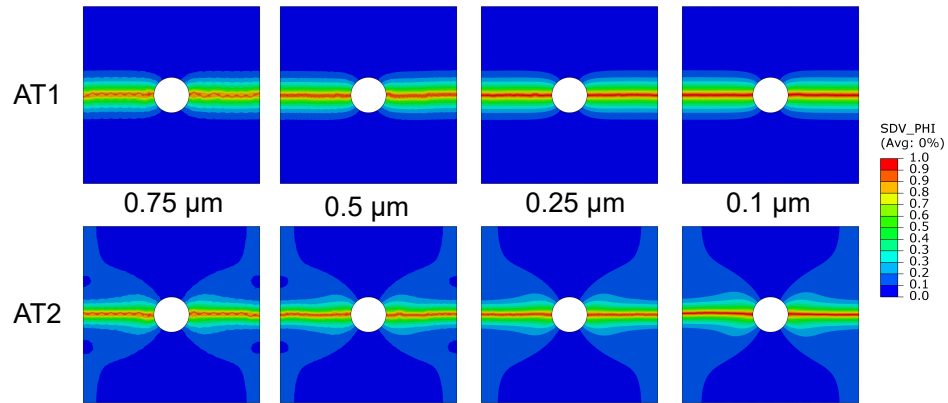


Figure 5.6: Crack patterns for AT1 and AT2 formulations under compression loading with different mesh sizes.

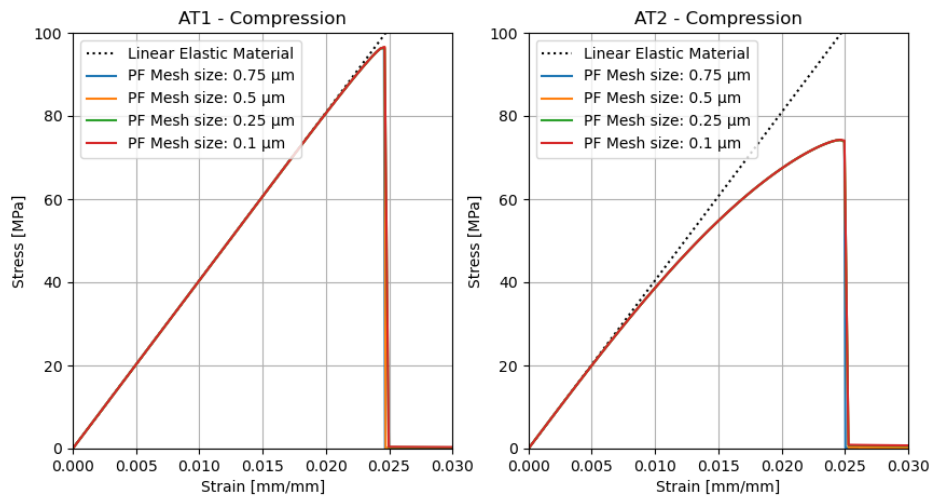


Figure 5.7: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different mesh sizes for the open-hole specimen under compressive loading in Fig. 5.1 c).

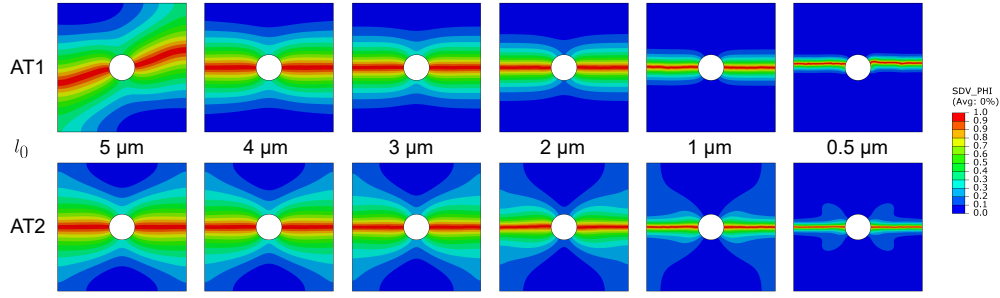


Figure 5.8: Crack patterns for AT1 and AT2 formulations under tensile loading and different values of the length scale parameter (l_0).

5.3.2 Influence of the length scale parameter

The influence of the length scale parameter is studied for the AT1 and AT2 formulations without using an energy split and under pure tension, pure shear and pure compression imposed through displacement BC, as shown in Fig. 5.1. The mesh size is 0.25 μm and the material properties used for comparison are shown in Table 5.1 when it is not explicitly stated. As before, the plots in this subsection are shown in the undeformed state and they do not explicitly show the mesh.

The crack patterns and global stress-strain curves are shown in Fig 5.8 and Fig 5.9, respectively, for tensile loading. As expected, when the value of the length scale parameter (l_0) is reduced, the damaged area gets gradually narrower (Fig 5.8) and the maximum stress increases (Fig 5.9). In this case, even if l_0 is equal to the hole diameter, localization is still achieved around the hole. The only particularity is related to the crack shape deviation in the AT1 formulation when l_0 reaches the size of the hole diameter due to the dispersed distribution of damage and initial struggle to reach damage localization. Besides, even though damage localization in AT1 is more difficult for large values of l_0 , there is a general trend for the AT2 formulation to generate damage patterns much more disperse. Thus, creating higher energy dissipation. This is the case even if the comparison between formulations is made using the same value of l_0 .

The crack patterns and global stress-strain curves are shown in Fig 5.10 and Fig 5.11, respectively, for shear loading. In this case, similar to loading in tension, localization is always present centred around the hole. The fracture pattern is consistent up to $l_0 = 1 \mu\text{m}$ in both formulations. However, as l_0 reaches the value of 0.5 μm , the fracture pattern changes dramatically. Namely while for larger values of l_0 , the shear loading created by the combined effect of simultaneous application of tension and compression creates a fracture pattern dominated by the maximum principal stress. For the AT1 formulation, critically low values of l_0 create fracture patterns that reflect individual contributions from tension and compression.

It is worth mentioning that unlike tension or compression loading, as localization is easier under shear loading, the spurious softening in the AT1 formulation due to difficulty of crack localization under large values of l_0 are not present in this loading scenario. However, spurious

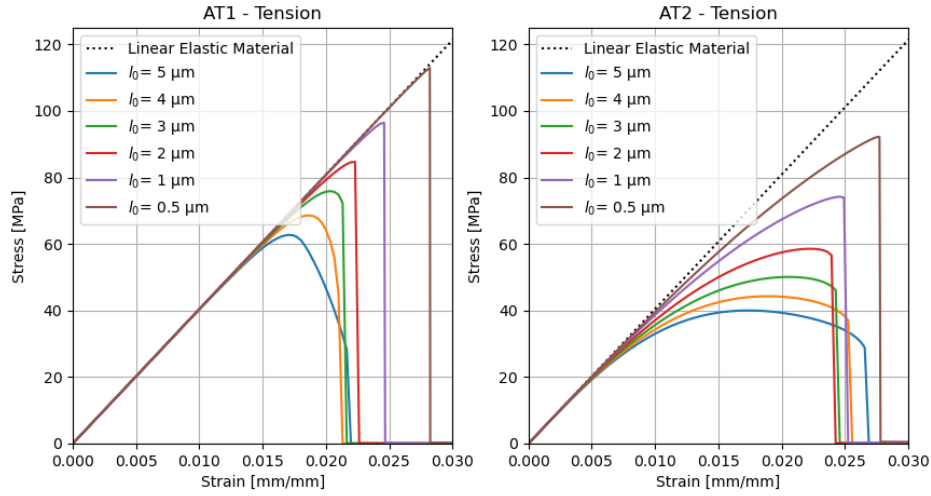


Figure 5.9: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different values of the length scale parameter (l_0) for the open-hole specimen under tensile loading in Fig. 5.1 a).

softening is still present for the AT2 formulation, even under shear when fracture localization happens much easier.

The crack patterns and global stress-strain curves are shown in Fig 5.12 and Fig 5.13, respectively, for compression loading. In this load scenario if no energy split is used the crack pattern and stress-strain behaviour in compression are very close to what is seen in tension. However, it seems that under compression loading, when the length scale reaches the size of the hole diameter, localization is not possible for the AT1 formulation.

At this point it is possible to see that even though the length scale clearly controls the maximum strength in all loading scenarios, the same cannot be said for the strain at complete specimen separation. Besides, there is inconsistency in the crack pattern found for the AT2 formulation, while for the AT1, modifying the value of l_0 can have an immediate effect on the shape and way of propagation of fracture.

It is clear from Fig 5.9, Fig 5.11 and Fig 5.13 that AT2 formulation yields highly non-linear response and apparent gradual failure of the specimen. However, as l_0 decreases, the non-linearity is reduced and the behaviour becomes dominantly fragile. This is because a sharper, more localized crack can be formed. One can say that AT1 experiences the same issues, regarding gradual failure previous to peak loads. However, this is only visible when the length scale parameter is truly close to the hole diameter.

In addition, from the stress strain curves (Fig 5.9, Fig 5.11 and Fig 5.13), it can be seen that regardless of the geometric localization of PF, there is a distinctive load drop at certain point. This is because in the case of crack localization, the specimen breaks at a certain region and when there is no localization, the whole specimen behaves similarly to the single element tests, still shown a characteristic peak load and posterior softening.

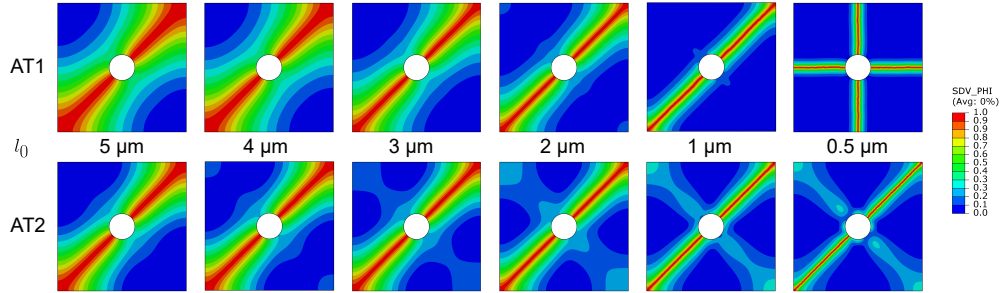


Figure 5.10: Crack patterns for AT1 and AT2 formulations under shear loading and different values of the length scale parameter (l_0).

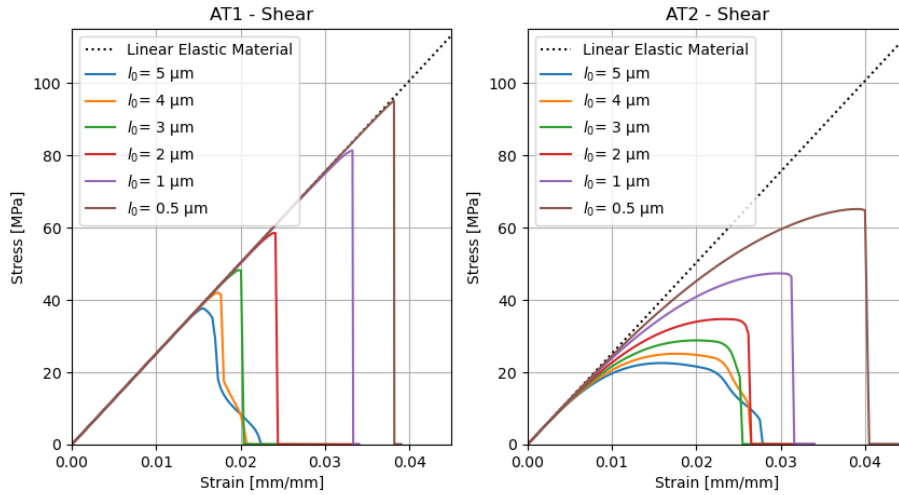


Figure 5.11: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different values of the length scale parameter (l_0) for the open-hole specimen under shear loading in Fig. 5.1 b).

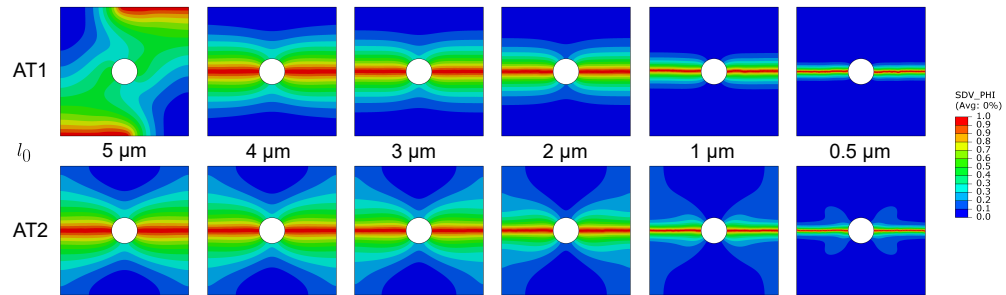


Figure 5.12: Crack patterns for AT1 and AT2 formulations under compression loading and different values of the length scale parameter (l_0).

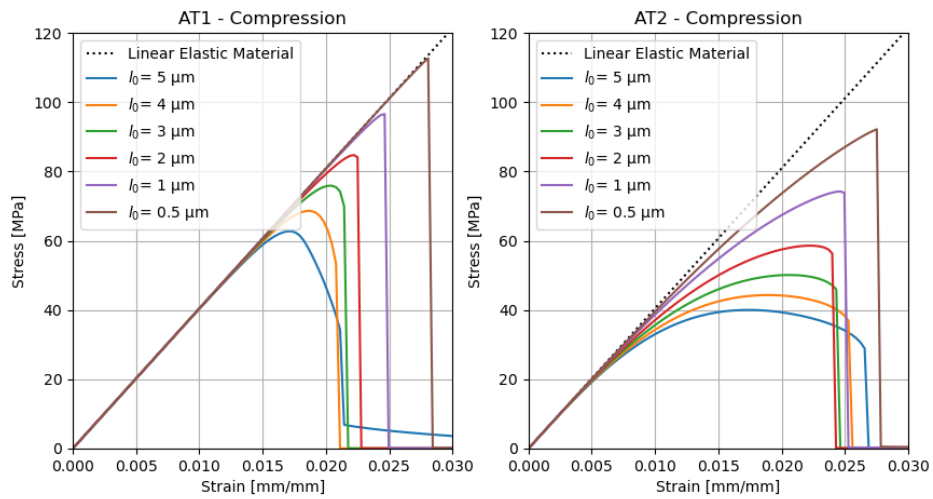


Figure 5.13: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different values of the length scale parameter (l_0) for the open-hole specimen under compressive loading in Fig. 5.1 c).

5.3.3 PF formulation and energy split

The influence of the energy split is studied for the AT1 and AT2 formulations using Miehe and Amor energy splits and for the sake of baseline reference also with no energy splits. The mesh size is $0.25 \mu\text{m}$ and the material properties used for comparison are shown in Table 5.1. Again, the open hole specimen is under pure tension, pure shear and pure compression imposed through displacement BC, as shown in Fig. 5.1. The curves in this subsection include the simulation using linear elastic material models without any sort of damage model in order to aid visualizing the deviation from a linear behaviour due to softening or fracture. In addition the fracture patterns in this subsection are also shown in the undeformed state and they do not explicitly show the mesh.

The crack patterns and global stress-strain curves are shown in Fig 5.14 and Fig 5.15, respectively, for tensile loading. As mentioned previously, the main purpose of the energy split is to prevent unrealistic fracture patterns under compressive dominated loading. However, in the case of Miehe's split, there is a clear disruption even in tensile dominated loading; in Fig 5.15 there is a clear increase in the maximum stress that can be reached in both formulations and in the case of the AT2 formulation there is even a reduction in the global softening. The reason for this is the fact that even though the loading is unidirectional deformation, the stress distribution is not uniform nor pure tension. Around the hole, even if tensile stresses dominate, there is a contribution of shear stresses that are taken into account in Amor and no split, but they are ignored in Miehe's split.

On the other hand, Amor split perfectly matches the solution with no energy split. With regard to the crack patterns shown in Fig 5.14 fracture still takes place around the centre of the hole in the direction perpendicular to the loading application. In this case, there is no clear difference between the Miehe, Amor or no energy split. Again the main difference still resides on the diffuse damage pattern and gradual softening of the AT2 formulation when compared to AT1, this effect occurs regardless of the split used.

The crack patterns and load-displacement curves are shown in Fig 5.16 and Fig 5.17, respectively, for shear loading. In this case, again there is no apparent difference between Amor split and no split, neither on the fracture pattern nor in the load-displacement curves. However, Miehe's split creates the largest disruption, more severe than in tension dominated loading, as the load carrying capacity increases as well as the gradual softening of AT2 diminishes. For Miehe's split, fracture still initiates around the hole, but it is triggered by the main tensile stress. In case of AT1, the whole crack is driven by the tensile deformation, while for AT2 only the initiation is triggered by the tensile deformation, after crack initiation there is a migration to a type of pattern similar to what is seen in Amor and no split. As the stress is computed from the vector sum of the reaction forces, in AT1 the vertical compressive component of the load keeps increasing, this is why there is no definite load drop. On the other hand AT2, there is a local minimum in the load-displacement curve created by the crack migration from the perpendicular to the diagonal direction, such phenomena largely increases the perceived load-carrying capacity if compared to Amor or no split.

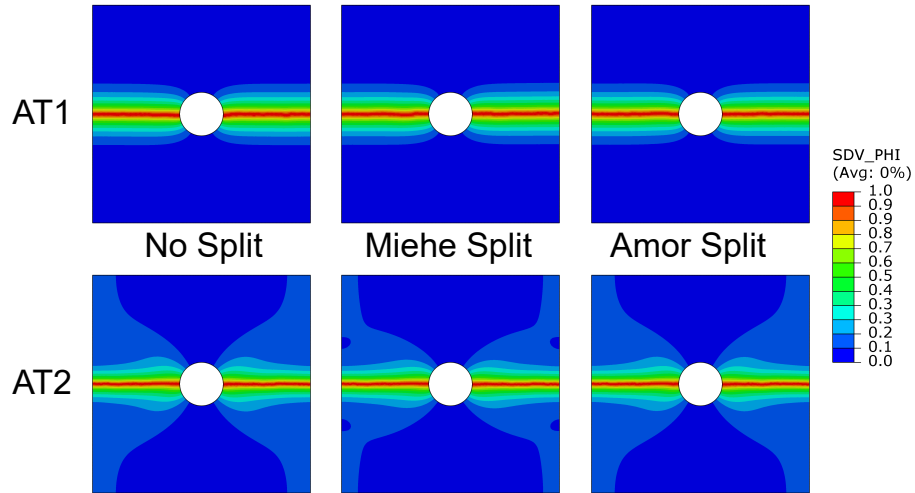


Figure 5.14: Crack patterns for AT1 and AT2 formulations under tensile loading and different energy splits.

The crack patterns and global stress-strain curves are shown in Fig 5.18 and Fig 5.19, respectively, for compression loading. As expected the largest differences are found in this load scenario. First, there is now a difference in the stress-strain response between Amor split and no split. Amor split delays crack initiation and propagation, and even though the crack patterns are similar, it means, that both run through the centre of the hole in the direction perpendicular to the load application, we can see that AT2 combined with Amor splits creates a larger damaged area than without a split. On the other hand, the strength estimated with Miehe's split is around double the one predicted by Amor's split in both AT1 and AT2 formulations, besides, once again the crack pattern shifts, but this time from the direction of maximum compressive stress to the direction of maximum shear, also passing through the centre of the hole. The lack of experimental evidence does not allow to rule out a specific damage pattern as unrealistic, as can be seen in UD FRP studies [179], both perpendicular and diagonal cracks can appear in compression tests.

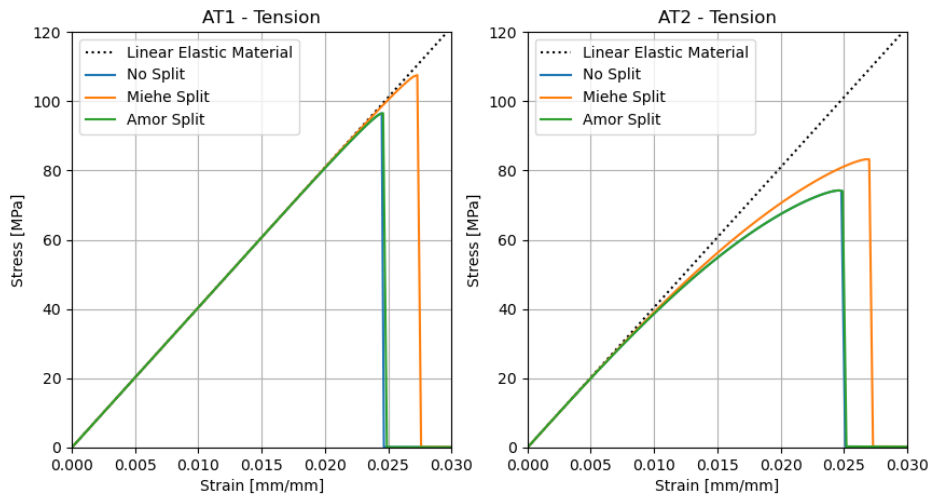


Figure 5.15: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different energy splits for the open-hole specimen under tensile loading in Fig. 5.1, a).

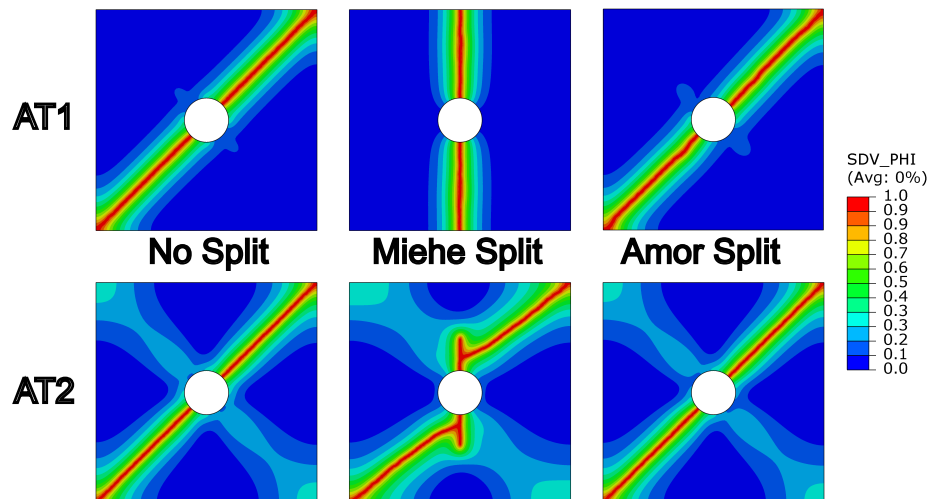


Figure 5.16: Crack patterns for AT1 and AT2 formulations under shear loading and different energy splits.

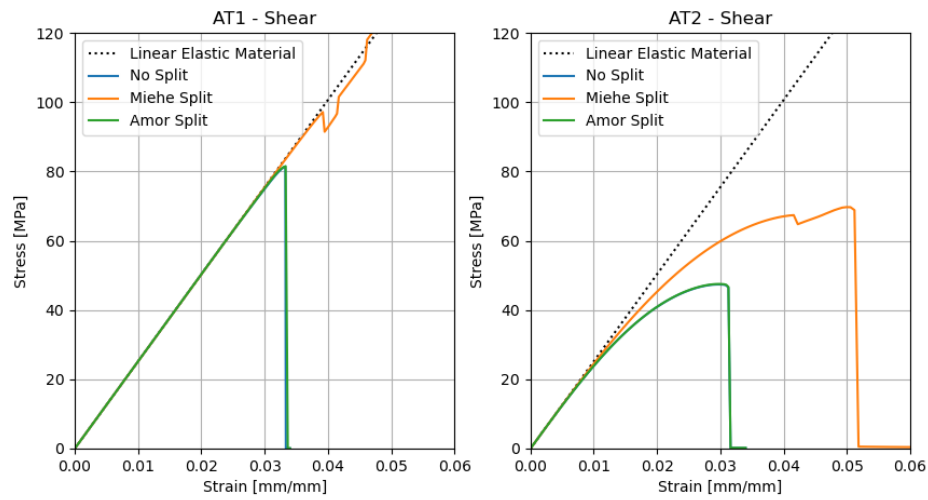


Figure 5.17: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different energy splits for the open-hole specimen under shear loading in Fig. 5.1 b).

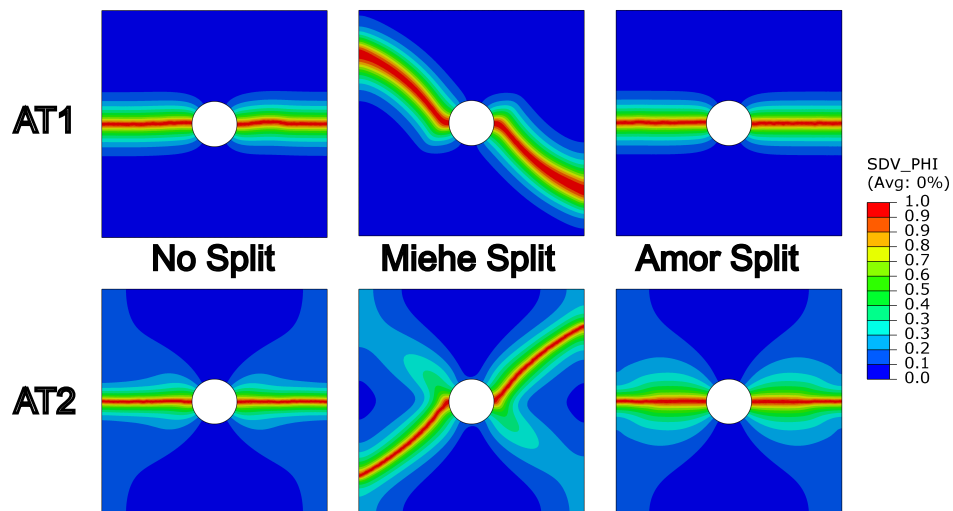


Figure 5.18: Crack patterns for AT1 and AT2 formulations under compression loading and different energy splits.

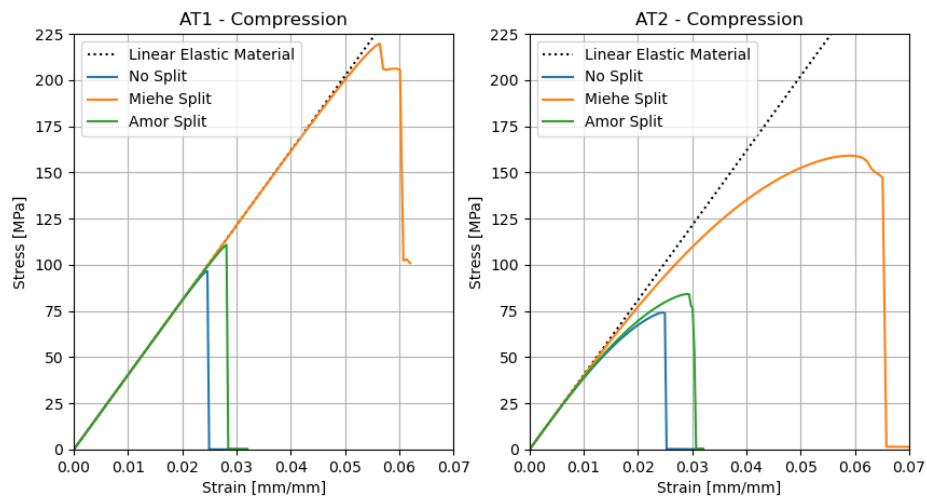


Figure 5.19: Stress-strain curves for linear elastic material model compared to AT1 and AT2 formulations with different energy splits for the open-hole specimen under compressive loading in Fig. 5.1 c).

5.4 Concluding remarks

This chapter presented an initial study of the numerical performance of a UEL and a UMAT subroutine implementation of PF inside Abaqus. It was concluded that the UEL provides much more control and implies a more clear understanding of the calculations performed by the software. Besides, it allows more flexibility in the configuration of the solver which translates into better numerical performance, the former given in terms of convergence rate and required number of iterations.

Once the UEL implementation was selected, the influence of the PF length scale, formulation and energy splits were studied in detail in an open-hole structure under different loading conditions. It was possible to individually identify the differences and limitations of each combination of parameters when representing micro-scale structures. The following chapter adds one additional parameter, it includes the fibre and its interfacial cohesive damage. A similar study is performed to gradually identify the individual contributions to the global response of larger RVE where the effect of such collection of variables could be obscured by the high amount of variability from geometrical as well as material origin.

One of the main ambiguities that could be directly identified in the implementation of PF as gradient-enhanced continuum damage model is the fact that, even though localization of the damaged area can be achieved most of the time, the brittle-like nature implied by the present formulation of PF is only perceived for values of l_0 which are much smaller than the characteristic geometric dimensions. In this case, the hole diameter is considered as the most relevant geometric parameter. As the value of l_0 increases, the global stress-strain behaviour tends to flatten prior to the main load drop, i.e., the whole specimen softens. This effect is created due to the struggle of the PF to localize in the form of a transverse crack when l_0 is too large. This behaviour is more severe for the AT2 formulation due to its inherent nature; which again, even if the softening behaviour is imposed locally, it can still influence the overall behaviour of the open hole specimen.

In summary, the ambiguity comes from the fact that even though damage localization takes place, defining or distinguishing such pattern as a crack resulting from a linear elastic brittle-like fracture formulation can be unclear specially if the global stress-strain response reflects gradual softening. Thus, for larger values of l_0 , PF analysis transforms into a sort of CDM approach. It is then, difficult to discriminate when is PF used properly if there is such strong limitation on the length scale, which is a "material" parameter that directly limits the geometric characteristics of the analysis.

Chapter 6

Single fibre Phase-Field modelling

6.1 Introduction

In this chapter a single fibre is included in the middle of the specimen. The fibre is considered to behave according to an isotropic linear elastic material model. Thus, any sort of damage is expected to take place in the bulk of this element. The interaction of the fibre and the surrounding matrix is given by a cohesive surface interaction with a bilinear behaviour and the Benzeggagh-Kenane (BK) fracture criteria. The surface interaction also accounts for normal contact after complete decohesion but without considering friction. The geometries and loading are such that the analysis is performed in the direction transverse to the fibre, so only transverse normal loading and shear are applied, see Fig. 6.1.

Within this chapter, all the models use micro-scale dimensions where the fibre has $5\text{ }\mu\text{m}$ diameter (typical of carbon fibre and Eglass in thin-ply composites) and its inside a square plate of $25\text{ }\mu\text{m}$ side length that represents the matrix. The material and interface properties are shown in Table 5.1, if not stated explicitly. The purpose of this section is to study the influence of the inclusion of the fibre and the cohesive interface both as the only failure mechanism as well as within the context of initial trigger of matrix PF fracture.

In all cases, the UEL implementation described in Chapter 5 is used for 2D plane strain elements and the infinitesimal deformation assumption is considered. The inclusion of the fibre and its interface create a more demanding convergence effort, which is potentiated by the loading scenario. For this reason models under tension and shear ran using *monolithic* solution scheme, while compression loading could only work with the *staggered* solution scheme. Besides, the studies of the different energy splits were done using a "hybrid" implementation.

Unlike the previous chapter, in this case, there is an initial analysis assuming cohesive damage is the only source on non-linearity. In this section mesh convergence as well as influence of loading are studied. Then PF damage is included in the matrix and similar studies are performed. In addition, there is an assessment of the influence of the PF formulation, energy split and of length scale in the variation of the single fibre model.

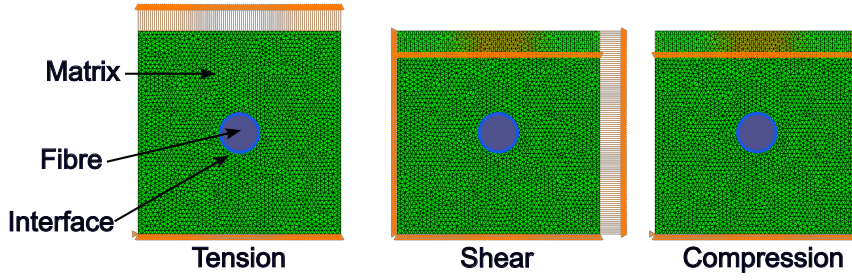


Figure 6.1: Mesh and BC for the Open Hole specimen under tensile, shear and compressive loading.

Similar to the previous chapter, the stress-strain curves are computed from the reaction forces divided by the cross-sectional area of the specimen and the normalized imposed displacement. This is why they are global measurements, no local stresses or strains are depicted in the present figures.

It should be clear that, at this point, there is no rigorous qualitative comparison with experimental data, as the required data is not available. Namely, there is no source of verified micro-scale properties that come alongside similar test specimens. Thus, at this point only a qualitative evaluation can be performed between the different variables in the PF formulation and cohesive properties. For this purpose the curves depicting specimens with a linear elastic material response and ideal fibre-matrix bonding are plotted alongside models that account for cohesive damage only and cohesive and PF damage together. These curves can easy visualization of the onset of non-linear response due to the different sources of damage.

6.2 Cohesive interface damage only

The mesh convergence as well as the study of the cohesive properties are initially done considering linear elastic material model in both the matrix and the fibre, and using cohesive interface damage under pure tension, pure shear and pure compression imposed through displacement BC, as shown in Fig. 6.1. Thus, at this stage the only source of non-linear behaviour is the decohesion of the fibre inside the matrix.

6.2.1 Mesh convergence

For the mesh convergence study, the global stress-strain curves alongside the polar plot of the cohesive damage distribution around the fibre are shown in Fig 6.2, Fig 6.3 and 6.4 for tensile, shear and compression loading. Purely linear elastic models ($\sigma_{I0/II0} = \infty$, $G_{Ic/IIc} = \infty$), it means, models that do not considering cohesive damage were also ran using the smallest mesh size in order to better appreciate the deviation from linearity due to the effect of the cohesive damage in the global stiffness degradation. It can be seen then, that non-linear behaviour is barely perceived in general, and it could be specially hidden in the case of compression. The main differences in

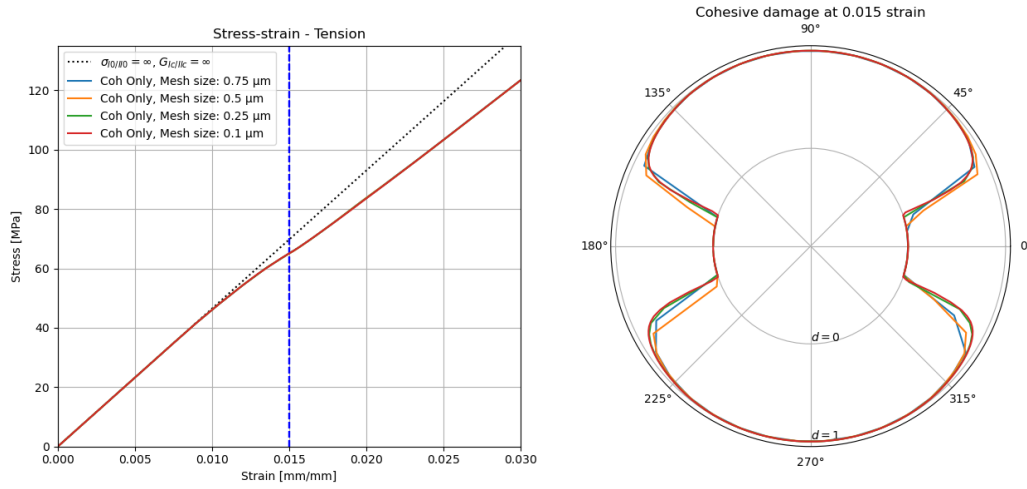


Figure 6.2: Stress-strain curves and cohesive damage (d) distribution around the fibre for a perfect interface connection ($\sigma_{I0/II0} = \infty, G_{Ic/IIc} = \infty$) compared to models considering a damageable cohesive interface. Different mesh sizes were used for the single-fibre specimen under tensile loading in Fig. 6.1 a). The blue dashed line represents the strain level at which the cohesive damage plot was evaluated.

mesh size are only visible in the polar plots, but only because smaller mesh sizes yield smoother curves, however the cohesive transition zone is fairly similar for all mesh sizes. In the case of shear loading, the differences are only in the location due to the propensity of this loading scenario to create asymmetries due to small perturbations, such as mesh irregularities. However, even in this case, the cohesive damage distribution can be considered in practical terms as equivalent.

On the other hand, it is clear that for such simple model the mesh size does not affect the results, thus, if the non-linear behaviour of the analysis is dominated by cohesive damage, coarse meshes can still be used without loss of accuracy.

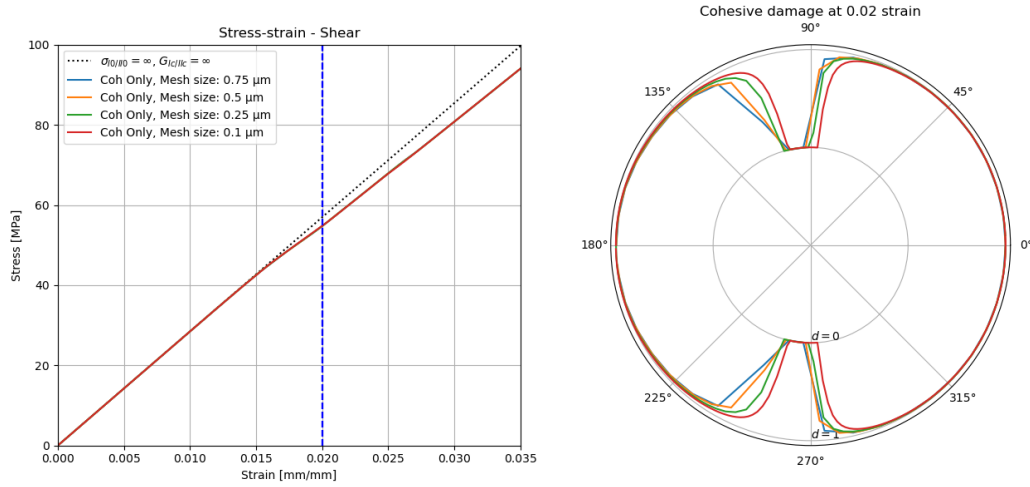


Figure 6.3: Stress-strain curves and cohesive damage (d) distribution around the fibre for a perfect interface connection ($\sigma_{I0/II0} = \infty, G_{Ic/IIc} = \infty$) compared to models considering a damageable cohesive interface. Different mesh sizes were used for the single-fibre specimen under shear loading in Fig. 6.1 b). The blue dashed line represents the strain level at which the cohesive damage plot was evaluated.

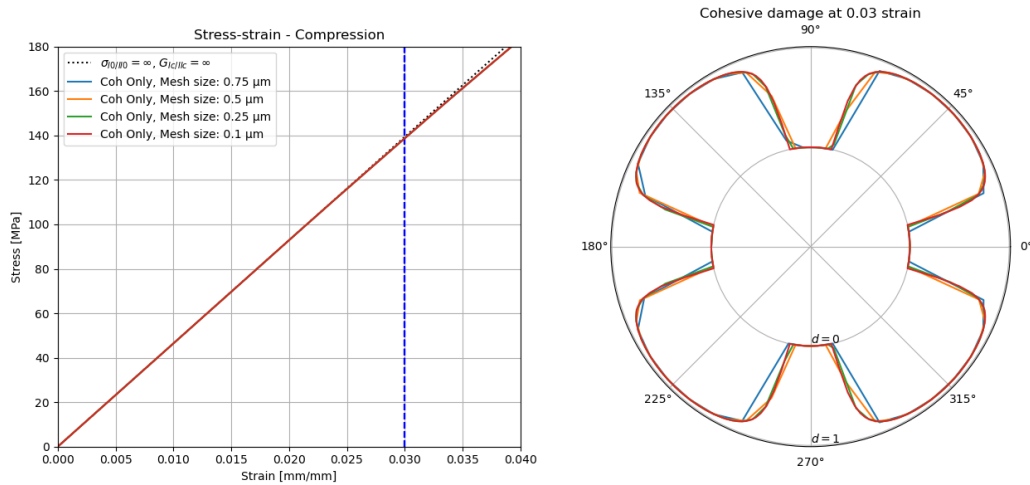


Figure 6.4: Stress-strain curves and cohesive damage (d) distribution around the fibre for a perfect interface connection ($\sigma_{I0/II0} = \infty, G_{Ic/IIc} = \infty$) compared to models considering a damageable cohesive interface. Different mesh sizes were used for the single-fibre specimen under compressive loading in Fig. 6.1 c). The blue dashed line represents the strain level at which the cohesive damage plot was evaluated.

6.2.2 Influence of the cohesive strength and fracture toughness

Once the mesh convergence is verified, the element size of $0.25 \mu\text{m}$ is used to study the influence of the strength and fracture toughness of the interface in the single fibre model response. For this study, the reference values for cohesive strength ($\sigma_{I0/II0}$) and cohesive fracture toughness ($G_{Ic/IIc}$) in Table 5.1 are defined to vary from 50 % to 150 %. The values represent the simultaneous and gradual reduction or increase in mode I and mode II properties, from the reference values given in Table 5.1 which represent 100 % of each property.

For the case of unidirectional tension, see Fig. 6.1, a), the global stress-strain response is shown in Fig. 6.5 to better appreciate the effect on the overall non-linearity of the single fibre model. Besides, Fig. 6.6 shows the cohesive damage distribution around the fibre at 0.015 of global strain for the given variation of interface properties. From Fig. 6.5 it can be seen that the cohesive strength ($\sigma_{I0/II0}$) controls the initiation of overall softening, it defines the knee point in the curve, while the cohesive fracture toughness ($G_{Ic/IIc}$) controls the "sharpness" of that knee point. Also, as seen in Fig. 6.6, the cohesive strength ($\sigma_{I0/II0}$) controls the length of the perimeter that is damaged at a given stage of global deformation, while the variation of the cohesive fracture toughness ($G_{Ic/IIc}$) does not immediately imply a different damaged perimeters around the fibre, the variation of these last parameters has more influence on how gradual the damage changes around the circumference of the fibre, but this effect is better perceived in the stress-strain curve.

One final point to notice is the fact that the cohesive properties do not seem to drastically change the sharpness of the damage profile in this loading scenario, which means the process zone does not seem to be heavily affected by the range of the variation of these parameters, this could also explain why the mesh convergence was so easily achieved.

The same study was performed for the case of shear loading, see Fig. 6.1, b). The global stress-strain response is shown in Fig. 6.7 in order to better appreciate the effect on the overall non-linearity of the single fibre model, while Fig. 6.8 shows the cohesive damage distribution around the fibre at a global strain level of 0.02. In this case, the effect of the overall non-linearity is very similar, however, the "knee point" is less marked for smaller values of $\sigma_{I0/II0}$. On the other hand, the variation on the cohesive properties seems to have a larger effect both on the symmetry as well as on the overall shape of the distribution of cohesive damage around the perimeter of the fibre. In this case, it can be seen that the cohesive strength ($\sigma_{I0/II0}$) has a clear effect on the length of the cohesive process zone, lower values of $\sigma_{I0/II0}$ produce sharper progressions from $d = 0$ to $d = 1$. In this case, the variation of $\sigma_{I0/II0}$ seems to disrupt more the shape of the cohesive perimeter if compared to the variation of $G_{Ic/IIc}$.

In general, for higher values of $\sigma_{I0/II0}$, the damaged perimeter is less, however, this can not be immediately assumed for the increased values of $G_{Ic/IIc}$. However, a gradual simultaneous increase in both properties does reduce the damaged perimeter in a larger proportion than increasing only the values of $\sigma_{I0/II0}$.

Finally, for the case of compressive loading, see Fig. 6.1, c). The stress-strain response is shown in Fig. 6.9 in order to better appreciate the effect on the overall non-linearity of the single

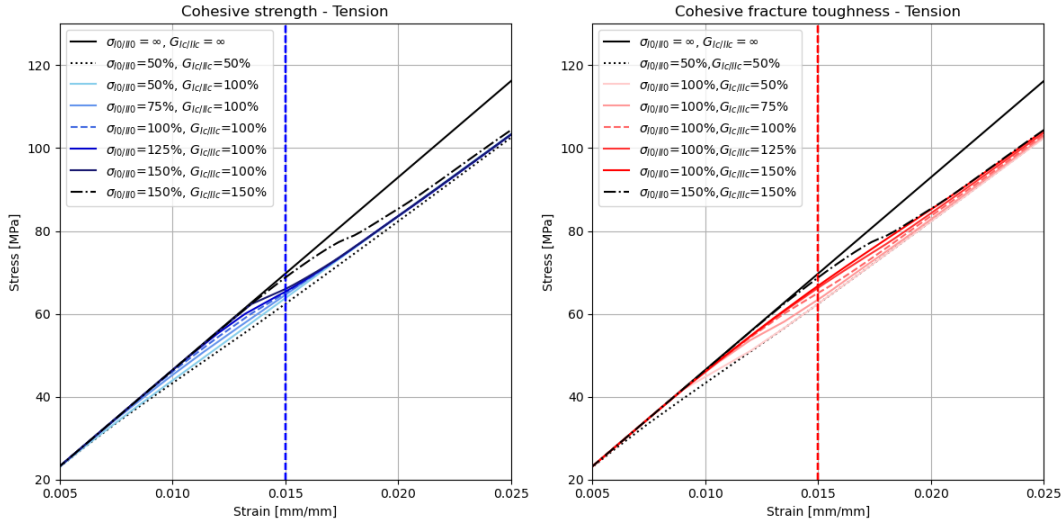


Figure 6.5: Stress-strain curves and cohesive damage (d) distribution around the fibre for a perfect interface connection ($\sigma_{I0/II0} = \infty, G_{Ic/IIc} = \infty$) compared to models considering a damageable cohesive interface with different values of cohesive strength and cohesive fracture toughness for the single-fibre specimen under tensile loading in Fig. 6.1 a).

fibre model, while Fig. 6.10 shows the cohesive damage distribution around the fibre at global strain level of 0.03. It is clear from Fig. 6.9 that the effect of the variation of properties is opposed to what was seen in the previous loading scenarios, it means, for compression loading, the variation of $\sigma_{I0/II0}$ seems to control how gradual is the softening taking place, while the variation of $G_{Ic/IIc}$ controls the location of the "knee point", which again is not very visible in this loading scenario. This behaviour is confirmed in Fig. 6.9, while changing $\sigma_{I0/II0}$ affects the transition distance (cohesive process zone) from damaged to undamaged interface, it also affects the longitude of the damaged area around the fibre. On the other hand, for the variation of $G_{Ic/IIc}$, the initial damaged perimeter is very similar, however, further damage progression seems to be abrupt and it is mainly controlled mainly by the fracture toughness rather than the strength.

At this point, the effect of the cohesive interface around the fibre seems to be understood, now the inclusion of the matrix PF damage can be added with confidence.

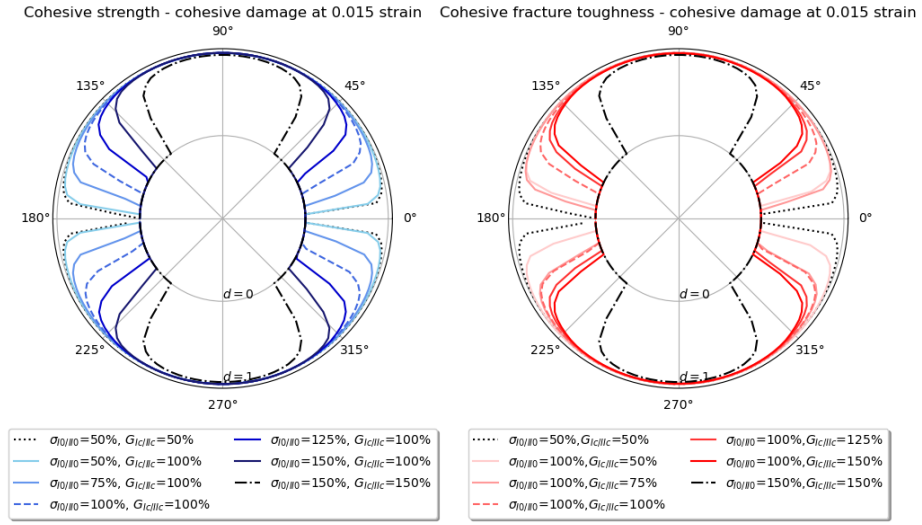


Figure 6.6: Cohesive damage (d) distribution around the fibre at 0.015 strain, for the models considering cohesive interface damage for different values of cohesive strength and cohesive fracture toughness for the single-fibre specimen under tensile loading in Fig. 6.1 a).

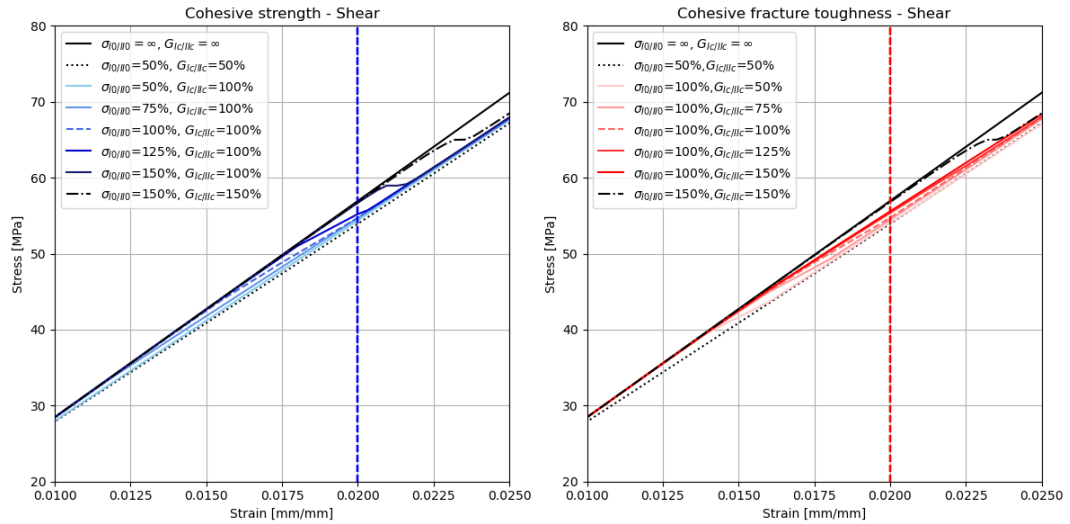


Figure 6.7: Stress-strain curves and cohesive damage (d) distribution around the fibre for a perfect interface connection ($\sigma_{I0/I0} = \infty$, $G_{Ic/Ic} = \infty$) compared to models considering a damageable cohesive interface with different values of cohesive strength and cohesive fracture toughness for the single-fibre specimen under shear loading in Fig. 6.1 b).

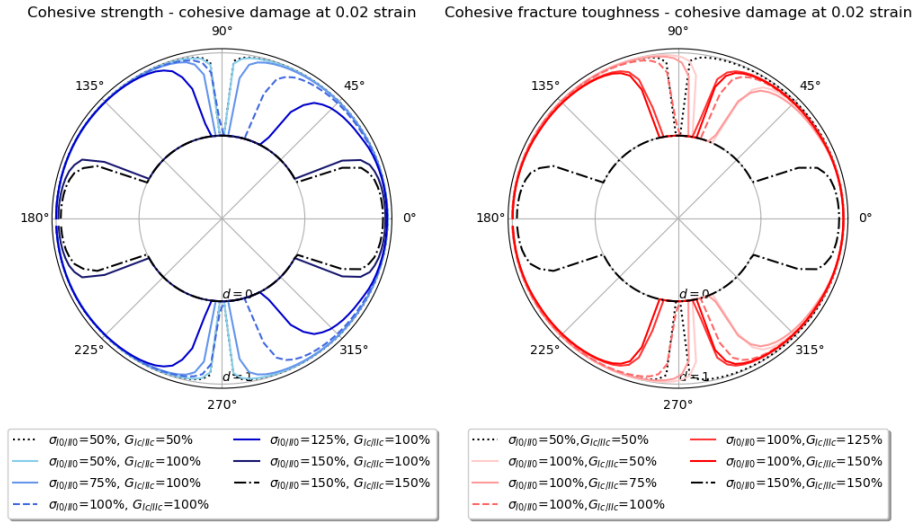


Figure 6.8: Cohesive damage (d) distribution around the fibre at 0.02 strain, for the models considering cohesive interface damage for different values of cohesive strength and cohesive fracture toughness for the single-fibre specimen under shear loading in Fig. 6.1 b).

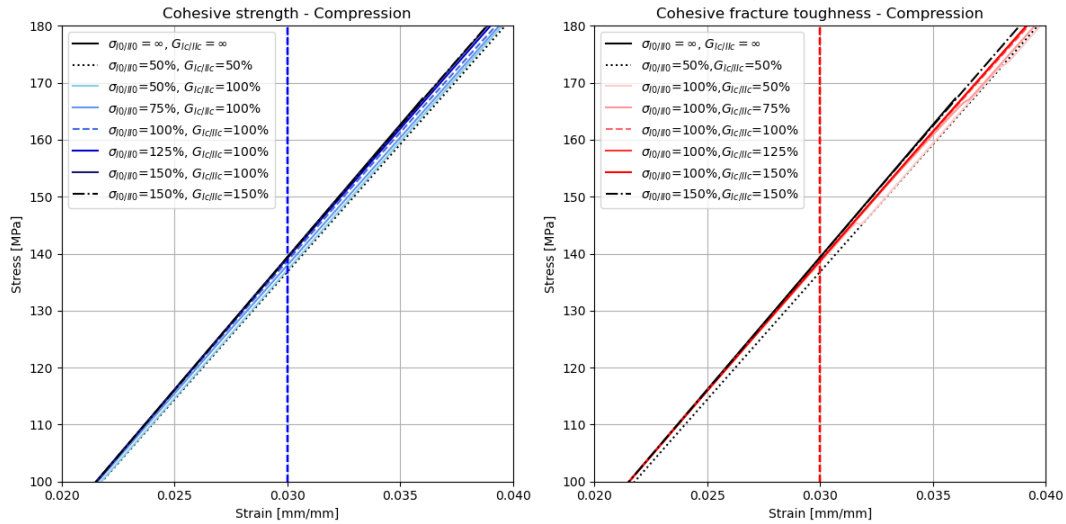


Figure 6.9: Stress-strain curves and cohesive damage (d) distribution around the fibre for a perfect interface connection ($\sigma_{I0/I0} = \infty$, $G_{Ic/Ic} = \infty$) compared to models considering a damageable cohesive interface with different values of cohesive strength and cohesive fracture toughness for the single-fibre specimen under compressive loading in Fig. 6.1 c).

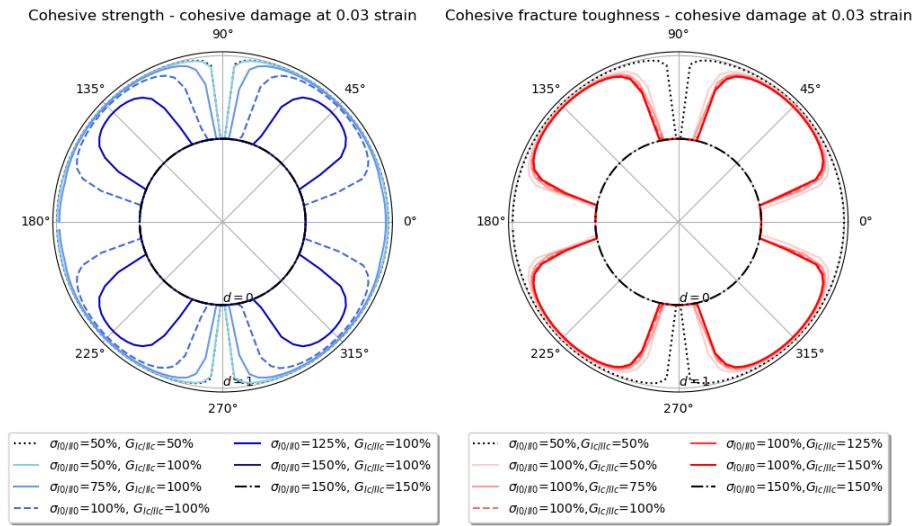


Figure 6.10: Cohesive damage (d) distribution around the fibre at 0.03 strain, for the models considering cohesive interface damage for different values of cohesive strength and cohesive fracture toughness for the single-fibre specimen under compressive loading in Fig. 6.1 c).

6.3 Cohesive interface damage and Phase-Field fracture

Now that it is clear how small is the influence of the mesh size in the softening due to only considering fibre-matrix decohesion. The next ingredient is the addition of the PF damage to the matrix. As it is difficult to plot PF damage distribution alongside cohesive damage, in the next subsections, the plots are shown in the deformed state, such as the gap between the fibre and the matrix gives an idea of the interface damage that is taking place in those areas. This is given in addition to the polar plots, where the cohesive interface damage variable (d) is plotted around the fibre perimeter.

The first study of fracture considers deformation-controlled tests on pure tension, pure compression, and pure shear; the objective is to compare AT1 and AT2 formulations as well as comparing the formulations without energy split and with Miehe and Amor energy splits. In the following, there is a brief summary and discussion on the tests of the single fibre models. As before, mesh convergence, effect of the PF length scale, energy split and formulation are compared in detail under different loading scenarios in order to better understand the disruption created by the inclusion of the fibre and its potential decohesion using cohesive elements.

6.3.1 Mesh convergence

According to different authors, the mesh size should be between 3 and 10 times lower than the length scale parameter. For this reason, mesh convergence is first studied for the AT1 and AT2 formulations without using an energy split and under pure tension, pure shear and pure compression loading imposed through displacement BC, as shown in Fig. 6.1. The material properties used for comparison are shown in Table 5.1 if not stated explicitly.

The deformed/damaged patterns are shown in Fig 6.11 while the stress-strain curves alongside the polar plots of cohesive damage are shown in Fig 6.12 for tensile loading. In this case, the polar plots represent the distribution of cohesive damage at peak stress. For tensile loading, similar to what happened in the open-hole model, the specimen fractures in the direction perpendicular to the load direction and the crack nucleates around the hole. However, the crack does not start from the centre of the hole, but it is slightly moved downwards or upwards as to start from the end of the decohesion. For the AT1 formulation, PF damage appears suddenly and the transversal crack is created from the tip of the cohesive crack. Thus, the initial softening is created only due to cohesive damage at the interface. However, in the AT2 formulation, softening in the matrix starts before the cohesive damage initiates, then once the interface starts to fail, the overall stiffness decrease is the sum of the contribution of decohesion and matrix damage.

Regarding mesh convergence, it is clear that a mesh size of $0.25 \mu\text{m}$ is required for accurate results in the case of the AT1 formulation, and $0.5 \mu\text{m}$ for AT2. The plots are different in terms of the stress-strain curves as well as cohesive damage distribution. The reason is because as larger mesh sizes promote premature PF fracture of the specimen they also delaying larger cohesive damaged areas. This effect, under tensile loading is clearly more severe for the AT1 than for the AT2 formulation.

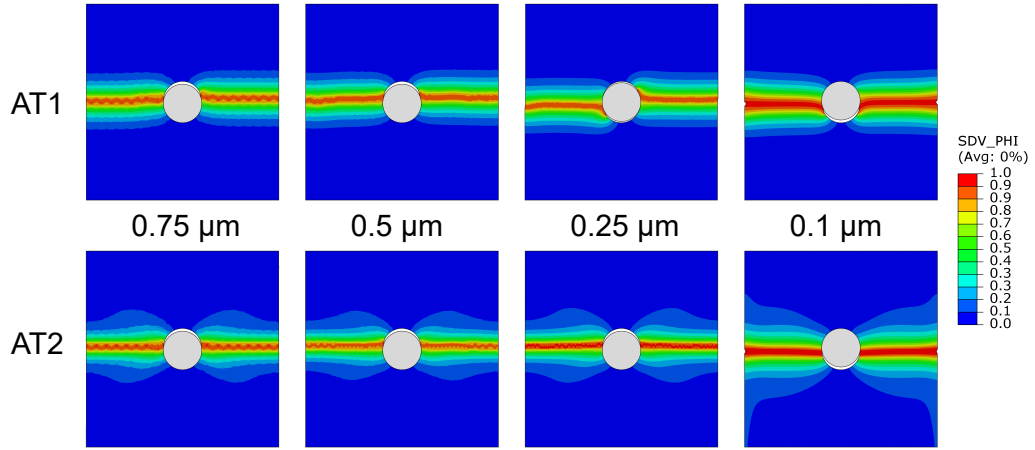


Figure 6.11: Crack patterns for single fibre models using AT1 and AT2 formulations under tensile loading and different mesh sizes.

In addition, the deformed/damaged patterns are shown in Fig 6.13 and stress-strain curves alongside the polar plots of cohesive damage around the fibre in Fig 6.14 for shear loading. In this case, the crack also goes in the diagonal direction, nucleating around the hole. However, in the case of the AT1 formulation, the crack initiates at the edge of the interface decohesion and it makes a turn to reach the specimen edges. Under this loading, there are two stages of softening, one that represents progression of the cohesive damage, that is somehow accelerated by the presence of the PF damage around the fibre, and one that represents progression of PF damage. This initial load drop was also found in the work of Guillén-Hernández et al. [27] and it was defined as a snap-back due to solely cohesive damage.

Similar to what happened in tension, the initial softening in the AT1 models is due to interface damage only, unlike the AT2 models that soften from the beginning (even before cohesive damage takes place). For AT1, larger mesh sizes seem to promote delayed PF damage, and at the same time reduce the cohesive damage. This is the case in both the first as well as the second load-drop of the stress-strain curves. On the other hand, for the AT2 formulation, there is an apparent difference in the stress-strain curves; coarse meshes underestimate the extension of cohesive damage. This is caused by the development of a PF damaged area around the contact region that does not seem to develop at the appropriate distance, delaying further progression of the interface damage.

Finally, the deformed/damaged patterns are shown in Fig 6.15 and stress-strain curves alongside the polar plots of cohesive damage around the fibre in Fig 6.16 for compression loading. This is the loading scenario that represents conflicting conclusions when compared to the shear or tensile loading. Under compression, the mesh size seems to have a lower influence on the overall results if we consider mainly the damage pattern, stress-strain curves and cohesive damage distribution. In this case, the results vary exclusively due to the formulation. Namely, with the inclusion of the fibre and the cohesive interface the specimens with AT1 formulation fracture in the direction

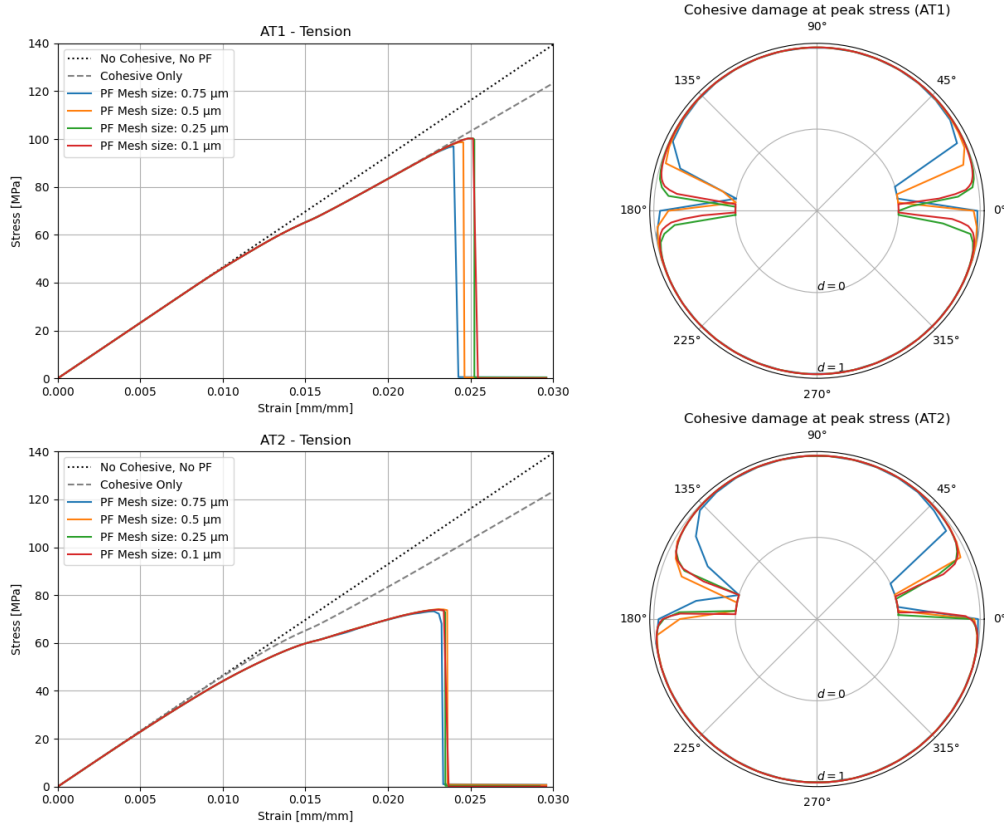


Figure 6.12: Stress-strain curves for a purely linear elastic material model (No Cohesive Damage, No PF) compared to models considering cohesive interface damage only (Cohesive Only) and Cohesive and PF damage for different mesh sizes. The results represent the single-fibre specimen under tensile loading in Fig. 6.1 a).

perpendicular to the loading direction. However, this time, the crack is shifted towards the bottom of the fibre/hole. On the other hand, fracture in the AT2 formulation does not happen around the fibre, it happens around the upper border and makes a turn avoiding the upper corners. It seems that the global softening of the AT2 model, which is evident in the stress-strain curve, prevents damage localization around the fibre even if the length scale is lower than the fibre diameter.

In all loading scenarios, there is a abrupt change in the thickness of the PF damaged region when the mesh size reaches 0.1 μm , this comes with a marked difference in the cohesive damage around the fibre. So far, there is evident explanation to relate the change of the PF damaged area based on the mesh size, when the mesh reaches very small values. This is specially intriguing, as the PF length scale is a predefined parameter and not a variable in the problem. For this reason, in the remaining sections, it is consider that a mesh size of 0.25 μm can reach results that could be representative for both formulations in the presence of cohesive and PF damage. This mesh size repects the most conservative rules explained previously in Chapter 2.

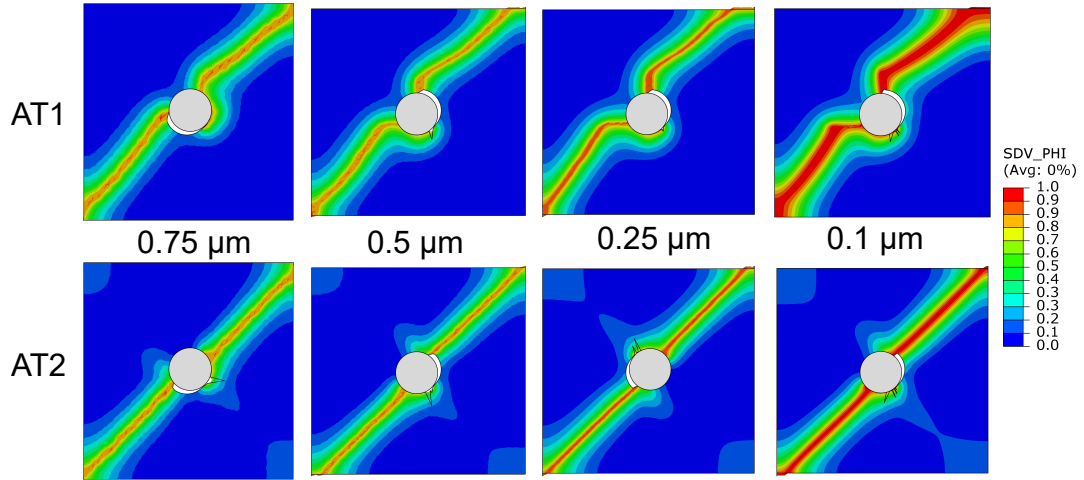


Figure 6.13: Crack patterns for single fibre models using AT1 and AT2 formulations under shear loading and different mesh sizes.

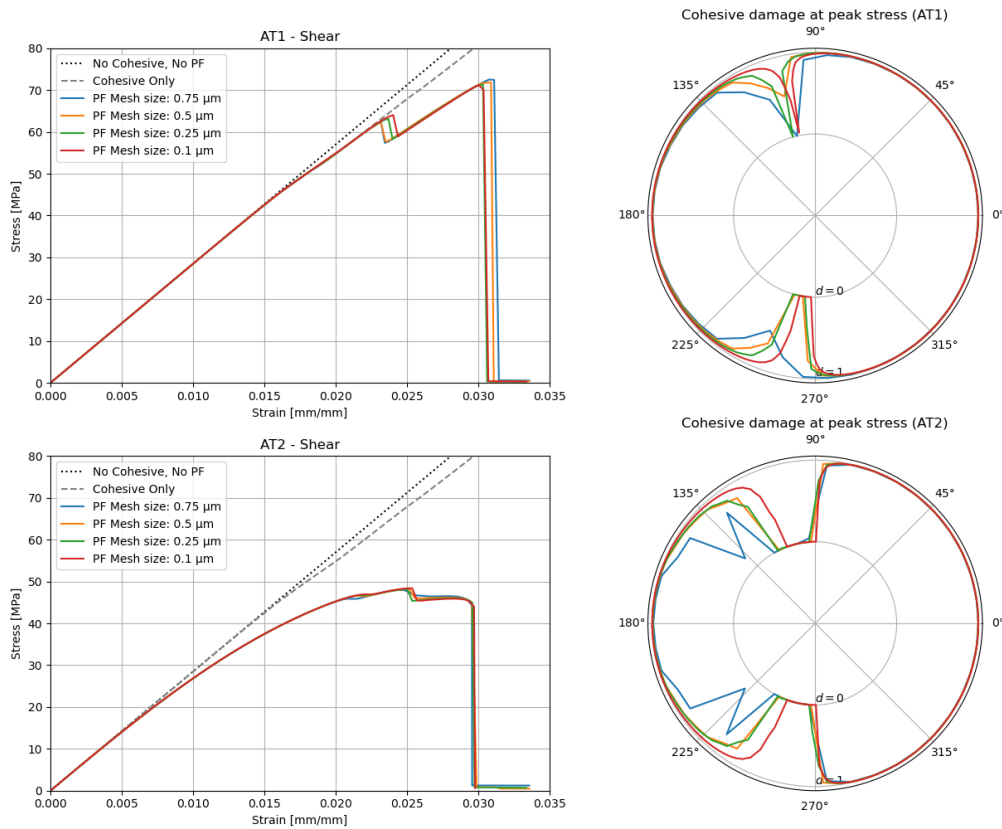


Figure 6.14: Stress-strain curves for a purely linear elastic material model (No Cohesive Damage, No PF) compared to models considering cohesive interface damage only (Cohesive Only) and Cohesive and PF damage for different mesh sizes. The results represent the single-fibre specimen under shear loading in Fig. 6.1 b).

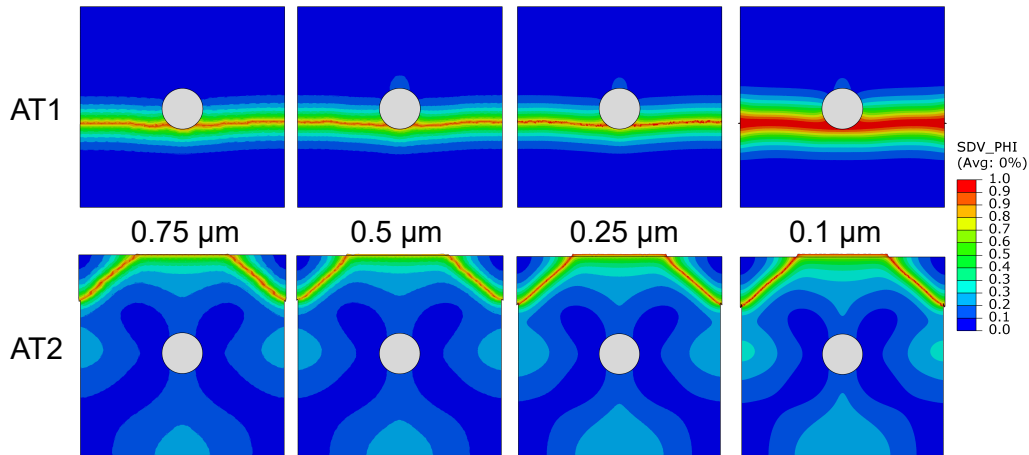


Figure 6.15: Crack patterns for single fibre models using AT1 and AT2 formulations under compressive loading and different mesh sizes.

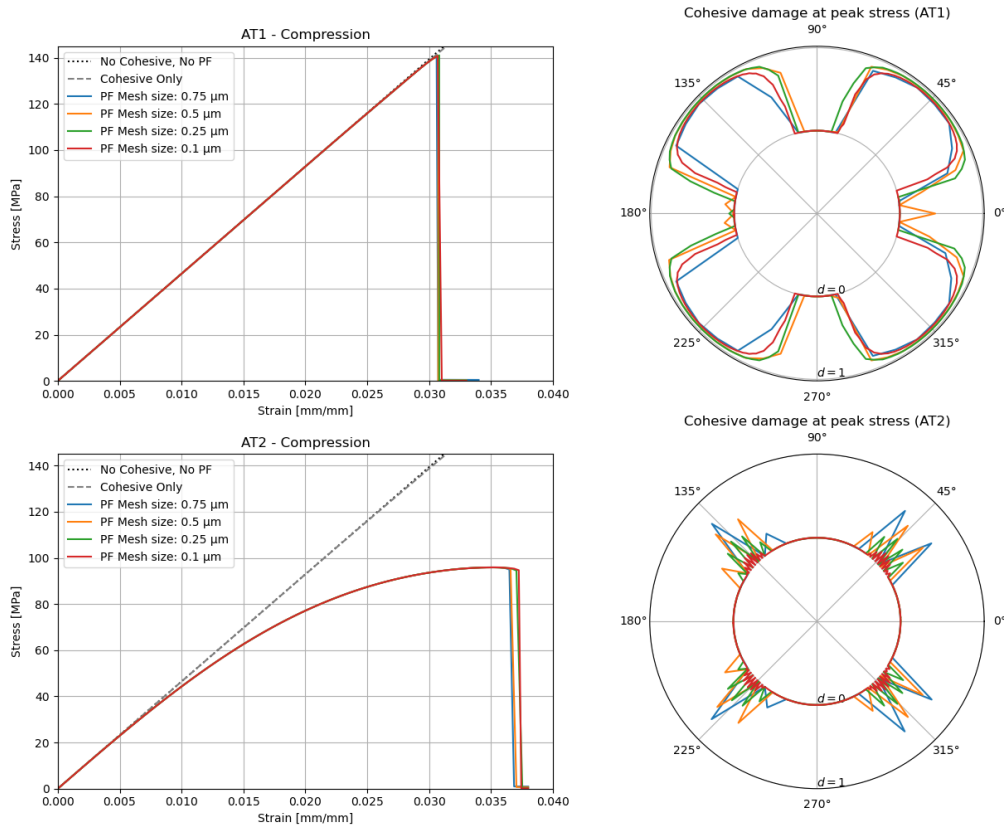


Figure 6.16: Stress-strain curves for a purely linear elastic material model (No Cohesive Damage, No PF) compared to models considering cohesive interface damage only (Cohesive Only) and Cohesive and PF damage for different mesh sizes. The results represent the single-fibre specimen under compressive loading in Fig. 6.1 c).

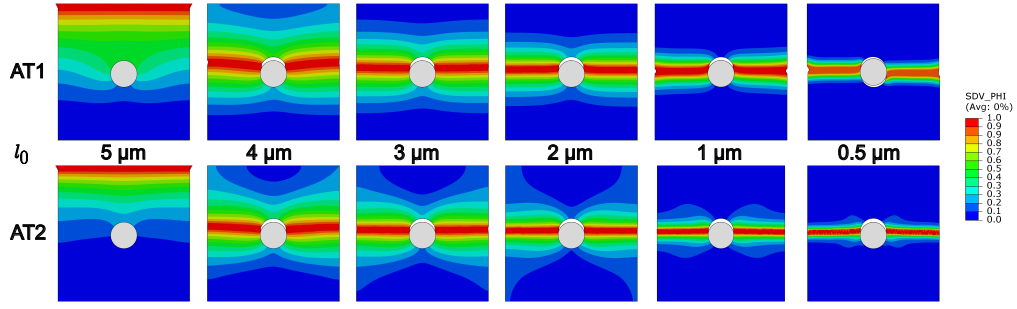


Figure 6.17: Crack patterns for AT1 and AT2 formulations under tensile loading and different values of the length scale parameter l_0 .

6.3.2 Influence of the length scale parameter

Similar to what was done for the Open-hole specimen, the influence of the length scale is studied for the AT1 and AT2 formulations without using an energy split and under pure tension, pure shear and pure compression BC, as shown in Fig. 6.1. The mesh size is $0.25 \mu\text{m}$ and the material properties used for comparison are shown in Table 5.1, except for the length scale parameter (l_0) which is set to vary from $5 \mu\text{m}$ to $0.05 \mu\text{m}$.

The crack patterns are shown in Fig 6.17 and the stress-strain curves, alongside the polar plots of cohesive damage are shown in Fig 6.18 for the case of pure tensile loading. The first thing to notice is that by adding the fibre and its cohesive interface, fracture localization around the hole is prevented for $l_0 = 5 \mu\text{m}$, even though significant decohesion can be observed, specially in the AT1 formulation. For values of l_0 lower than $5 \mu\text{m}$, the fracture pattern is fairly similar to the case of open-hole this is due to the fact that decohesion goes almost all around the fibre interface before the specimens completely separates into two pieces. Namely, by the moment of fracture, the fibre is almost completely separated from the matrix and all that remains is in fact the circular hole. For the AT1 formulation, decohesion is larger and it does not seem to strongly diminish by increasing the values of l_0 , at least up to $l_0 = 5 \mu\text{m}$, where it seems that lower decohesion happens before fracture of the specimen. This is owed to the fact that the crack does not localize around the hole, it does it at the edges of the specimen.

Besides, for the AT1 formulation, for values of l_0 larger than $1 \mu\text{m}$, softening before fracture is present due to the contribution of both decohesion and PF damage around the fibre, namely, only when l_0 is lower than $2 \mu\text{m}$ the global behaviour can be described as dominantly fragile. On the other hand, gradual softening is always present in the AT2 formulation, the initiation of the non-linear response does not seem to depend strongly on the length scale. However, l_0 does influence the intensity of the overall softening of the specimen. In general, for AT2 and for smaller values of l_0 , the behaviour is stiffer and larger stresses can be reached, at the same time larger decohesions accompany this trend.

Next, the crack patterns are shown in Fig 6.19 and the stress-strain curves, alongside the polar plots of cohesive damage are shown in Fig 6.20 for shear loading. This is a clear example of how

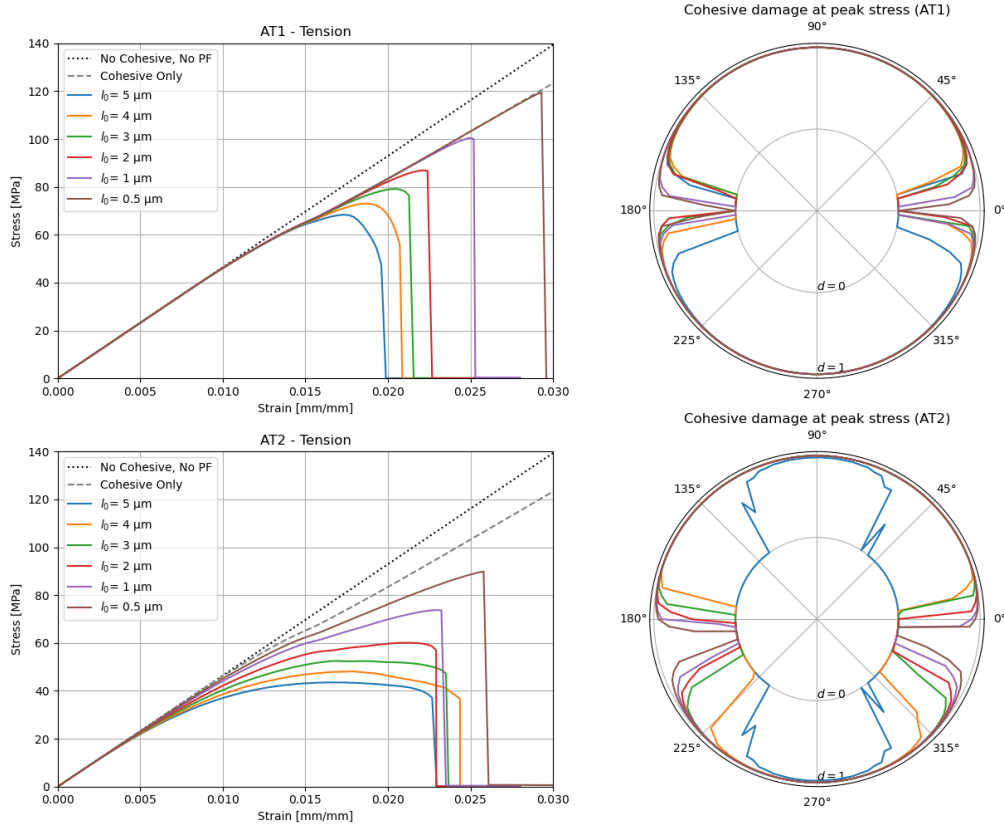


Figure 6.18: Stress-strain for AT1 and AT2 formulations under tensile loading and different values of the length scale parameter l_0 .

unpredictable PF results can be, specially when additional damage mechanisms such as cohesive damage are present. In this case, fracture localization around the fibre is prevented for intermediate values of l_0 (2 and 3 μm) in the AT2 formulation. Besides, for the AT1 formulation and $l_0 = 0.5 \mu\text{m}$ two transversal cracks are obtained instead of the diagonal crack observed in most of the other scenarios.

It is notorious that the so called "snap back" in the work of Guillén-Hernández et al. [27] is only present for values of $l_0 = 1 \mu\text{m}$ or smaller. If the length scale is larger than this, there is, in addition to the softening due to decohesion, some more softening caused by PF damage. This additional PF softening can be explained by observing that, for large values of l_0 , the crack struggles to localize around the fibre decohesion (main stress concentrator) and it rather distributes around the fibre before moving into the edges of the plate. This process of delayed crack localization is responsible for additional softening in the AT1 formulation.

For the AT2 formulation, the delayed crack localization is amplified by the fact that there is lower decohesion which causes further delay in crack nucleation and the overall softening is augmented not just by the contribution of decohesion but by the nature of the AT2 formulation. The severity of this last factor is augmented by larger values of l_0 . In fact, if the length scale is larger than 2 μm there is barely any cohesive damage and this is why for $l_0 = 4$ and $l_0 = 5 \mu\text{m}$, the

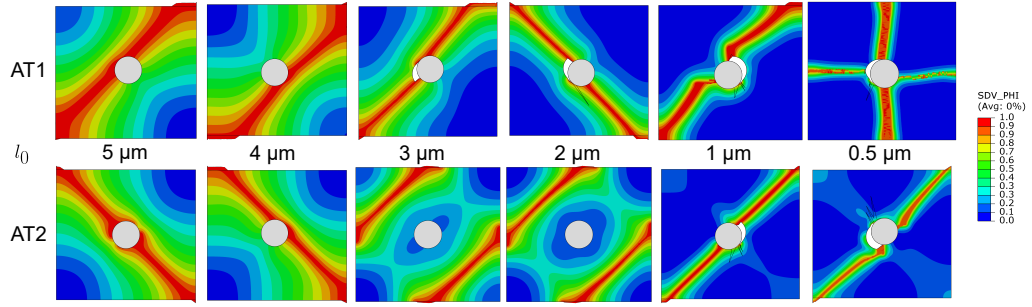


Figure 6.19: Crack patterns for AT1 and AT2 formulations under shear loading and different values of the length scale parameter l_0 .

PF damage shade goes round the fibre instead of jumping from one side of the fibre to the other one.

Finally, the crack patterns are shown in Fig 6.21 and the stress-strain curves, alongside the polar plots of cohesive damage are shown in Fig 6.22 for compression loading. This is the loading scenario where crack localization around the fibre is more difficult to reach, the AT1 formulation requires a length scale parameter of at least $3 \mu\text{m}$. It seems that cohesive damage around the fibre is necessary in order to nucleate the crack in the centre. Apparently the same logic can be applied to the AT2 formulation, however only for $l_0 = 0.5 \mu\text{m}$ the cohesive damage reaches an area that is sufficient to trigger PF fracture around the fibre and it does in an unsymmetrical way.

The stress-strain plot for compression give the most intuitive response regarding the relationship between the length scale parameter and the maximum stress and maximum strain (strain at null load-carrying capacity). It means, only for compression loading, reducing l_0 increases the maximum stress and the maximum strain proportional, even if such proportion is non-linear. This is considerably different for the other loading scenarios where, reducing l_0 does increase the maximum stress; however, the maximum strain or strain for sudden crack propagation does not seem to scale in an intuitive manner, it can in fact increase and decrease as l_0 changes progressively (see Fig. 6.20). In this work the length scale was set to $1 \mu\text{m}$ in order to ease crack localization while without heavily overestimating the material strength given in the work of Camanho et al. [18].

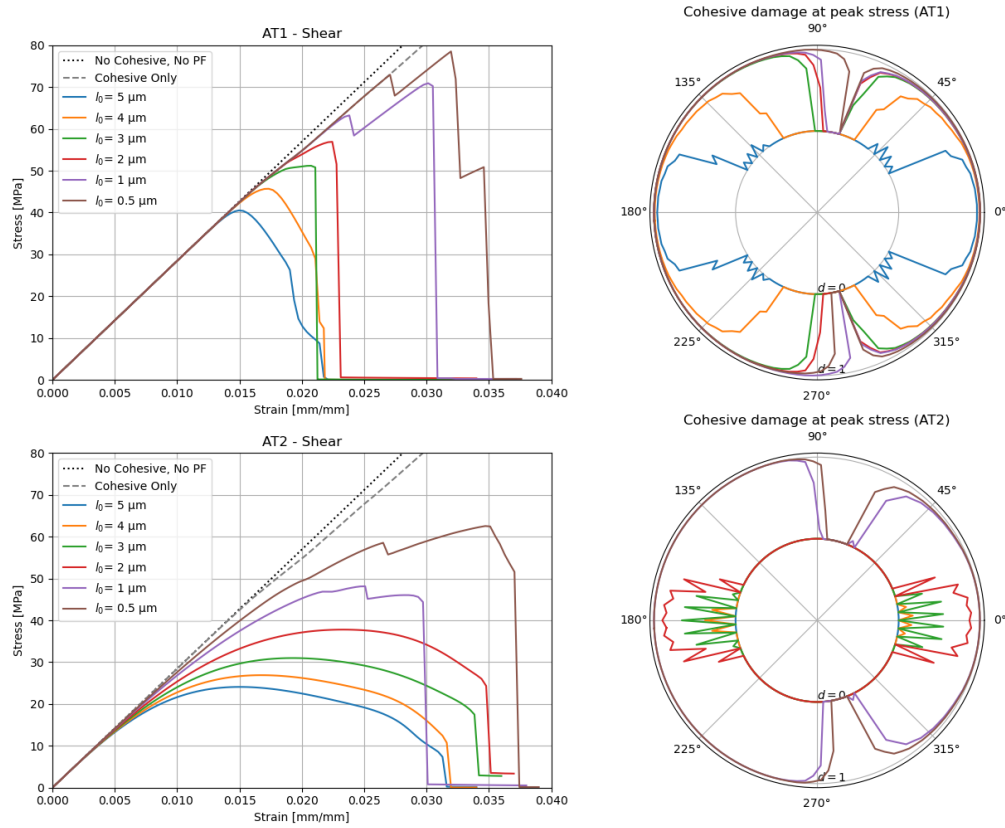


Figure 6.20: Stress-strain for AT1 and AT2 formulations under shear loading and different values of the length scale parameter l_0 .

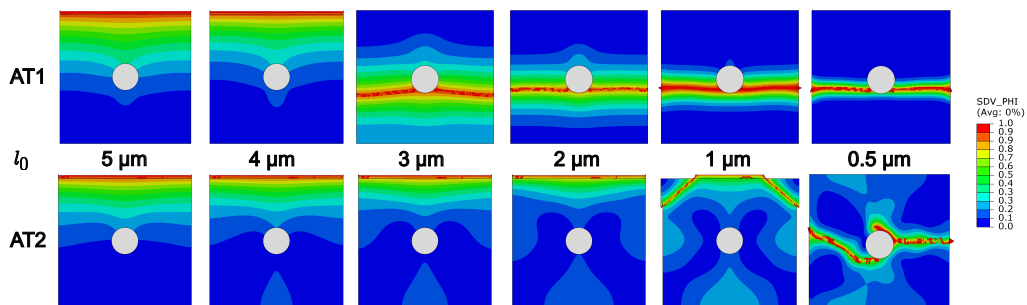


Figure 6.21: Crack patterns for AT1 and AT2 formulations under compressive loading and different values of the length scale parameter l_0 .

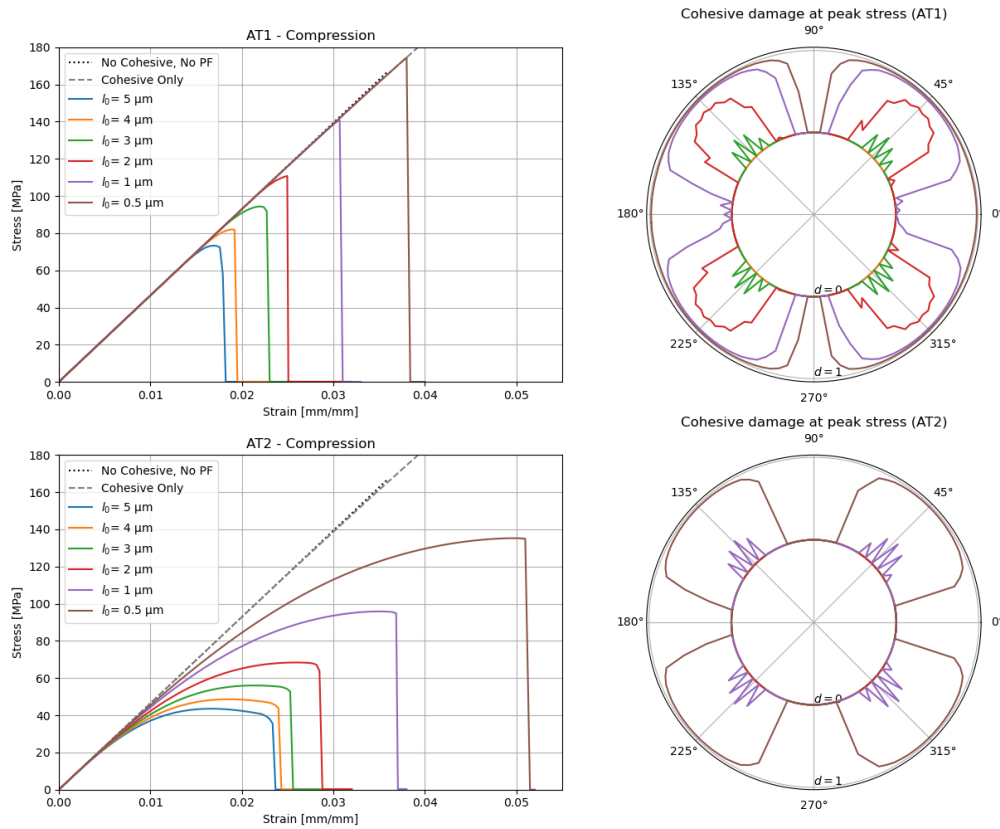


Figure 6.22: Stress-strain for AT1 and AT2 formulations under compressive loading and different values of the length scale parameter l_0 .

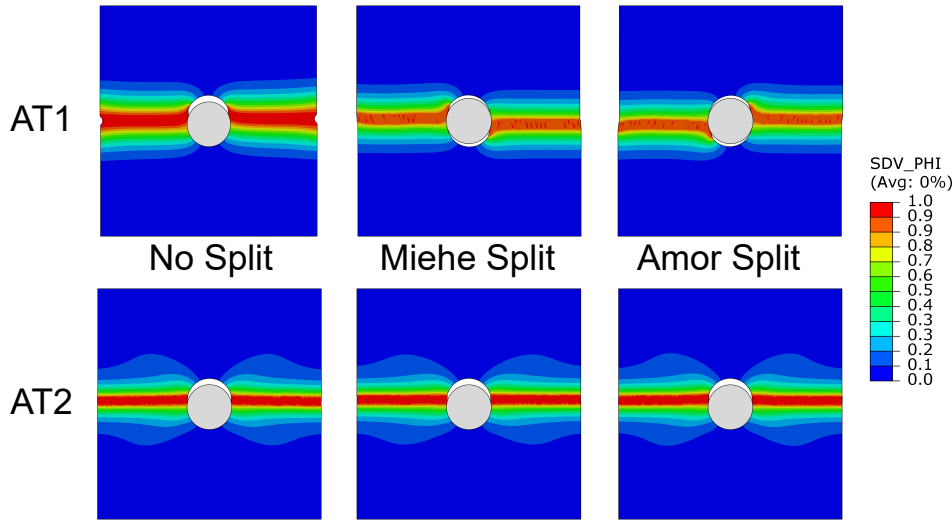


Figure 6.23: Crack patterns for AT1 and AT2 formulations under tensile loading and different energy splits.

6.3.3 PF formulation and energy split

The influence of the energy split is studied for the AT1 and AT2 formulations with Miehe and Amor energy splits and no energy splits. The mesh size is $0.25 \mu\text{m}$ and the material properties used for comparison are shown in Table 5.1. Again, the single fibre specimen is under tension, pure shear and pure compression loading imposed through displacement BC, as shown in Fig. 6.1.

The crack patterns are shown in Fig 6.23 and the stress-strain curves, alongside the polar plots of cohesive damage are shown in Fig 6.24 for tensile loading. Similar to the open-hole specimens, Amor's split and no split present almost identical results while Miehe's split delays crack propagation and reduces AT2 softening. In this case, the inclusion of the fibre and its interface imply a larger decohesion for Miehe's split. In addition, for the AT1 formulations Amor and Miehe's split seem to be more prone to asymmetrical responses as the crack patterns show in Fig 6.23. Decohesion is significant specially for the AT1 formulation, thus, fracture of the specimen takes place very close to the hole's centre.

The crack patterns are shown in Fig 6.25 and the stress-strain curves, alongside the polar plots of cohesive damage are shown in Fig 6.26 for shear loading. Again, decohesion is large and it is the first damage mechanism for the AT1 models. While for the AT2, overall softening is noticeable before interface damage takes place. Due to the large decohesion, the final resulting crack patterns are similar to the open-hole specimen. However, crack deviation due to the presence of the fibre is mainly noticed for Amor split and no split. Under this loading, Amor split and no split resemble but are not equal as in the case of the open-hole specimen. In particular, Amor split reduces the so called "snap back" while such phenomena is not present for Miehe's split.

The crack patterns are shown in Fig 6.27 and the stress-strain curves, alongside the polar plots

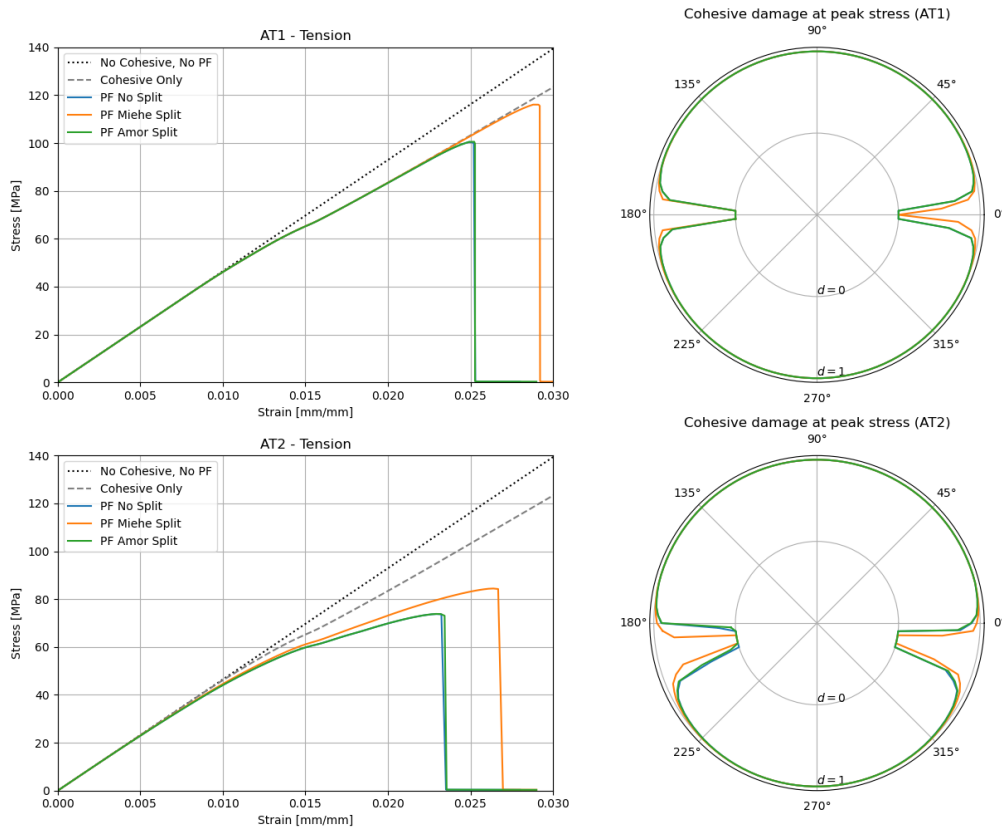


Figure 6.24: Stress-strain for AT1 and AT2 formulations under tensile loading and different energy splits.

of cohesive damage are shown in Fig 6.28 for compression loading. In this case, result vary significantly depending on the formulation as well as the energy split. The AT1 formulation nucleate cracks around the fibre, Amor split and no split create cracks in the direction perpendicular to the imposed displacement; this time the cracks are not centred as compared to the open-hole models instead they bend around the fibre, specially in Amor split. On the other hand, models with Mieke's split fracture in a diagonal direction going through the fibre regardless of the formulation.

In the AT2 formulation the crack nucleates around the hole only for Mieke's split. No split or Mieke's split create a crack on the top edge that makes a sharp turn away from the corners of the specimen. This effect is more pronounced in Amor split.

Stress strain response as well as decohesion patterns also vary significantly depending on the formulation and energy split. For AT1, no split creates a partial decohesion in a simetrical pattern in the vertical and horizontal axis. Amor split brings an increased cohesive damage and its simetry goes only with respect to the vertical axis. Finally, the decohesion in Mieke's split goes all around the fibre. Thus, matrix fracture occurs only in an equivalent open-hole specimen. For the AT2 formulation, significant decohesion is obtained only for Mieke's split, while Amor and no split heavily prevent the evolution of coherent interface damage.

Unlike the other loading scenarios, in this case, there is a clear difference in the strength based

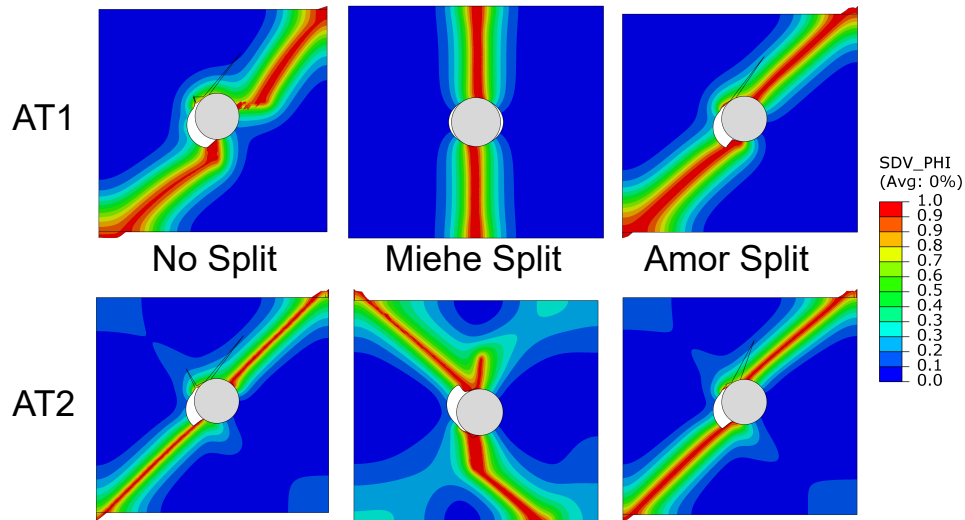


Figure 6.25: Crack patterns for AT1 and AT2 formulations under shear loading and different energy splits.

on the formulation. Fig 6.28 shows the highest strength in the case of Miehe's split, followed by Amor and the no split. This tendency is the same regardless of the formulation.

In all cases, the strength using Miehe's split is much larger. However, the difference increases as we move from tension, to shear and compression.

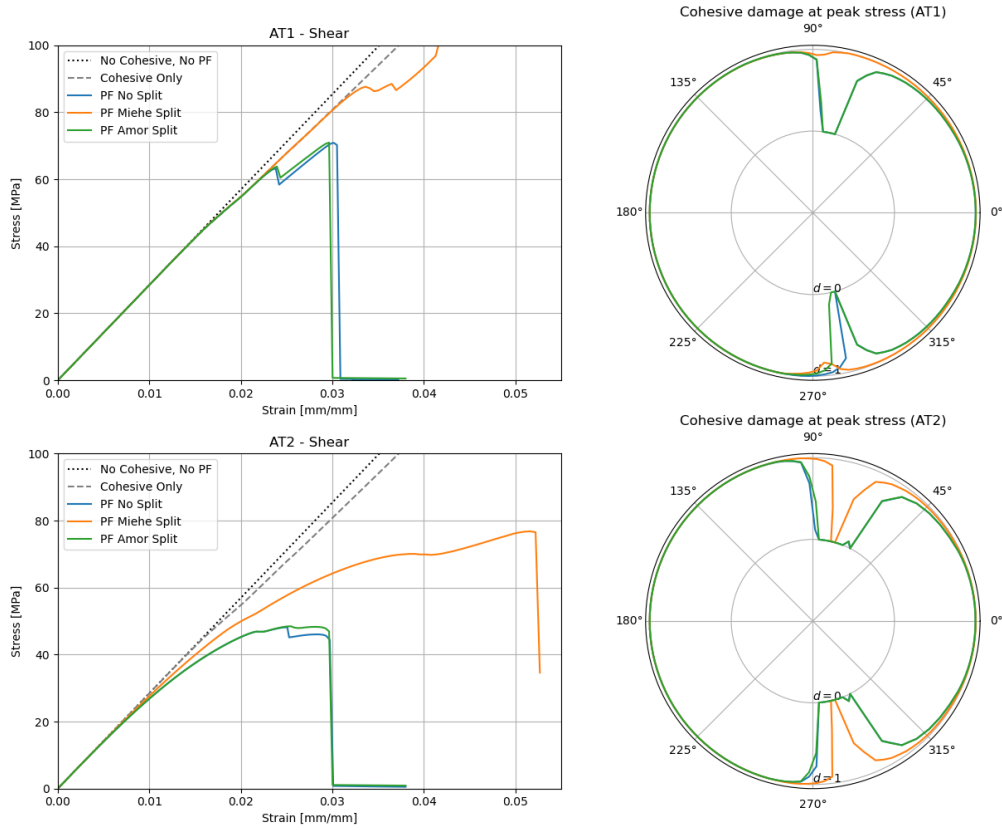


Figure 6.26: Stress-strain for AT1 and AT2 formulations under shear loading and different energy splits.

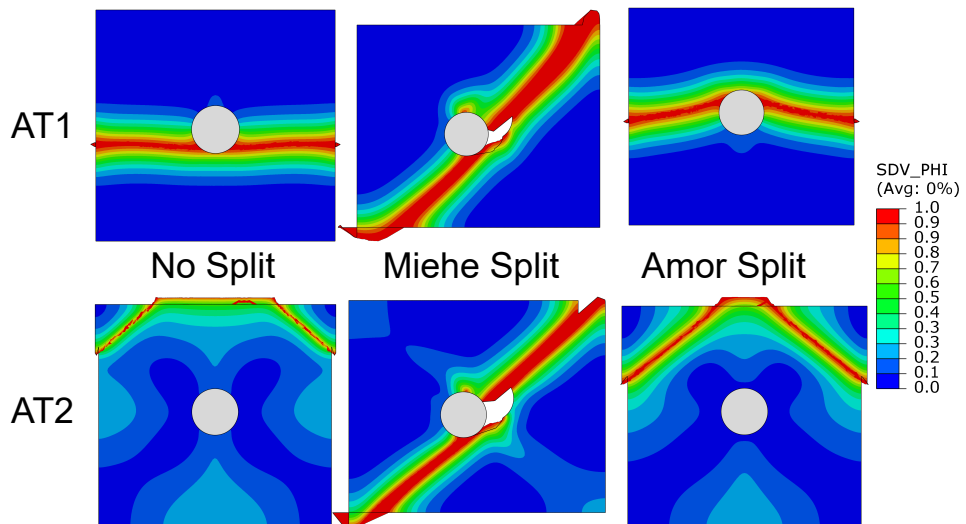


Figure 6.27: Crack patterns for AT1 and AT2 formulations under compressive loading and different energy splits.

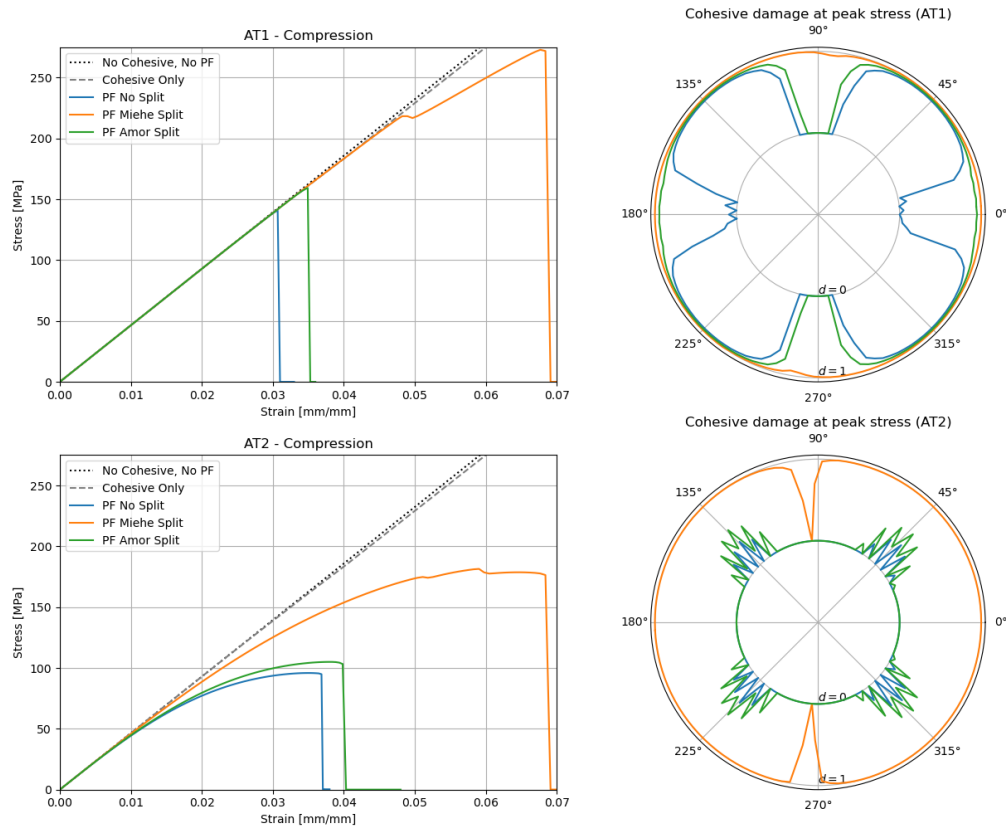


Figure 6.28: Stress-strain for AT1 and AT2 formulations under compressive loading and different energy splits.

6.4 Concluding remarks

This chapter presented a study of a single fibre model using cohesive damage around the fibre-matrix interface and PF damage in the matrix. Mesh convergence was verified once again in the case of the models accounting only for cohesive damage as well as cohesive and PF damage. It is clear that mesh size requirements can vary if PF or interface damage are considered and specially if they are applied simultaneously. Besides, even the loading condition can be an influencing factor of the mesh convergence.

The influence of the PF length scale, formulation and energy splits were also studied in detail under different loading conditions. From here, one of the main observations in the study of the length scale variation under tensile and shear loading is the fact that for large values of l_0 the crack takes longer to localize and global softening takes place even in the AT1 formulation. These cases highlight the potential problem of using PF in micromechanics. If the length scale is close to the geometric features of the model the behaviour is not as brittle as we should expect according to the PF theoretical background and damage is not sufficiently distributed as it would be expected in CDM. This ambiguity can be amplified or diminished based on the loading scenario, formulation and energy split that are considered.

Another main finding in this section, is the bulk material softening generated by the AT2 formulation. As the softening is initially concentrated around the fibre, it distorts the evolution of cohesive damage around it, creating interface damage distributions such as the zigzag that is shown in Fig. 6.16, Fig. 6.20 and Fig 6.28. Such behaviour has not been reported so far in models that use cohesive damage combined with PF or CDM to predict damage in the matrix.

In this chapter, there is a detailed study of the effect of different parameters in a single fibre model using cohesive damage around the fibre-matrix interface and PF damage in the matrix. Such study can be used to further analyse and question some literature results [27]:

- There are some combination of parameters that can prevent fracture localization around the fibre, where the so-called "crack kink" [27] does not occur and it may invalidate the failure envelopes that can come as results of such studies.
- No fully symmetrical interface crack propagation was found to take place in tensile loading under any combination of parameters, unlike previous literature results [27]. Micromechanical analysis of a single fibre are extremely sensitive to small perturbations even if they are only given by mesh distribution. Thus, decohesion tends to snap to one of the sides.
- Finally, it was shown that all results are highly sensitive to the cohesive parameters, the PF formulation and energy split. Thus, conclusions maybe biased if a single combination of parameters and properties are used in the study of geometric variables or loading conditions.

In general, the AT1 formulation always predicts a stiffer response, and for shear and tension loading it is also tougher. In the case of the AT2 formulation, if crack localization is not promoted by the loading or geometry configuration, spread damage and excessive softening are presented.

So far, "*realistic*" crack patterns can be obtained for tensile and shear loading; in the case of compression, the use of an energy split is no guarantee of agreement with other numerical approaches.

Chapter 7

Phase-Field analysis of Representative Volume Elements (RVEs)

7.1 Introduction

In this chapter, all models use micro-scale dimensions where the fibre has 5 microns diameter (typical of carbon fibre and E-glass in thin-ply composites). The material and interface properties in all scenarios are the ones shown in Table 5.1 (unless stated explicitly), extracted from the micro-mechanical simulations used to cross-validate the failure criteria from the work of Camanho et al. [18] and from Refs. [14, 83]. The studies are performed using RVEs with 60% fibre volume fraction and the fibre distributions are generated using the random sequential absorption method already included in the software Digimat [180].

This chapter seeks to explore the accuracy of the AT1 and AT2 formulations combined with the different energy splits in comparison with meso-scale failure criteria. Therefore, in these formulations, the material strength is controlled by the length scale parameter l_0 , which is set to 1 μm for the linear-elastic AT1 and AT2 formulations. This yields a higher matrix strength than that given in Ref. [18]. Camanho et al. [18] used a matrix tensile strength of 93 MPa. This would imply a length scale of 3.8 μm for AT1 and 1.08 μm for AT2. However, as shown in previous chapters, there is a geometrical limitation given by the fibre dimensions, related to the fact that there is a minimum length scale required to simulate crack localization, which can also be promoted, or prevented, by the boundary conditions, PF formulation and even the energy split. The length scale can be gradually reduced to achieve a more crack-like fracture pattern, but it would come at the cost of a potential overestimation of the material strength. This has shown that for standard PF formulations there is a geometrical bias imposed by the micro-scale dimensions on the length scale parameter that can influence the material strength.

In all cases, the UEL implementation described in Chapter 5 is used for 2D plane strain elements and the infinitesimal deformation assumption is considered. To overcome convergence issues, the *staggered* solution scheme is used, following a sensitivity study of the minimum required time step to obtain time-step independent results previously to all analyses. Besides, the

studies of the different energy splits were done using a "hybrid" implementation. The geometries and loading are such that the analysis is performed in the direction transverse to the fibre, so only transverse normal loading and shear are applied (22, 33 and 23 directions). Cohesive surface interaction is used to model fibre-matrix interface damage with a bilinear behaviour and the Benzeggagh-Kenane (BK) fracture criteria. The surface interaction also accounts for normal contact after complete decohesion but without considering friction. Besides, periodic boundary conditions are used, considering the dependence on the RVE size which is studied for different loading conditions.

Similar to Chapter 6, first there is an analysis assuming cohesive damage is the only source on non-linearity. In this chapter mesh convergence as well as influence of the RVE size is studied. Then PF damage is included in the matrix and similar studies are performed. In addition, there is an assessment of the influence of the PF formulation, energy split and of length scale in the variation of the computed failure envelopes.

In this chapter, the *global stress-strain* curves are the main source for comparison and evaluation. The term *global stress* refers to the stress computed from the reaction loads on the edges of the RVE divided by its transversal area. In the same way, the *global strain* is computed from the displacement of the reference node divided by the side-length of the RVE. Thus, we are following the methodology in [12, 133, 82, 136, 31, 30, 7, 181] in contrast to [131, 114, 44, 111, 115], that compute average values from integration points within matrix and fibres. In addition to stress-strain curves and fracture patterns, we have included *plots of distributed cohesive damage*. These plots show the percentage of the cohesive surfaces that have reached values of damage higher than 95%. It means, these plots show from the total interface perimeter, how much of the interface has reached critical damage for a given state of deformation.

As explained before, a 2D plane strain model representing a transverse random fibre distribution with periodic BCs is employed, and a σ_{22} – σ_{23} loading is applied in an RVE according to Fig. 7.1. Thus, from this point the results from a single fibre distribution may not be fully representative in many of the analyses at hand. Therefore, we have decided to present the mean values from six different distributions on RVEs of the same size for analysis of RVE size and the computation of failure envelopes.

It should be clear that, at this point, there is no rigorous qualitative comparison with experimental data, as the required data is not available. Namely, there is no source of verified micro-scale properties that come alongside the macro-scale measurements for the exact same material systems tested in the required loading scenarios. Therefore, "*verification*" is limited to the comparison with the failure envelope given in Camanho et al. [18] and qualitative comparison with some other approaches. Then, the failure envelope obtained using the criteria proposed by Camanho et al. [18] considered as the reference result, is obtained by solving:

$$\alpha_1 I_1 + \alpha_2 I_2 + \alpha_3 I_3 + \alpha_{32} I_3^2 - 1 = 0 \quad (7.1)$$

where:

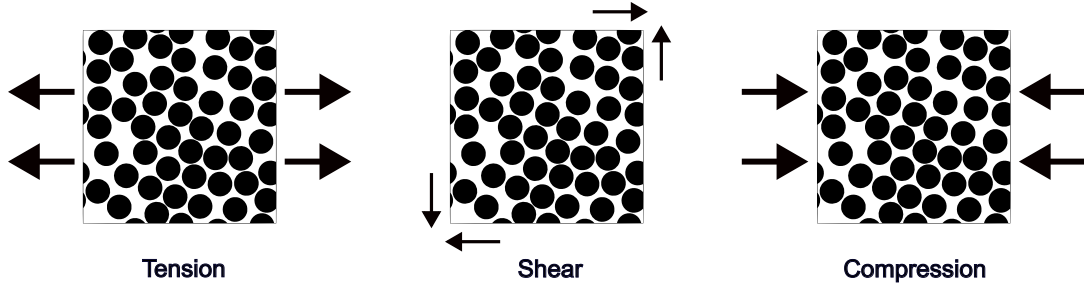


Figure 7.1: Schematic BC for the Composite RVE under tensile, shear and compressive loading.

$$\begin{aligned}
 I_1 &= \frac{1}{4}\sigma_{22}^2 - \frac{1}{2}\sigma_{22}\sigma_{33} + \frac{1}{4}\sigma_{33}^2 + \sigma_{23}^2 \\
 I_2 &= \sigma_{12}^2 + \sigma_{13}^2 \\
 I_3 &= \sigma_{22} + \sigma_{33} \\
 \alpha_1 &= \frac{1}{S_T^2} \\
 \alpha_2 &= \frac{1}{S_L^2} \\
 \alpha_3 &= \alpha_3^t = \frac{1}{2Y_{BT}} - 2\alpha_{32}^t Y_{BT} \text{ if } I_3 > 0 \\
 \alpha_3 &= \alpha_3^c = \frac{1}{2Y_{BC}} - 2\alpha_{32}^c Y_{BC} \text{ if } I_3 \leq 0 \\
 \alpha_{32} &= \alpha_{32}^t = \frac{1 - \frac{Y_T}{2Y_{BT}} - \alpha_1 \frac{Y_T^2}{4}}{Y_T^2 - 2Y_{BT}Y_T} \text{ if } I_3 > 0 \\
 \alpha_{32} &= \alpha_{32}^c = \frac{1 - \frac{Y_C}{2Y_{BC}} - \alpha_1 \frac{Y_C^2}{4}}{Y_C^2 - 2Y_{BC}Y_C} \text{ if } I_3 \leq 0
 \end{aligned}$$

Besides, S_T and S_L are respectively the transverse and in-plane shear strengths, Y_T and Y_C are respectively the transverse tensile and compressive strengths, and Y_{BT} and Y_{BC} are respectively the biaxial transverse tensile and compressive strengths, obtained from computational micro-mechanics [18]. This analytical model, which predicts the strength of homogenized transversely isotropic fibre-reinforced composites for multiaxial stress states, has been validated through direct comparison with experimental data from the literature for several polymer-matrix composite materials. For that reason, it is used to benchmark the predictions of the micro-mechanical simulations that employ the phase-field method to model fracture of the polymer matrix. A similar approach is proposed by Camanho et al. [18] to perform cross-validation of the analytical model and computational micro-mechanics. Hence, in the present work, the failure criteria proposed by Camanho et al. [18] is compared with the PF analyses using the AT1 and AT2 formulations without energy split, with Amor's split [66] and with Miehe's split [67]. In addition, the initial sections of this chapter depict curves of "*cohesive interface damage only*", which is an analysis that is added to delimit the influence where the load drop used to estimate the composite strength is dominated by fibre-matrix decohesion. This curves are computed using RVEs where the matrix is considered linear elastic and no matrix damage is accounted for, with the load drop exclusively dominated by the sudden accumulation of decohesions. The purpose is to show that, if the strength of the matrix is very high due to the value of the length scale parameter, due to the formulation, or due to the energy split, the matrix behaviour loses relevance because the whole phenomenon is dominated by the fibre-matrix interface strength and fracture toughness.

7.2 Cohesive interface damage only

As mentioned in the introduction, the first mesh convergence study as well as the sensitivity analysis of the RVE size are initially done considering linear elastic material model in both the matrix and the fibre, and using cohesive interface damage under pure tension, pure shear and pure compression imposed through periodic BC, as shown in Fig. 7.1. Thus, at this stage the only source of non-linear behaviour is the decohesion of the fibre inside the matrix.

7.2.1 Mesh convergence

For the mesh convergence study, a single RVE distribution of 25 μm square side is used to compute the *global stress-strain* curves alongside the *plots of distributed cohesive damage* which are shown in Fig 7.2, Fig 7.3 and 7.4 for tensile, shear and compression loading respectively. Purely linear elastic models ($\sigma_{I0/II0} = \infty$, $G_{Ic/IIc} = \infty$), it means, models that do not considering cohesive damage were also ran using the smallest mesh size in order to better appreciate the deviation from linearity due to the effect of the cohesive damage in the global stiffness degradation. In addition, these plots depict a comparison of the mesh convergence using elements of different degrees of interpolation. As it will be shown later, only quadratic formulations allow reasonable mesh sizes given the properties and geometry at hand.

The first thing to notice is that, the required minimum element type to reach mesh convergence is highly dependent on the loading scenario and not just on the degree of interpolation of the element. Taking the elements of linear interpolation as reference, while for compressive loading, the results overlap for mesh sizes lower than 0.5 μm , tensile loading requires a minimum element size of 0.25 μm to obtain mesh independent results. However, for shear loading the minimum element type can be as low as 0.1 μm . Larger mesh sizes usually yield inconsistent results as they overestimate the stiffness even though the percentage of decohesion is larger as well.

From these initial results, several observations can be made. First, there is an initial deviation from linearity that coincides with the raising point of the "percentage of cohesive damage over 0.95 in the RVE" curve, which indicates that this metric is appropriate to display significant or representative levels of cohesive damage in the RVE. On the other hand, it is possible to see that tensile and shear loading display a global maximum or peak stress. However, the percentage of cohesive damage to reach this critical point is load-dependent, being larger in shear than in tension. In the case of compressive loading, there is no local maximum but rather, the critical stress and strains are defined based on the inflection point of the stress-strain curves. Such inflection point is reached only at very large percentages of cohesive damage. In fact at this stage, a non-linear analysis would probably result in geometric bucking of the RVE. The same trend can be seen from the deviation of the results with respect to the reference strength of Camanho et al. [18]. It means, the deviation is larger as loading moves from tension to shear and then to compression. This topic is analysed in more detail in the computation of failure envelopes in the following sections.

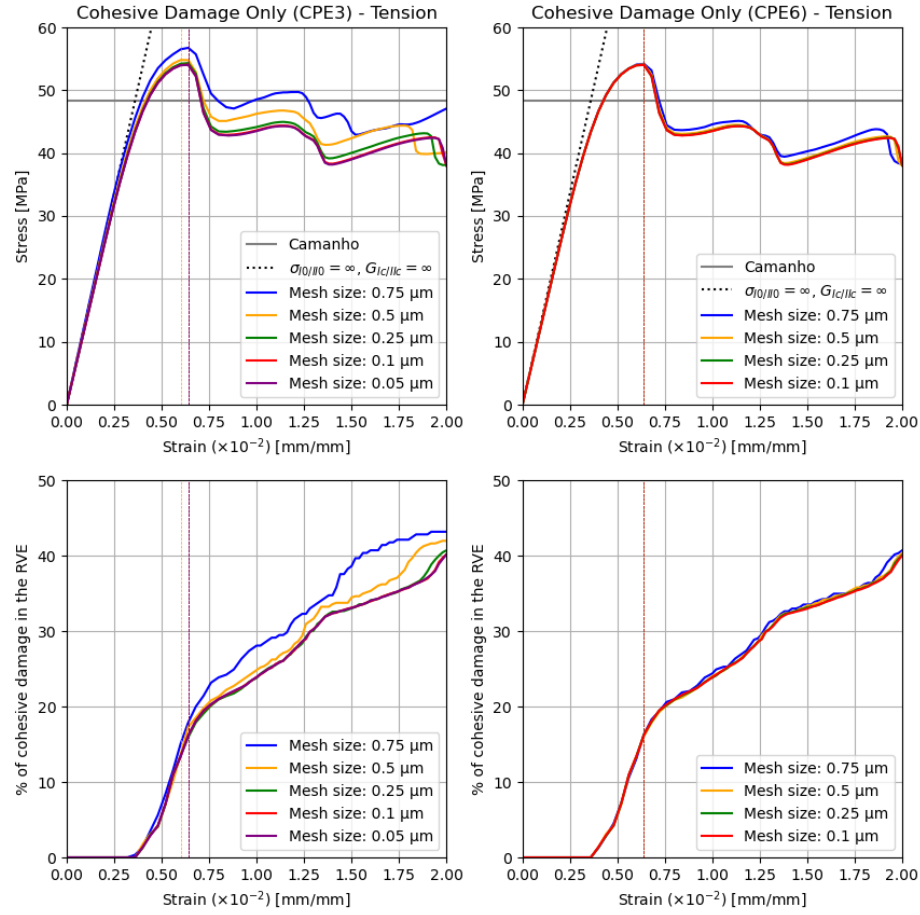


Figure 7.2: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection ($\sigma_{I0/II0} = \infty, G_{Ic/IIc} = \infty$) compared to models considering a damageable cohesive interface. Different mesh sizes were used for the RVE specimen under tensile loading in Fig. 7.1 a). Vertical lines indicate the strains at peak stresses.

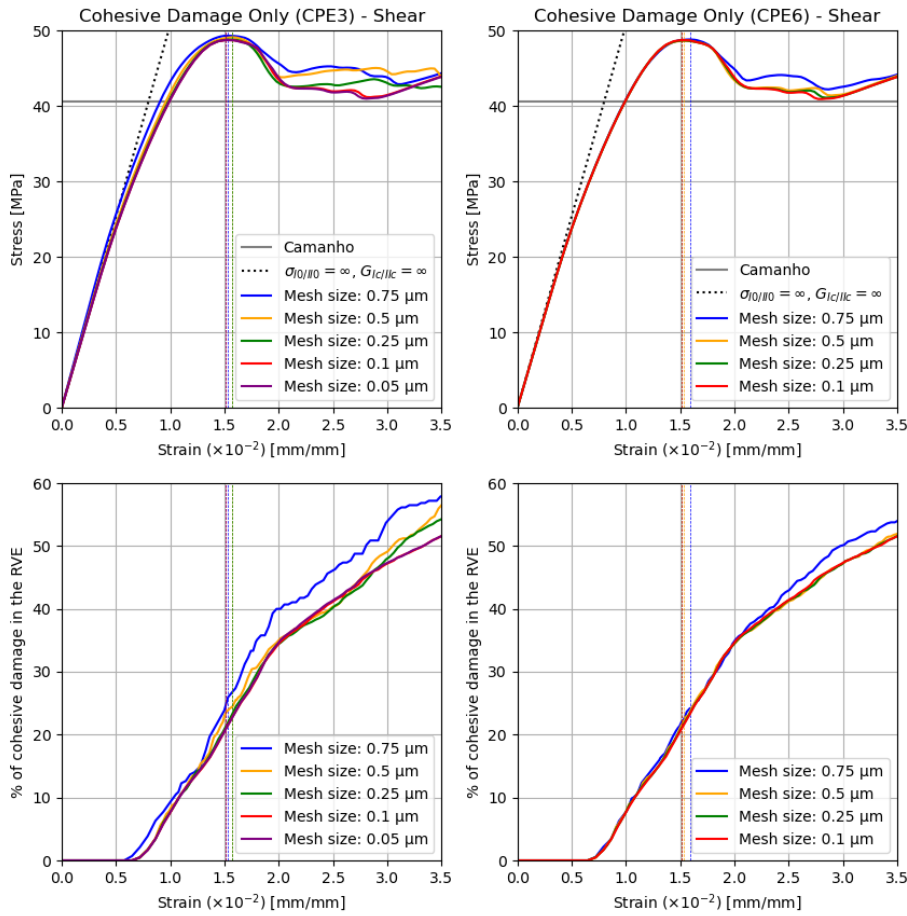


Figure 7.3: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection ($\sigma_{I0/II0} = \infty$, $G_{Ic/IIc} = \infty$) compared to models considering a damageable cohesive interface. Different mesh sizes were used for the RVE specimen under shear loading in Fig. 7.1 b). Vertical lines indicate the strains at peak stresses.

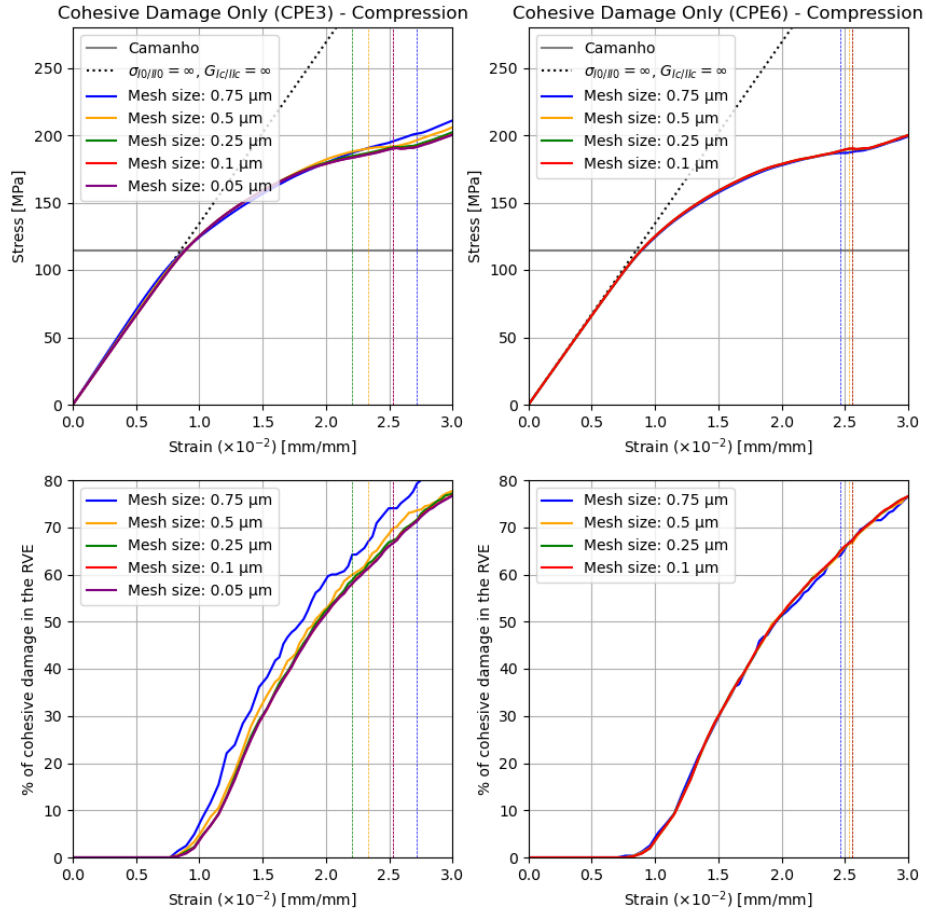


Figure 7.4: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection ($\sigma_{I0/I10} = \infty$, $G_{Ic/I1c} = \infty$) compared to models considering a damageable cohesive interface. Different mesh sizes were used for the RVE specimen under compressive loading in Fig. 7.1 c). Vertical lines indicate the strains at the stress inflection points.

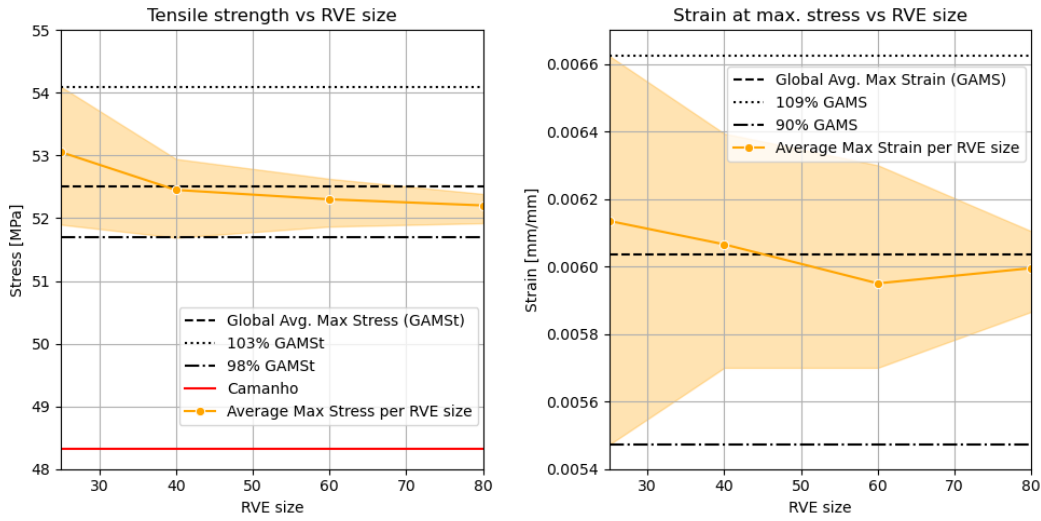


Figure 7.5: Evolution of tensile strength and strain at maximum tensile stress for different RVE sizes.

7.2.2 Influence of the RVE size

As mentioned in the bibliographic review, periodic boundary conditions cannot properly capture localization phenomena. Thus, in this subsection there is a study of the influence of the RVE size and dispersion of results given by different random distributions under different loading conditions. Fig. 7.5, Fig. 7.6 and Fig. 7.7 show the evolution of the strength and strain at peak stress for RVEs of size $25\ \mu\text{m}$ up to $80\ \mu\text{m}$ for different loading conditions. These plots show the results of six different fibre distributions for each RVE size. Thus, it is possible to depict both mean values as well as variation of the results for each RVE and the overall maximum and mean values for all 24 RVEs. In addition, the strength values given in Camanho et al. [18] are used for comparison.

For tension and shear loading the behaviour is asymptotic, namely, as the RVE size increases both dispersions narrow down and the mean values tend to diminish their oscillations. This is opposite to what happens in compression, when there is no clear trend as the RVE size increases. The reason for this behaviour is explained in later sections when PF damage is introduced. In all cases, the results overestimate the reference values given by Camanho et al. [18]. However, this is highly dependent on the loading scenario. It means, for tensile and shear loading the overestimation is much lower if compared to compression. Regarding the variability of the overall results, it is clear that the variation of stresses is much narrower than the variations of strains; the exact values are highly dependent on the loading type. However, one can see that the range of overall variation of strains is around double the overall variation of stresses in the best scenario.

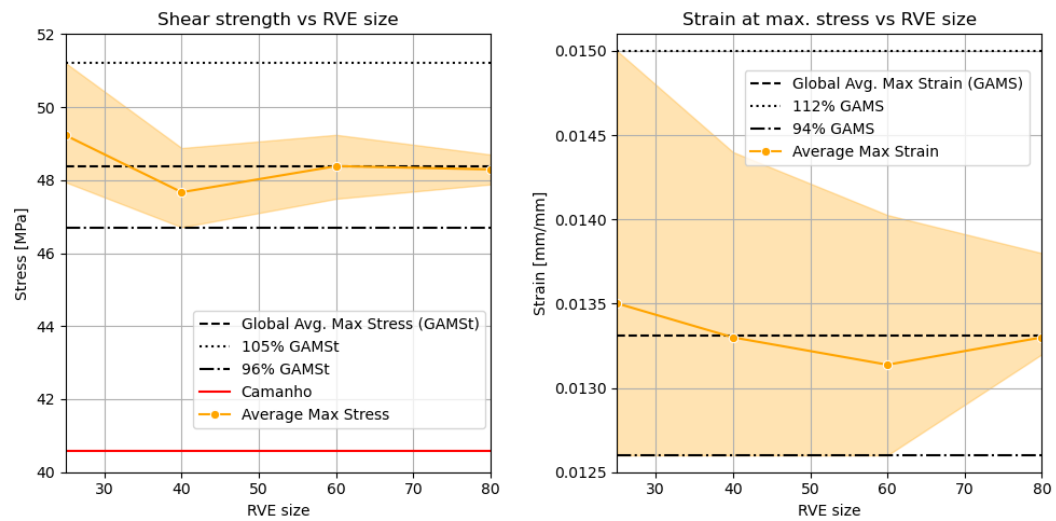


Figure 7.6: Evolution of shear strength and strain at maximum shear stress for different RVE sizes.

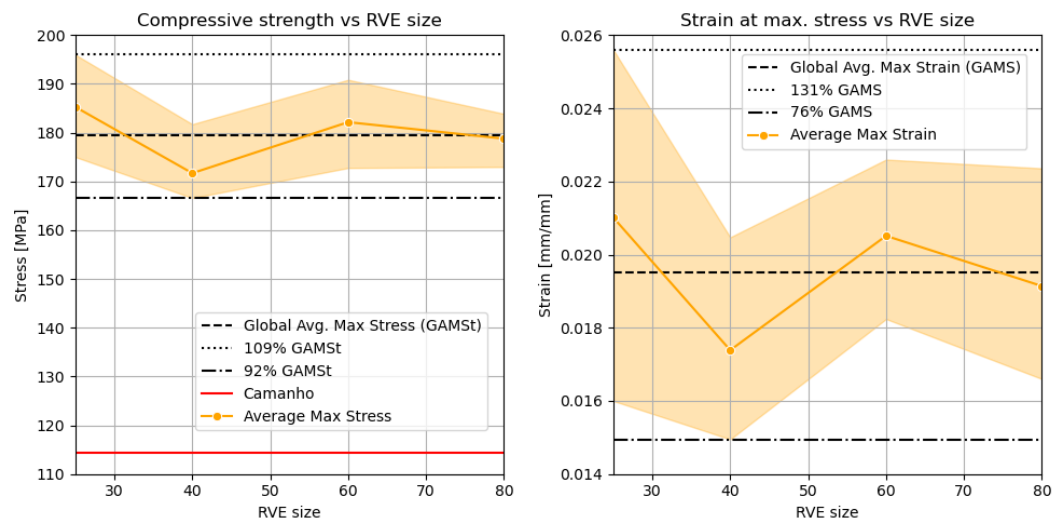


Figure 7.7: Evolution of compressive strength and strain at maximum compressive stress for different RVE sizes.

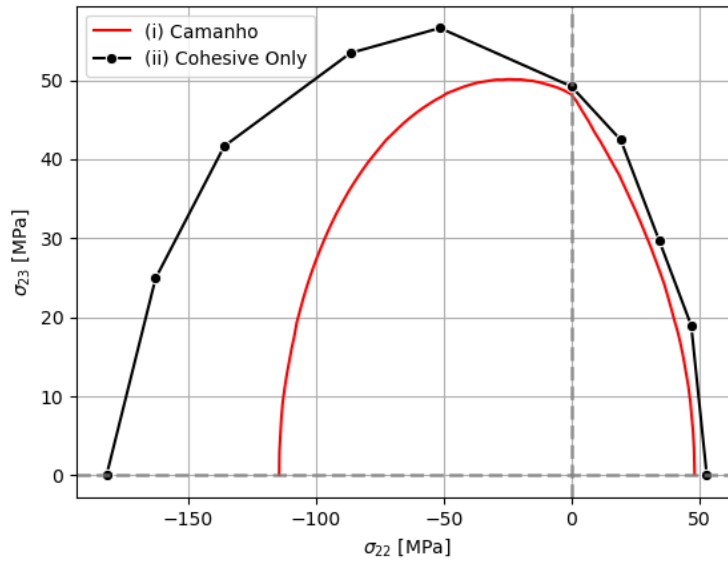


Figure 7.8: Failure envelopes of: (i) Camanho et al. [18] and (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only).

7.2.3 Failure envelopes

The first failure envelope that can be approximated is the one shown in 7.8. This failure envelope was computed using the RVE size of $25 \mu\text{m}$ and it is given as a reference or threshold for the analysis that follow in the inclusion of PF damage. Initially one can observe that Even though the failure envelope of Camanho et al. [18] is contained inside the "Cohesive only" envelope, the initial estimation yields close results in the tensile dominated region, as this is the area where decohesion is expected to be the main failure trigger of the RVE. On the other hand, the curve of the initial estimation opens up much more in the compressive region if compared to the reference envelope. The inclusion of a matrix damage model plays a mayor role in the "correction" of such initial overestimation.

7.3 Cohesive interface damage and Phase-Field fracture

For the RVE analysis using PF for matrix bulk damage and cohesive damage of the fibre-matrix interface, a study on the mesh convergence is initially performed in order to estimate the required mesh size. Then, the RVE size influence is assessed to estimate the dimensions required to obtain representative strengths and maximum strain values. Once the minimum size is defined, a comparative study using the results of the analytical model of Camanho et al. [18] is used to verify the predictive capabilities of the different energy splits and PF formulations. The influence of the length scale parameter and interface cohesive interaction is also analysed in order to verify the accuracy of all the assumptions within this methodology.

7.3.1 Mesh convergence

For the mesh convergence study, a single RVE distribution of $25\ \mu\text{m}$ square side is used to compute the *global stress-strain* curves alongside the *plots of distributed cohesive damage*. Purely linear elastic models (*No Cohesive, No PF*), it means, models that do not considering cohesive or PF damage were also ran using the smallest mesh size in order to better appreciate the deviation from linearity due to the effect of the cohesive damage in the global stiffness degradation. In addition, models using only cohesive interface damage (*Cohesive only*) are also plotted in order to better appreciate the moment at which point in the deformation PF damage becomes truly relevant in the global RVE response. For tensile loading the results are shown in Fig 7.9 and Fig 7.10 using elements of linear (CPE3) and quadratic (CPE6) formulation respectively. In this case, mesh convergence is achieved for a mesh size of $0.5\ \mu\text{m}$ regardless of the element formulation. Larger mesh sizes, overestimate the peak stresses and the amount of cohesive damage. Under tension loading, it is clear that the initial softening, stress peak and first load drop is fully controlled by cohesive damage regardless of the PF formulation. Up to 0.75×10^{-2} normal strain, the stress-strain curve and cohesive damage distribution is exactly the same for all models that account for cohesive damage. PF becomes relevant only as a post peak behaviour when the accumulation of cohesive cracks coalesce into a single transversal crack through the matrix. In this case, there is no spurious global softening due to the AT2 formulation as compared with single fibre models.

For shear loading the results are shown in Fig 7.11 and Fig 7.12 using elements of linear and quadratic formulation respectively. In this case, mesh convergence is different depending on the PF and element formulations. Namely, for linear elements and the AT1 formulation the minimum element size is $0.1\ \mu\text{m}$, while for the AT2 formulation a mesh size lower than $0.25\ \mu\text{m}$ suffices. On the other hand, for elements with a quadratic formulation, if the AT1 model is used, the mesh needs to be at least $0.25\ \mu\text{m}$, while for AT2 $0.5\ \mu\text{m}$ is enough. Thus, in general, AT1 models require smaller mesh sizes, and quadratic elements achieve mesh convergence faster. Furthermore, one can already see that for this loading scenario, interface damage still plays a major role. However, matrix behaviour becomes more relevant as now PF is responsible for a more drastic load drop in the case of AT1 and increased global softening in the case of AT2. One of the immediate causes

of global softening in the AT2 formulation is the prediction of lower peak stresses and reduced cohesive damage in the whole RVE.

Finally, for compression loading the results are shown in Fig 7.13 and Fig 7.14 using elements of linear and quadratic formulation respectively. In this case, similar to shear loading, mesh convergence is different depending on the PF and element formulations. For linear elements and the AT1 formulation the minimum element size is at least $0.05 \mu\text{m}$, while for the AT2 formulation the mesh size should be $0.1 \mu\text{m}$ or lower. On the other hand, for elements with a quadratic formulation, if the AT1 model is used, the mesh needs to be at least $0.25 \mu\text{m}$, while for AT2 $0.5 \mu\text{m}$ is enough. For this type of load, distributed cohesive damage is much smaller, thus, the role of matrix behaviour is more relevant and can even dominate the global response. For the AT1 formulation, softening before the load drop is only due to cohesive damage, while for the AT2 formulation, global softening is a consequence of the combined action of cohesive distributed damage and local softening inherent from AT2.

In general, as loading moves from pure tension to shear and then to compression, matrix behaviour starts to play a major role compared to the influence of interface damage. This tendency comes from a reduced amount of distributed cohesive damage and an increased global softening in the RVE as loading changes from tension to shear and then to compression. As matrix behaviour becomes more relevant, mesh size dependency is altered in a similar fashion, reduced mesh sizes are required for compression, than for shear and tension. Finally, it is worth to notice that while deviation from linear behaviour in the AT1 models is always due to cohesive damage; for the AT2 models, such deviation is also due to PF damage. However, it is present only for shear and compressive loading. softening under tensile loading is always fully dominated by cohesive damage, matrix fracture plays a minor role.

After this study, it is concluded that for the remaining analyses of this work the use of quadratic elements with a mesh size of $0.2 \mu\text{m}$ should give the desired accuracy and it should be free from mayor inaccuracies due to mesh dependency.

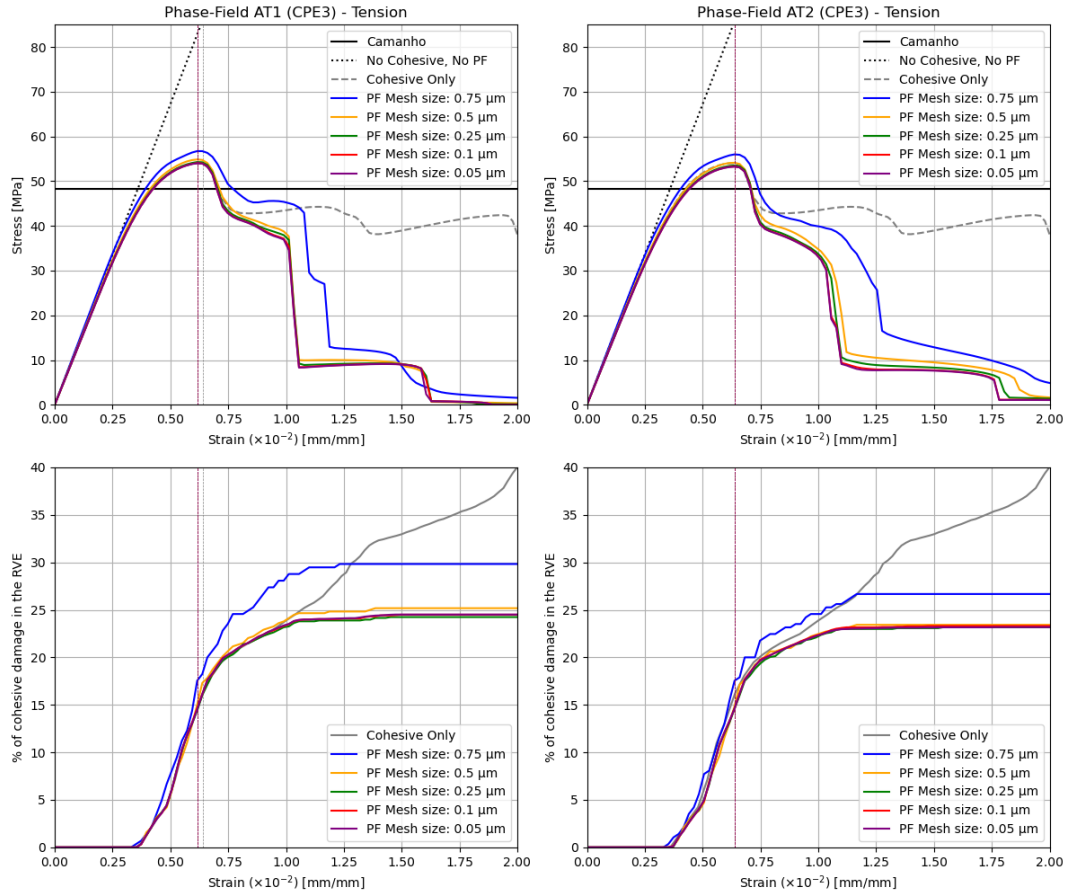


Figure 7.9: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage. Different mesh sizes were used for the RVE specimen under tensile loading in Fig. 7.1 a) using a linear element formulation. Vertical lines indicate the strains at peak stresses.

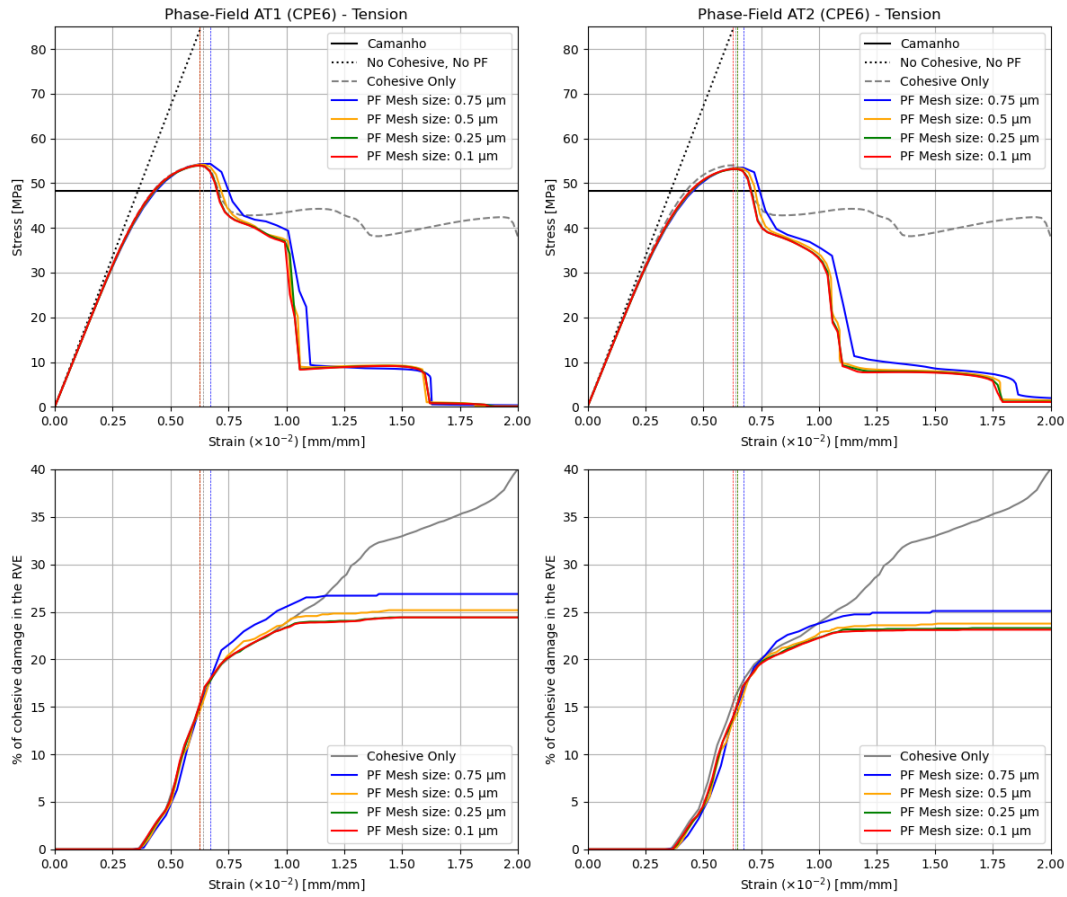


Figure 7.10: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage. Different mesh sizes were used for the RVE specimen under tensile loading in Fig. 7.1 a) using a quadratic element formulation. Vertical lines indicate the strains at peak stresses.

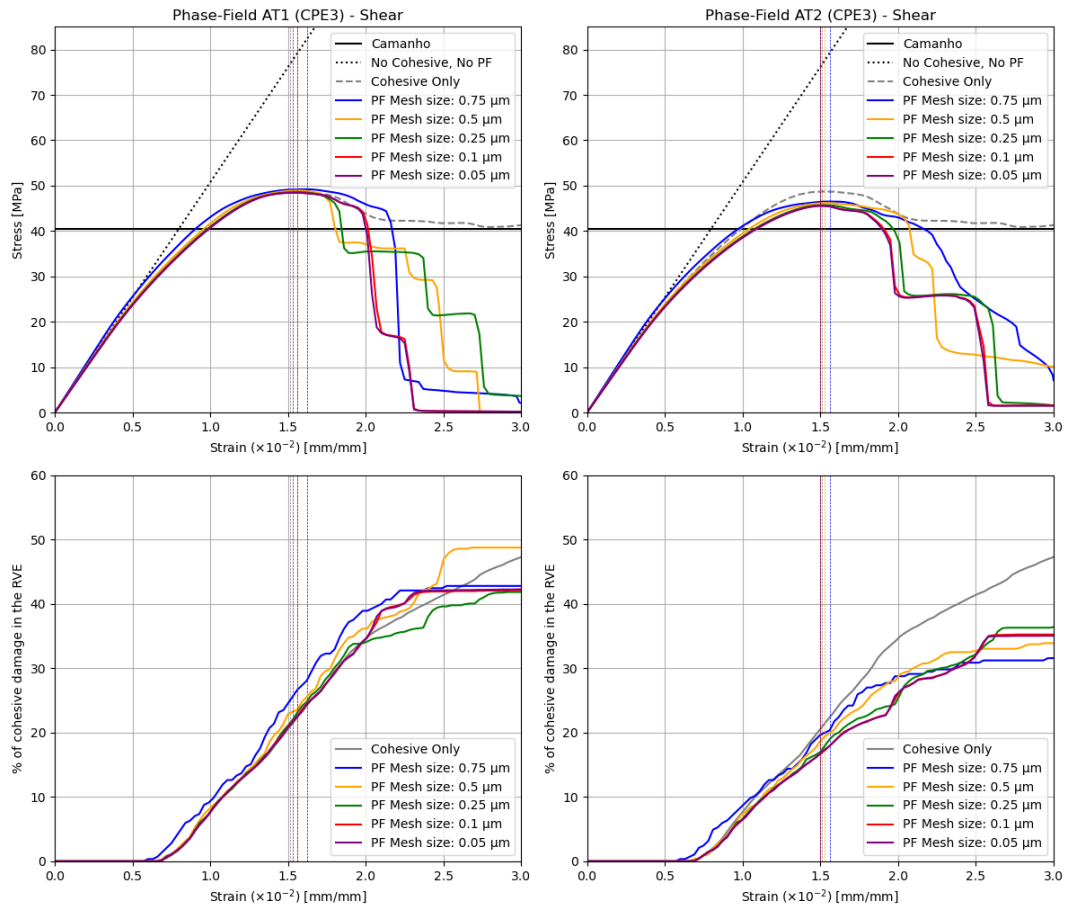


Figure 7.11: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage. Different mesh sizes were used for the RVE specimen under shear loading in Fig. 7.1 b) using a linear element formulation. Vertical lines indicate the strains at peak stresses.

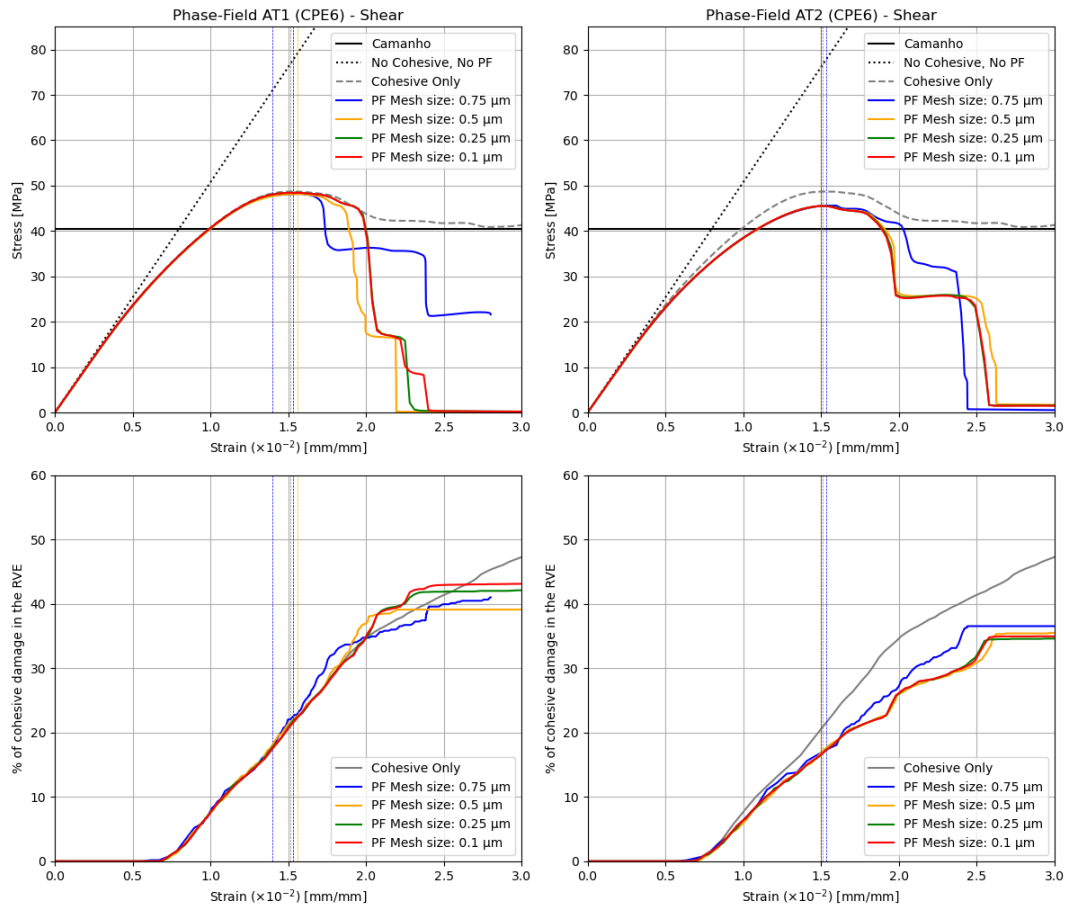


Figure 7.12: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage. Different mesh sizes were used for the RVE specimen under shear loading in Fig. 7.1 b) using a quadratic element formulation. Vertical lines indicate the strains at peak stresses.

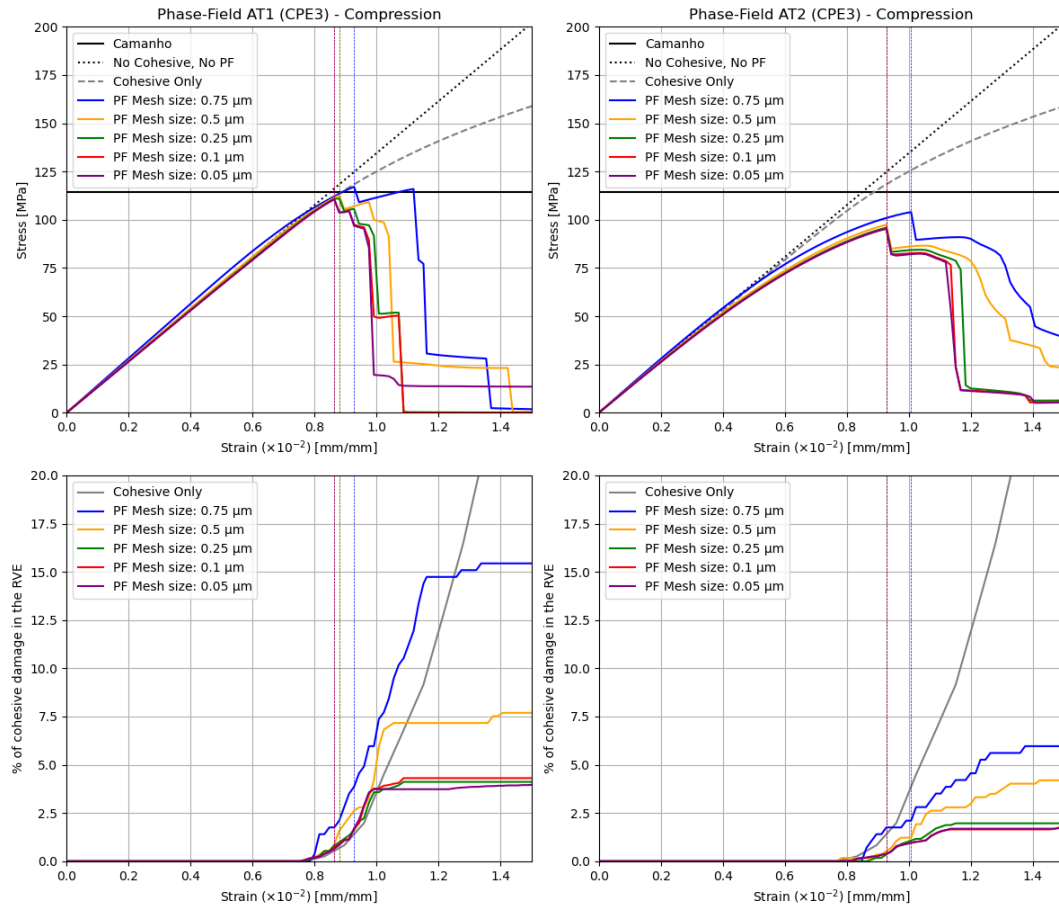


Figure 7.13: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage. Different mesh sizes were used for the RVE specimen under compressive loading in Fig. 7.1 c) using a linear element formulation. Vertical lines indicate the strains at peak stresses.

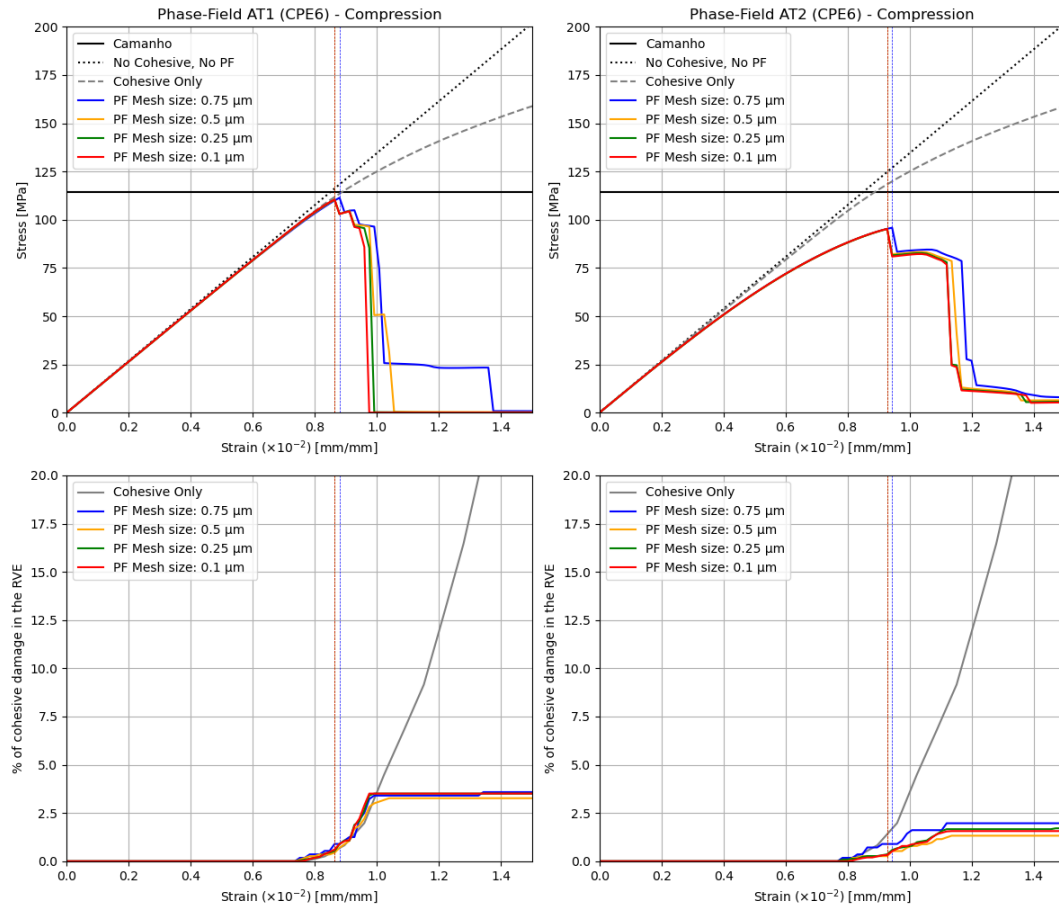


Figure 7.14: Stress-strain curves and plots of distributed cohesive damage for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage. Different mesh sizes were used for the RVE specimen under compressive loading in Fig. 7.1 c) using a quadratic element formulation. Vertical lines indicate the strains at peak stresses.

7.3.2 Influence of the RVE size

To estimate the minimum size that can be used and to obtain meaningful strength and maximum strain measurements, transverse tensile, shear and compressive deformation are applied on square RVEs of side length from $25\ \mu\text{m}$ (RVE size close to the one used by Espadas-Escalante et al. [29]) to $80\ \mu\text{m}$, or from a ratio $L/r_{\text{fibre}} = 10$ to $L/r_{\text{fibre}} = 32$, where L is the length of the sides of the RVE and r_{fibre} is the fibre radius. In this example, only the AT1 formulation with Miehe's energy split is used. For each value of L/r_{fibre} , six different random distributions are generated and simulated. From that, average, minimum and maximum values of strength and strain at peak stress are plotted for RVE size as well as for all the RVE that were tested. The plots are shown in Fig. 7.15, Fig. 7.16 and Fig. 7.17 for tensile, shear and compressive loading respectively. The values of strength and strain at peak stress for the largest RVEs where only small variation is obtained by increasing the size of the RVE are called "*asymptotic values*", which are considered to be the most accurate approximation obtained. The strength predictions in tensile loading do not match the strength predicted by Camanho et al. [18] using computational micro-mechanics, see Fig. 7.15. An overestimation of 8% is observed even for the largest RVEs. In addition, the average value has an asymptotic behaviour with the increase of the RVE size. This behaviour is expected as it follows the trend observed in the results of Van der Meer [133]. The results presented in Ref. [133] showed that the variation of the average strain from a small RVE to the asymptotic value can reach 7% which is still lower than the variation obtained by RVEs of medium size. In the present results, this is also the case for the predicted strength, where a 2% variation of the average value with increasing RVE size is obtained. But the asymptotic value of strain at maximum stress has a 17% difference with respect to the smallest RVE size. Besides, the asymptotic value is outside the variability obtained in the smallest RVEs. This is expected as the stiffness of smaller RVEs after failure initiation is highly polluted by spurious gradual softening due to the periodic BC after damage onset.

The strength predictions in shear loading do not match the strength predicted by Camanho et al. [18] using computational micro-mechanics, see Fig. 7.16. An overestimation of 18% is observed for the largest RVEs. The maximum difference between the smallest and largest RVE size is 1 % for the strength and 0.06 % for the strains at peak stress. Thus, a very low variation of the results is obtained as the RVE size increases.

The strength predictions in compression loading also do not match the strength predicted by Camanho et al. [18] using computational micro-mechanics, see Fig. 7.17. An overestimation of 226% is observed for the largest RVEs. The maximum difference between the smallest and largest RVE size is 8 % for the strength and 9 % for the strains at peak stress. Thus, a significant variation of the results is obtained as the RVE size increases.

In compressive, shear and tensile loading, the scatter of the results narrows down and the average values tend to become smaller as the RVE size increases. Such decrease in the scatter and average values is more visible in the strains at peak stress than in the strength predictions. An "*asymptotic value*" is clearly reached in the case of tensile loading. However, such trend cannot be

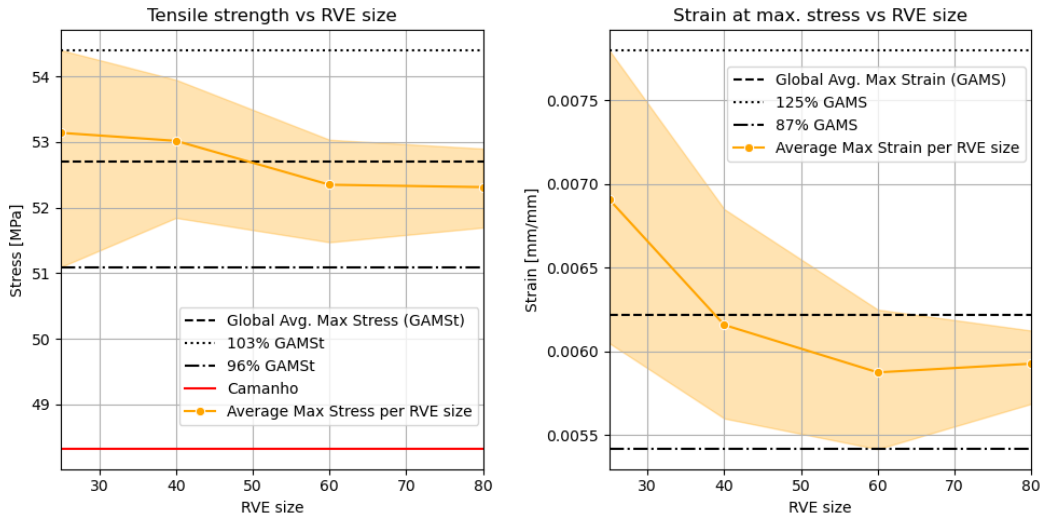


Figure 7.15: Maximum, minimum, average and standard deviation of (a) the peak stress values and (b) the strains at peak stress for different RVE sizes under tensile loading, Phase-Field AT1 formulation and Miehe's energy split.

immediately concluded from the strength plots for shear and compression loading (See Fig. 7.16 and Fig. 7.17). Therefore, these kind of loading scenarios may require even higher RVE size to reach results that can be considered fully independent from the RVE size. In general, these results agree with the conclusions of Trias et al. [111], showing that different metrics require different ratios L/r_{fibre} ; even though a square RVE of $25 \mu\text{m}$ side length can be enough for the prediction of maximum stress, the RVE size necessary to predict the strain to failure can be at least three times higher.

The representative stress-strain curves for each RVE size are shown in Fig. 7.18, Fig. 7.19 and Fig. 7.20 for tensile, shear and compressive loading respectively. These provide an overall representation of the difference in the post-peak behaviour as the RVE size increases. In all stress-strain curves, the strength reported by Camanho et al. [18] is also shown. As explained previously, smaller RVEs under shear or tensile loading tend to produce a more gradual failure, because the periodic BCs produce spurious interactions, especially if it is close to the edges of the RVE; it means that periodic BCs make a crack tip on one side to interact and even gets arrested by the tip of the same crack on the other side, see Fig. 7.21. This is why for small RVEs the last part of the stress-strain curves in Fig. 7.18 and Fig. 7.19 have a tendency to flatten. This effect clearly diminishes with the increase of the RVE size, but the behaviour is dominantly brittle only for the RVEs with $L = 80 \mu\text{m}$. These results clearly show the inadequacy of periodic BCs to model fracture in RVEs, supporting the claim of Coenen et al. [143] of the need for special kinematics that allow strain localization, especially within smaller RVEs. One particular issue that is more visible in compression loading than in the other loading scenarios, is that as periodic BC can delay crack propagation, the strength and strains at peak stress predictions can be highly underestimated for smaller RVEs, see Fig. 7.17. For compressive loading, the shape of the stress-strain curve is

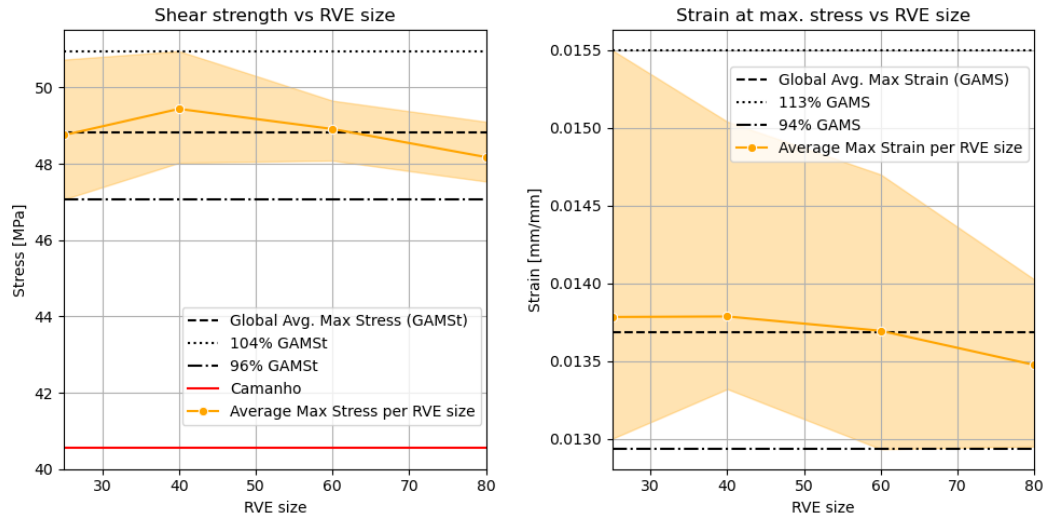


Figure 7.16: Maximum, minimum, average and standard deviation of (a) the peak stress values and (b) the strains at peak stress for different RVE sizes under shear loading, Phase-Field AT1 formulation and Miehe's energy split.

rather consistent. However, as the RVE size increases, the maximum stress and strain at peak load decrease, see Fig. 7.20.

Such unrealistic post-peak behaviour due to the periodic BCs renders the analysis of a single RVEs of small dimensions, e.g., $L/r_{\text{fibre}} = 10$ [29], not necessarily representative of the meso-scale composite behaviour. In fact, as it is shown in the results of Fig. 7.18, Fig. 7.19 and Fig. 7.20 if periodic BCs are used, the post-peak behaviour is highly affected by the size of the RVE, as well as the PF formulation and energy split. In addition, if the fibre distribution is randomly generated, a large variability in post-peak behaviour can be observed, especially if values of L/r_{fibre} are small. As shown in Fig. 7.22, where the meso-scale stress-strain curves of six RVEs with different random fibre distributions are plotted for $L/r_{\text{fibre}} = 10$ using the AT1 formulation and Miehe's split [67]. In this figure, it is shown that some fibre patterns yield an "apparent" tougher material response, while others could be seen as more brittle. Another important aspect is the fact that cohesive interface damage in such small RVEs can also promote gradual failure, while assuming a perfect fibre-matrix interaction [29] can promote a more brittle behaviour, yielding sharper stress-strain curves (this is further explored in the following sections). Finally, it should be noted that, despite the recent efforts to define appropriate boundary conditions in the presence of localization [143, 182, 183], the complex, interacting failure mechanisms observed in composite laminates still pose challenges to the definition of accurate boundary conditions for RVEs after localization takes place. This is a particularly relevant problem for multiscale analysis where information is transferred between different scales.

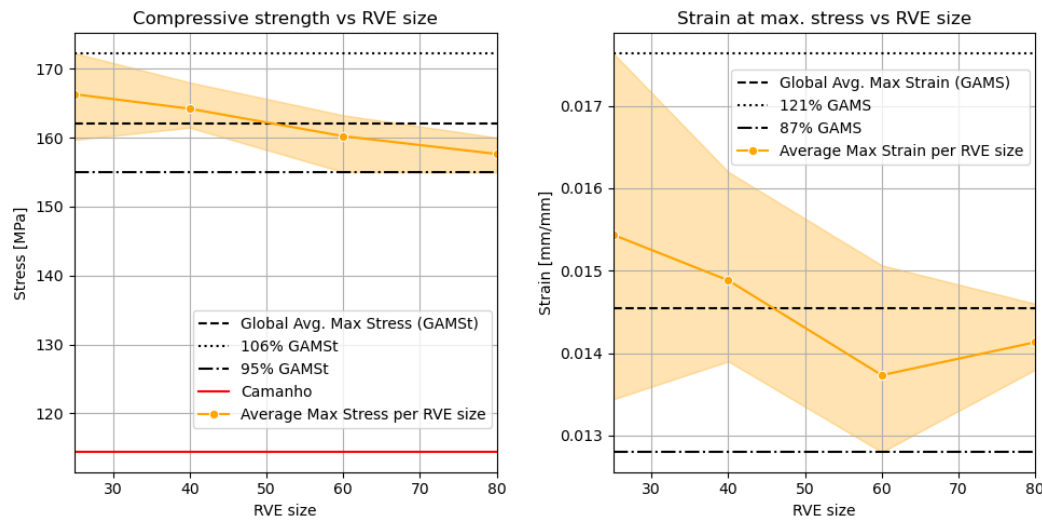


Figure 7.17: Maximum, minimum, average and standard deviation of (a) the peak stress values and (b) the strains at peak stress for different RVE sizes under compressive loading, Phase-Field AT1 formulation and Miehe's energy split.

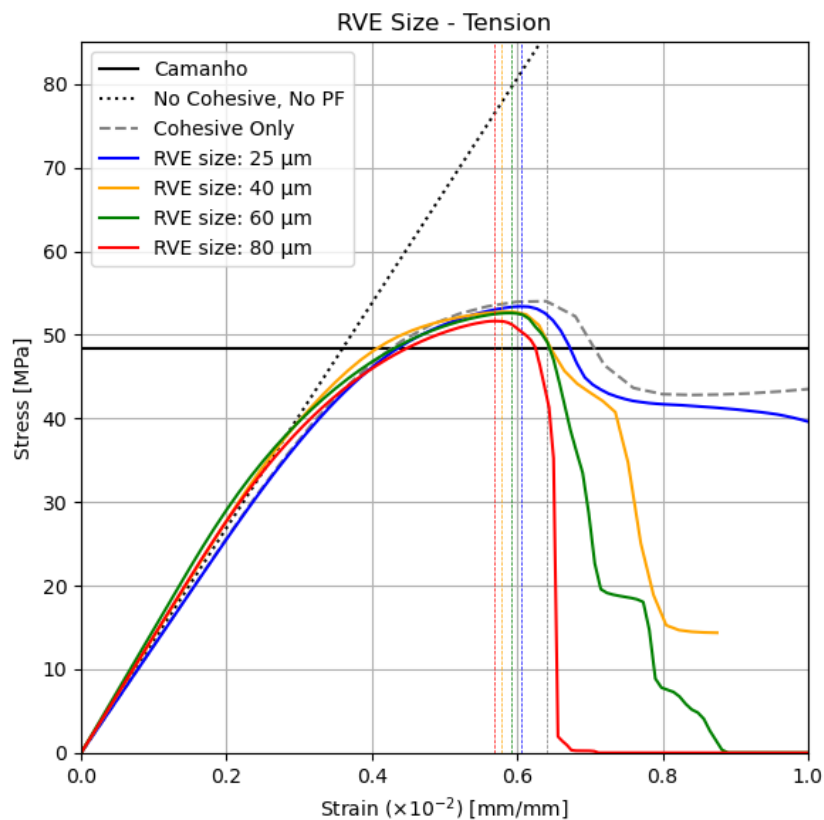


Figure 7.18: Stress-strain curves for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage using the AT1 formulation and Miehe's energy split. Different RVE sizes were used for tensile loading as depicted in Fig. 7.1 a).

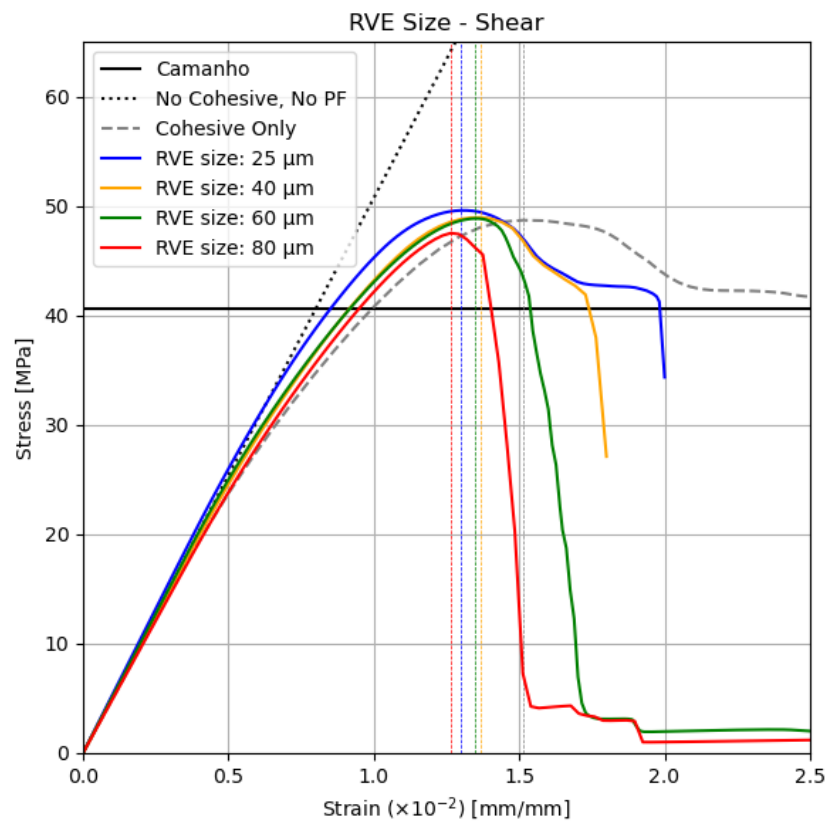


Figure 7.19: Stress-strain curves for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage using the AT1 formulation and Miehe's energy split. Different RVE sizes were used for shear loading as depicted in Fig. 7.1 b).

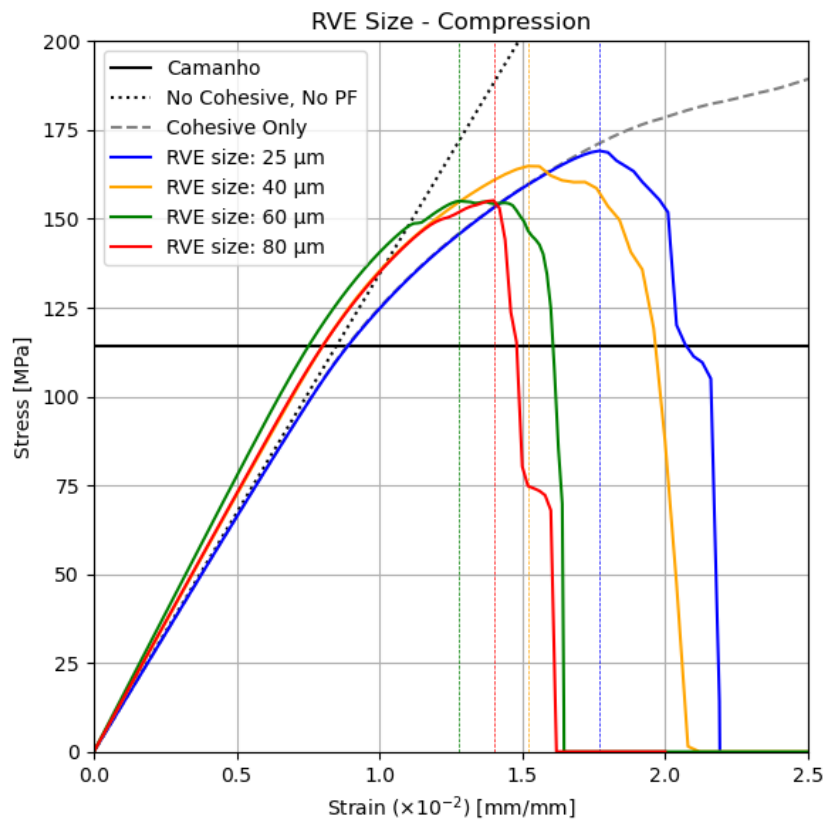


Figure 7.20: Stress-strain curves for a perfect interface connection (No Cohesive, No PF) compared to a model considering a damageable cohesive interface only (Cohesive Only) and models considering cohesive and PF damage using the AT1 formulation and Miehe's energy split. Different RVE sizes were used for compressive loading as depicted in Fig. 7.1 c).

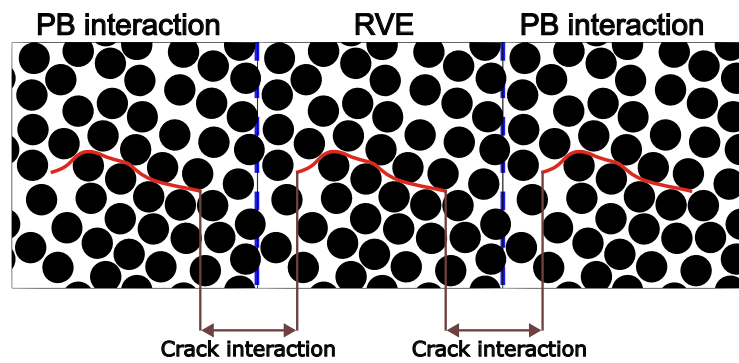


Figure 7.21: Effect of periodic boundary (PB) interaction on crack propagation.

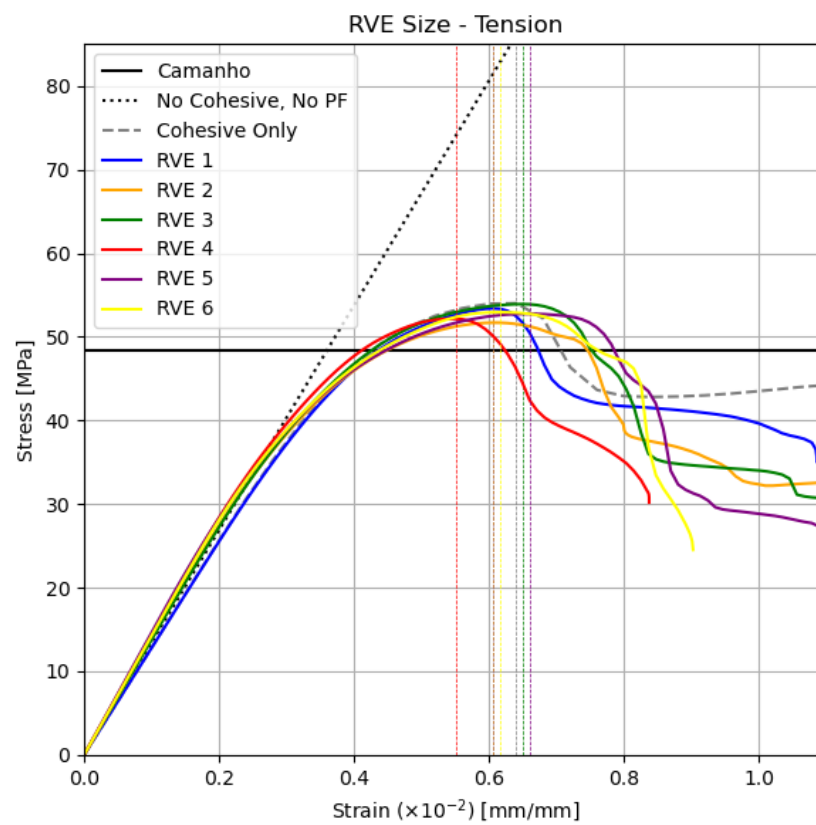


Figure 7.22: Stress-strain curves for tensile loading of RVEs of $25 \mu\text{m}$ size with cohesive interface damage, AT1 formulation and Miehe's energy split.

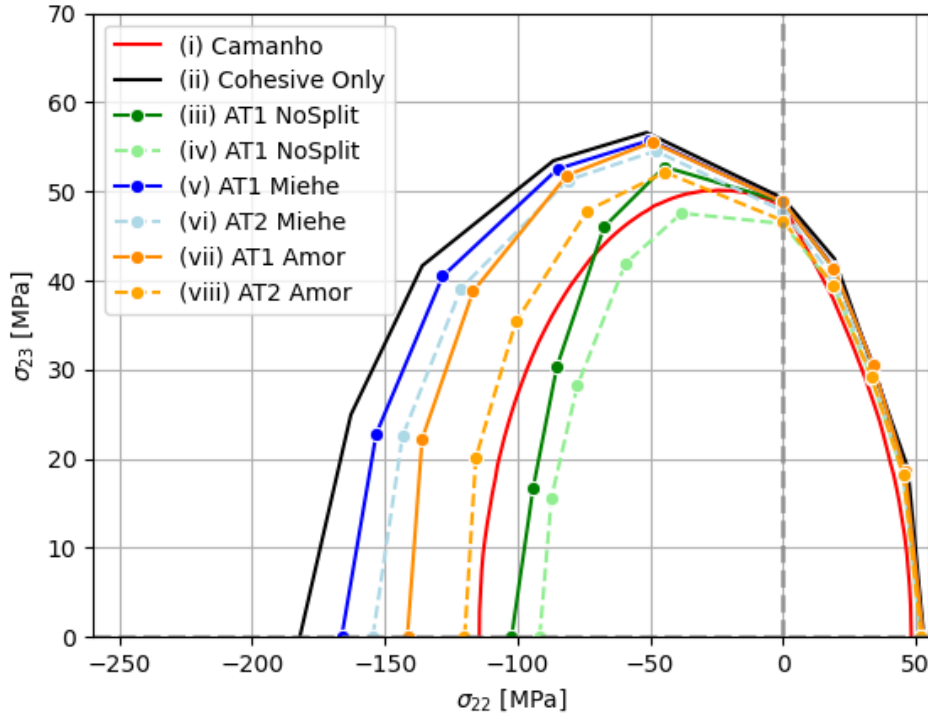


Figure 7.23: Failure envelopes of: (i) Camanho et al. [18] and (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only), (iii) AT1 No Split, (iv) AT2 No Split, (v) AT1 Miehe's split, (vi) AT2 Miehe's split, (vii) AT1 Amor's split and (viii) AT2 Amor's split.

7.3.3 PF formulation and energy split

According to the discussion presented in the previous section, for stress analysis, since the average strength of a square RVE of dimensions $L = 25 \mu\text{m}$ is less than 5% higher than the asymptotic values, then these dimensions can be considered to give the desired trade off between accuracy and running time for the following studies. Similar to the previous analyses, the results presented here are the mean values from six different distributions on RVEs of the same size. The complete σ_{22} – σ_{23} failure envelopes are plotted in Fig. 7.23; in addition, the crack patterns and close-up observation of the intersections with the coordinate axes are shown for pure tension in Fig. 7.24, pure compression in Fig. 7.26, and pure transverse shear in Fig. 7.25.

If an energy split is used, the AT1 formulation overpredicts the failure envelopes of Camanho et al. [18], especially when Miehe's split is used. On the other hand, the AT2 formulations cross the reference envelope of Camanho et al. [18] on the shear-dominated loading, because the AT2 formulation struggles to localize fracture under shear, which generates spurious softening all over the RVE, reducing the maximum stress that can be reached; this can be observed in the crack patterns of Fig. 7.25. In addition, the AT2 formulation under shear loading is more prone to plastic-like fracture patterns where the crack tends to run perpendicular to the shear orientation, similar to the crack patterns in the RVE analyses of Totry et al. [124, 125]. However, if the split of

Miehe et al. [67] is used, brittle-like crack patterns can still be obtained with the AT2 formulation. On the other hand, the AT1 formulation predicts fracture along the plane of maximum principal stress, similar to what is expected from RVE analyses using pressure-dependent plasticity-damage models [46, 129, 117, 134] and the crack band model of Pineda et al. [138]. Under tensile-dominated loading, initial fibre-matrix decohesion promotes fracture localization. Then, spurious softening is less severe and all formulations and splits give very close results in terms of stress distribution and crack patterns. They also match the fracture patterns of RVE analyses following a "weak interfaces" assumption [119], where the interface fracture toughness is significantly lower than that of the matrix (see Table 5.1). For tensile-dominated loading, from pure tension to pure transverse shear, failure is dominated by fibre-matrix decohesion, and all the curves are close to the "Cohesive Only" limit, which is dominated by the "weak interfaces". Due to the linear behaviour of the AT1 formulation, the PF predictions match the "Cohesive Only", as matrix fracture is triggered after the cohesive damage instability occurred. On the other hand, due to the softening of the AT2 formulation, the stresses inside the RVE are slightly diminished before the cohesive instability is triggered.

In general, for compressive-dominated loading, the difference in the matrix strength due to the formulation and energy split plays a more important role. In this case, not accounting for an energy split implies an underestimation of the strength. If an energy split is used, the effect is the opposite, the composite strength is overpredicted, and such overestimation is increased by using Miehe's split or the AT1 formulation. The AT1 formulation combined with Amor's split, and both AT1 and AT2 formulations with no energy split yield crack patterns perpendicular to the loading direction that are considered unrealistic, in the sense that disagree with both experimental as well as previous numerical observations. Miehe's split, regardless of the formulation, and Amor's split with the AT2 formulation yield fracture angles (with respect to the normal to the load direction) clearly larger than 45° , as observed in previous numerical results [117] and in the experimental results of Puck and Schürmann [184]. If no energy split is used, the maximum compressive strength is lower than the failure envelope of Camanho et al. [18].

From the preliminary study of fracture on the RVEs using different sizes and loading conditions, it can be concluded that the current models, alongside the assumed mechanical properties, overestimate the meso-scale strength in tension and compression if an energy split is used, with the predictions of compressive strength yielding the highest differences. As explained in the next section, one of the most evident reasons for the overestimation is the fact that a higher strength is assumed on the resin in order to reduce the length scale parameter so that the damage pattern can actually resemble a fracture-like shape. For simulations where the length scale is further reduced, the failure surfaces are expected to enlarge proportionally up to the "Cohesive Only" surface limit. However, if the length scale is increased, even though a better fit could be obtained on the strength prediction, damage localization could not be achieved, and failure could not be visualized in the form of crack formation, but rather diffuse damage. This indicates that if the length scale parameter could be interpreted as a material property associated to the material strength and fracture toughness, which is the case of the AT1 and AT2 formulations, the "usability" of such parameter

for the specific geometric arrangement and dimensions that need to be studied in the context of computational micro-mechanics can become an important limitation on both the spatial scales that can be modeled as well as the accuracy of the results that can be obtained.

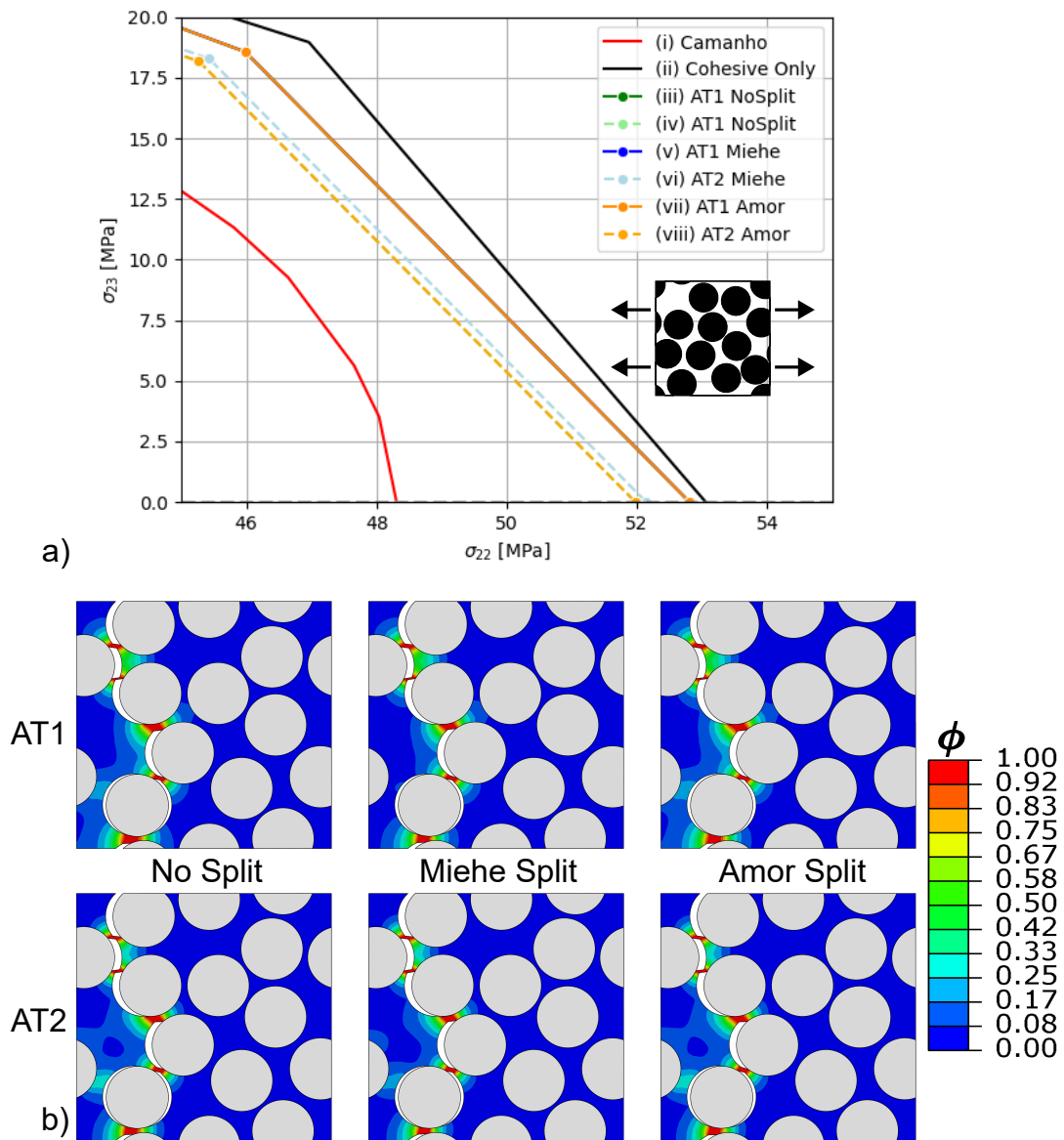


Figure 7.24: a) Failure envelopes and b) crack patterns for pure tensile load of: (i) Camanho et al. [18] and (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only), (iii) linear-elastic AT1 formulation without energy split, (iv) linear-elastic AT2 formulation without energy split, (v) linear-elastic AT1 formulation with Miehe's energy split, (vi) linear-elastic AT2 formulation with Miehe's energy split, (vii) linear-elastic AT1 formulation with Amor's energy split and (viii) linear-elastic AT2 formulation with Amor's energy split.

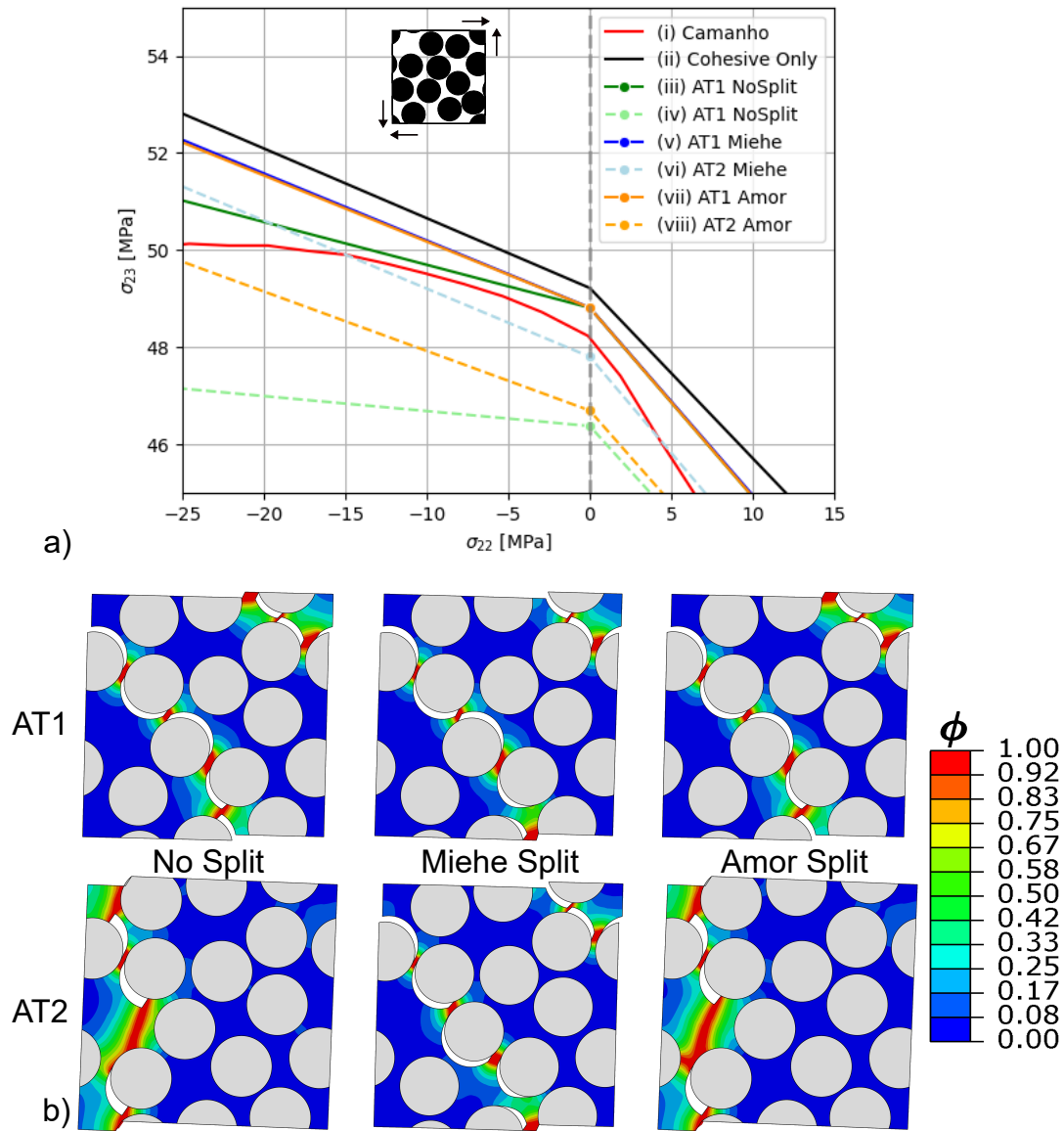


Figure 7.25: a) Failure envelopes and b) crack patterns for pure transverse shear load of: (i) Camanho et al. [18] and (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only), (iii) linear-elastic AT1 formulation without energy split, (iv) linear-elastic AT2 formulation without energy split, (v) linear-elastic AT1 formulation with Miehe's energy split, (vi) linear-elastic AT2 formulation with Miehe's energy split, (vii) linear-elastic AT1 formulation with Amor's energy split and (viii) linear-elastic AT2 formulation with Amor's energy split.

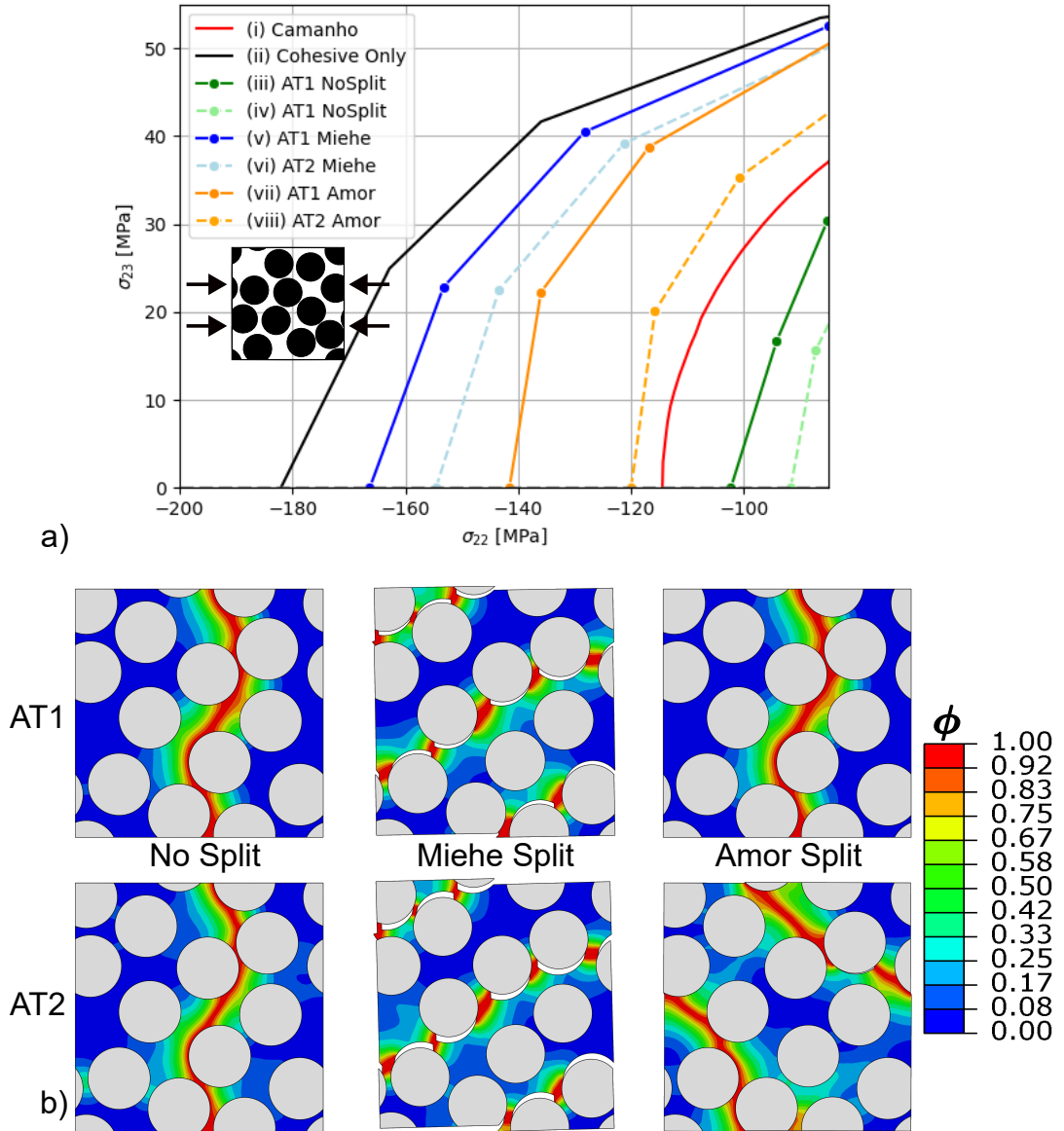


Figure 7.26: a) Failure envelopes and b) crack patterns for pure transverse compression load of: (i) Camanho et al. [18] and (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only), (iii) linear-elastic AT1 formulation without energy split, (iv) linear-elastic AT2 formulation without energy split, (v) linear-elastic AT1 formulation with Miehe's energy split, (vi) linear-elastic AT2 formulation with Miehe's energy split, (vii) linear-elastic AT1 formulation with Amor's energy split and (viii) linear-elastic AT2 formulation with Amor's energy split.

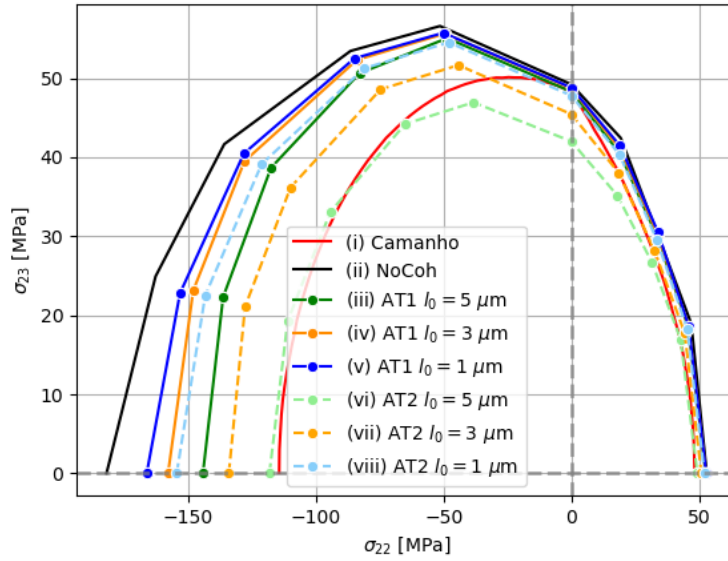


Figure 7.27: Failure envelopes computed using: (i) Camanho et al. [18], (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only). AT1 and Miehe's split formulation with length scale (l_0) equal to (iii) $5 \mu\text{m}$, (iv) $3 \mu\text{m}$ and (v) $1 \mu\text{m}$. AT2 and Miehe's split formulation with length scale (l_0) equal to (vi) $5 \mu\text{m}$, (vii) $3 \mu\text{m}$ and (viii) $1 \mu\text{m}$

7.3.4 Influence of the length scale parameter

To study the effect of the length scale parameter on the transverse failure predictions, new envelopes are calculated using values of length scale equal to $1 \mu\text{m}$, $3 \mu\text{m}$ and $5 \mu\text{m}$; see Fig. 7.27. Again, the results are compared with the case "*Cohesive Only*" to assess if failure is triggered by decohesion or matrix damage. If the curves computed using a PF formulation are very close to the case "*Cohesive Only*", then PF damage does not significantly affect the behaviour of the RVE. As the length scale is further reduced, the curves approximate the "*Cohesive Only*" solution, showing that when the matrix strength is much higher than the interface strength, the maximum meso-scale stress is conditioned by the instability created by decohesion. The matrix fracture strength dictated by the length scale parameter and fracture toughness becomes relevant mainly for the post-peak behaviour and is highly dependent on the loading scenario. Increasing the length scale brings the curves closer to the solution of Camanho et al. [18] but the fracture-like pattern that represents a brittle fracture is gradually lost and replaced by a diffuse damage area whose physical interpretation can become ambiguous.

In the case of tensile loading, representative stress-strain curves for different lengths scales are shown in Fig. 7.28, and the crack patterns in Fig. 7.29. Maximum stress under this type of loading is fully dominated by the interface properties, as the peak is the same for all values of length scale and coincides with the peak stress of the "*Cohesive Only*" curve. The length scale mainly affects the post-peak behaviour. In this case, a lower value of l_0 implies a higher strength, thus a material that fails gradually, while increasing l_0 promotes a brittle-like curve, similarly to increasing the

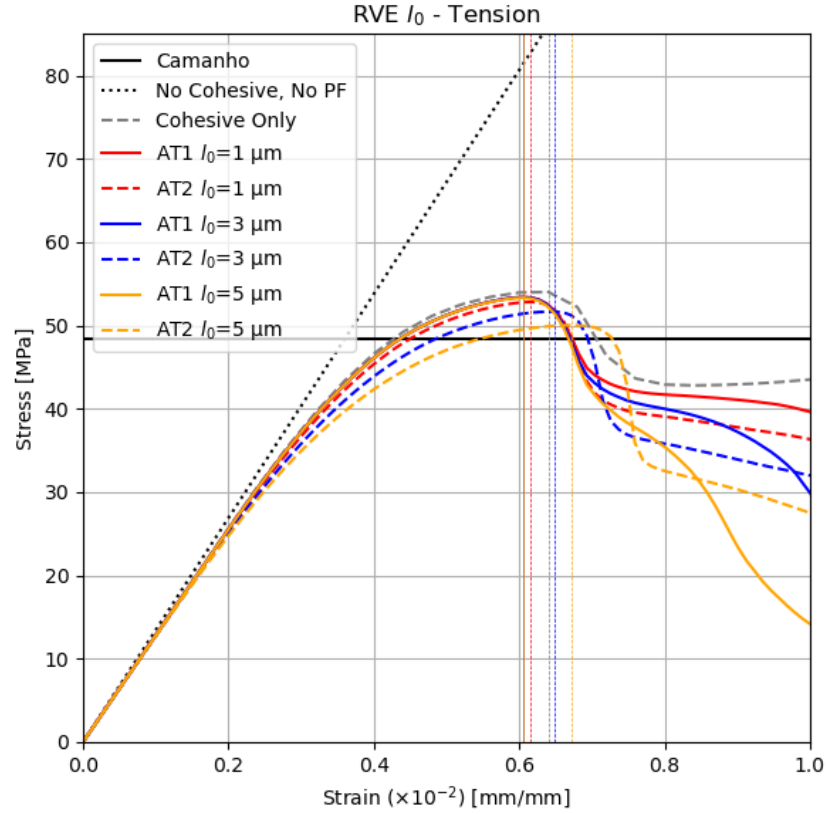


Figure 7.28: Stress-strain curves for tensile loading comparing: (i) strength according to Camanho et al. [18], (ii) RVE with perfect interface connection (No Cohesive, No PF), (iii) RVE with linear elastic materials and damageable interface (Cohesive only), (iv) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 1$, (v) RVE with PF damage using Miehe's split, AT2 formulation and $l_0 = 1$, (vi) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 3$, (vii) RVE with PF damage using Miehe's split, AT2 formulation and $l_0 = 3$, (viii) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 5$, and (ix) RVE with PF damage using Miehe's split, AT12 formulation and $l_0 = 5$. μm ,

size of a periodic RVE, proving that the study of material parameters can be highly dependent on the RVE size and BCs. In addition, increasing the length scale can change the damage pattern and prevent damage localization in an RVE micro-structure. Thus, the damage pattern created by the PF variable does not resemble a crack like-pattern when the length scale is larger than $1 \mu\text{m}$. This is observed even in the case of tensile loading, which is the loading scenario that more easily promotes crack localization.

For transverse shear loading, representative stress-strain curves for different length scales are shown in Fig. 7.30, and the crack patterns in Fig. 7.31. The maximum stress under this type of loading is also mainly dominated by fibre-matrix decohesion for the AT1 formulation, but matrix behaviour is dominant in the AT2 formulation, because this formulation struggles to localize fracture under shear, as explained in Sect. 7.3.3. In this case, higher values of l_0 can modify the damage topology. For the AT1 formulation, if l_0 is smaller than $3 \mu\text{m}$, the crack patterns coinci-

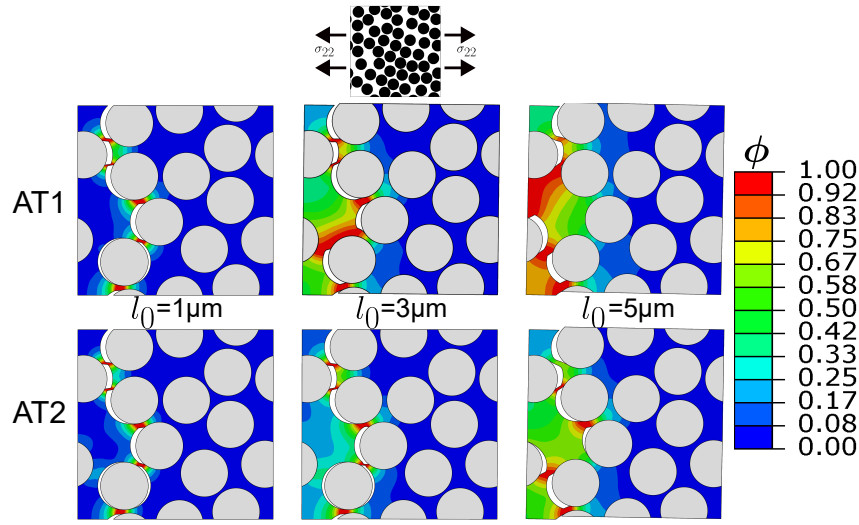


Figure 7.29: Crack patterns for tensile loading using AT1 and AT2 formulations with length scale (l_0) equal to: (i) $1 \mu\text{m}$, (ii) $3 \mu\text{m}$ and (iii) $5 \mu\text{m}$.

dent with the plane of maximum principal stresses, if the length scale is larger, failure can change to plastic-like damage patterns where damage follows the shear direction. For the AT2 formulation this transition happens at lower values of l_0 .

In the case of compressive loading, representative stress-strain curves for different lengths scales are shown in Fig. 7.32, and the crack patterns in Fig. 7.33. The maximum stress under this type of loading is dominated by the matrix behaviour, but there is still matrix decohesion that can take place if the length scale is sufficiently small. The amount of decohesion decreases as the length scale increases, and the damage patterns for small values of l_0 go from crack-like patterns where decohesions are joined by small areas of matrix damage, to diagonal patches of matrix damage, with reduced damage at the interfaces for larger values of l_0 .

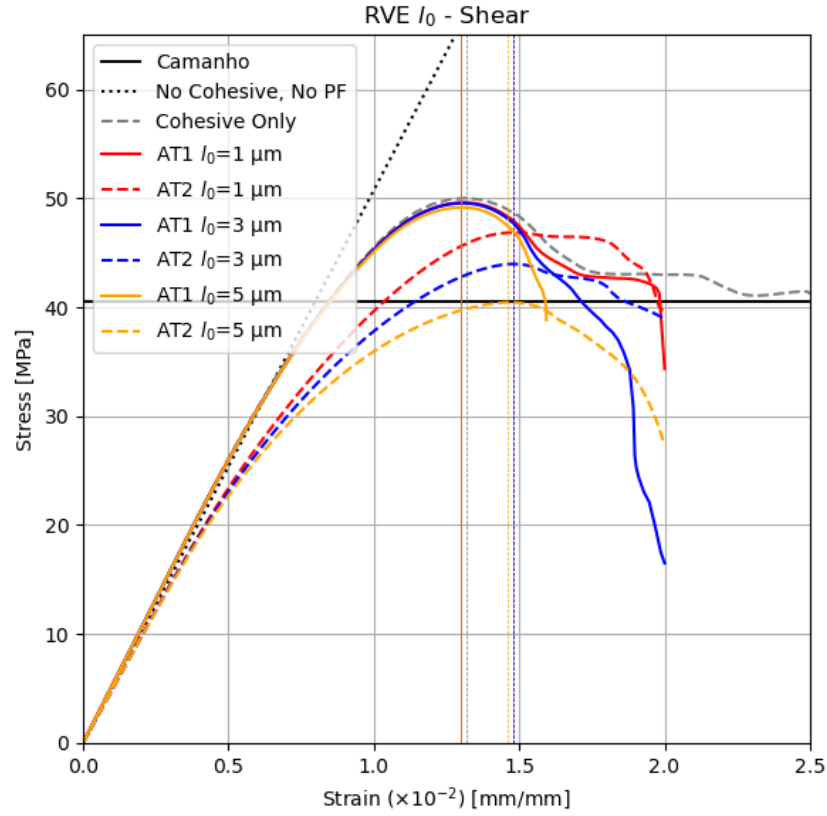


Figure 7.30: Stress-strain curves for shear loading comparing: (i) strength according to Camanho et al. [18], (ii) RVE with perfect interface connection (No Cohesive, No PF), (iii) RVE with linear elastic materials and damageable interface (Cohesive only), (iv) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 1$, (v) RVE with PF damage using Miehe's split, AT2 formulation and $l_0 = 1$, (vi) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 3$, (vii) RVE with PF damage using Miehe's split, AT2 formulation and $l_0 = 3$, (viii) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 5$, and (ix) RVE with PF damage using Miehe's split, AT12 formulation and $l_0 = 5$.

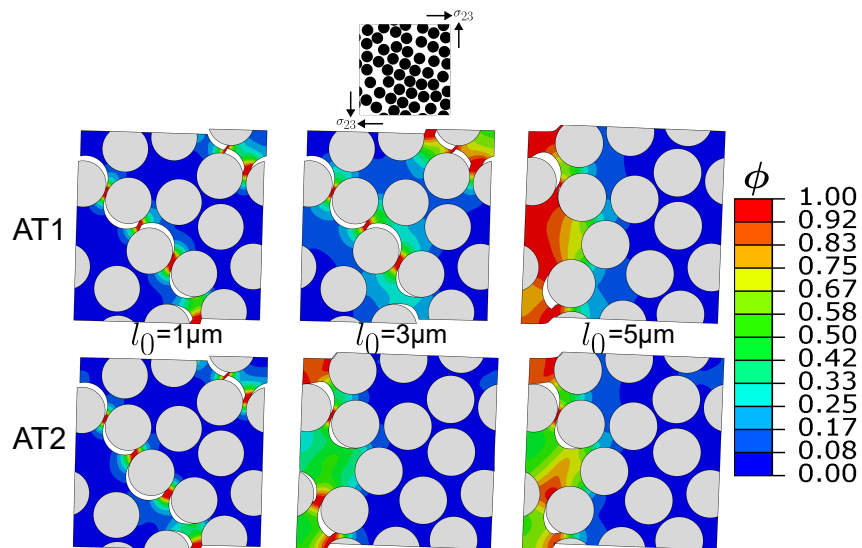


Figure 7.31: Crack patterns for transverse shear loading using AT1 and AT2 formulations with length scale (l_0) equal to: (i) $1\mu\text{m}$, (ii) $3\mu\text{m}$ and (iii) $5\mu\text{m}$.

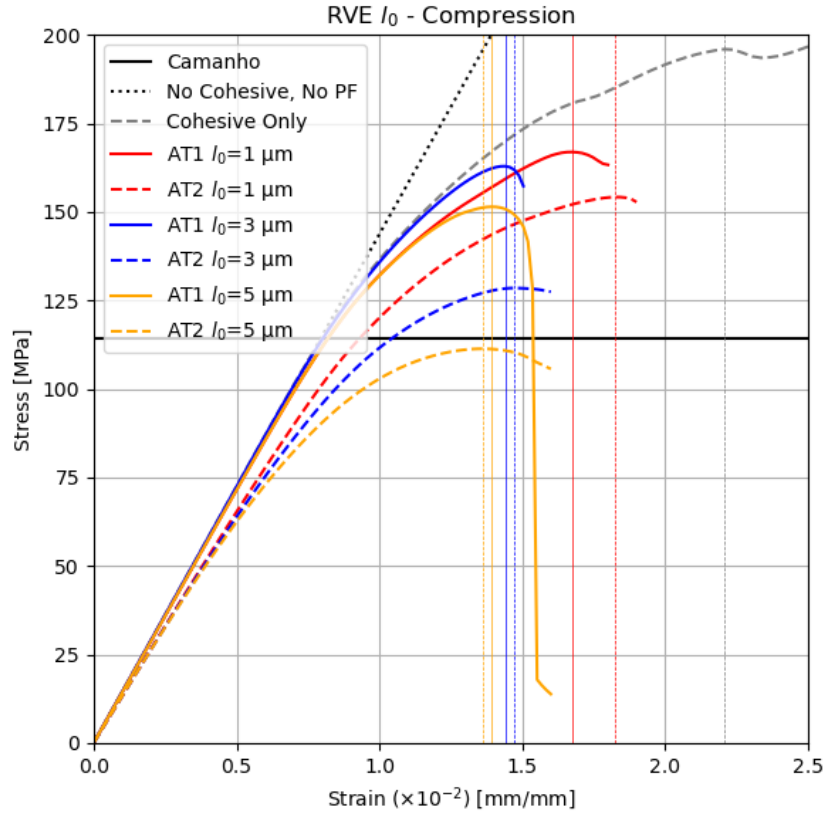


Figure 7.32: Stress-strain curves for compressive loading comparing: (i) strength according to Camanho et al. [18], (ii) RVE with perfect interface connection (No Cohesive, No PF), (iii) RVE with linear elastic materials and damageable interface (Cohesive only), (iv) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 1$, (v) RVE with PF damage using Miehe's split, AT2 formulation and $l_0 = 1$, (vi) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 3$, (vii) RVE with PF damage using Miehe's split, AT2 formulation and $l_0 = 3$, (viii) RVE with PF damage using Miehe's split, AT1 formulation and $l_0 = 5$, and (ix) RVE with PF damage using Miehe's split, AT12 formulation and $l_0 = 5$.

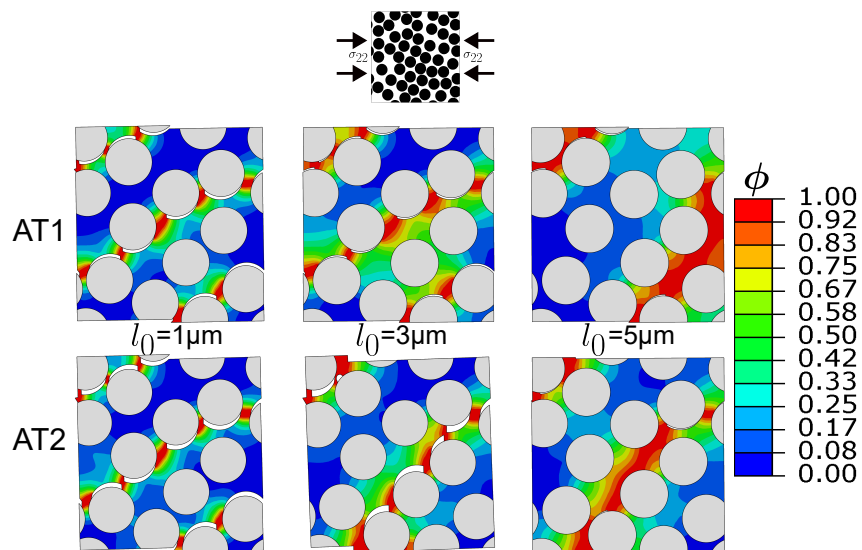


Figure 7.33: Crack patterns for transverse compressive loading using AT1 and AT2 formulations with length scale (l_0) equal to: (i) $1 \mu\text{m}$, (ii) $3 \mu\text{m}$ and (iii) $5 \mu\text{m}$.

7.3.5 Influence of the fibre-matrix interface

The last verification involves removing the cohesive interface interaction and replacing it with a perfect bonding to study failure initiation triggered purely by PF damage. This is an assumption followed in previous micro-mechanical studies of composites using PF for pure transverse tension and pure transverse compression [29]. In the case of tensile loading [29], it was found that the behaviour was dominantly brittle even for small RVEs, a behaviour that can be attributed mainly to the very low matrix fracture toughness that was obtained from calibration in combination with the perfect interface bonding assumption.

Fig. 7.34, Fig. 7.35 and Fig. 7.36 compare the tensile, shear and compressive stress-strain curves from RVEs with and without cohesive interface damage. All pairs of RVEs possess the same size and fibre distribution. It can be seen that, since cohesive damage is the first failure mechanism, removing the cohesive interaction implies a larger meso-scale strength. This trend can be better visualized in the failure envelopes that can be estimated by removing the cohesive interaction and replacing it by a tie constraint, see Fig. 7.37. Failure envelopes computed using the matrix properties in Table 5.1 and ignoring interface damage lead to large global overprediction when compared with the failure criteria of Camanho et al. [18], and even the case of "*Cohesive Only*".

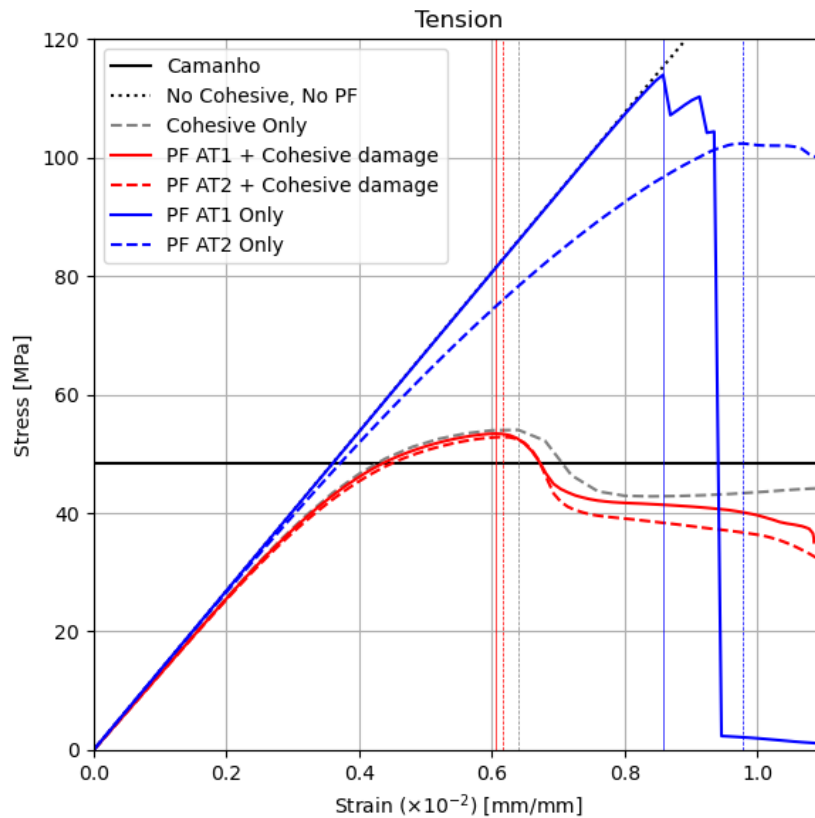


Figure 7.34: Stress-strain curves for tensile loading comparing: (i) strength according to Camanho et al. [18], (ii) RVE with perfect interface connection (No Cohesive, No PF), (iii) RVE with linear elastic materials and damageable interface (Cohesive only), (iv) RVE with PF damage using Miehe's split, AT1 formulation and interface cohesive damage, (v) RVE with PF damage using Miehe's split, AT2 formulation and interface cohesive damage, (vi) RVE with PF damage using Miehe's split, AT1 formulation and tie constraint between fibre and matrix, (vii) RVE with PF damage using Miehe's split, AT2 formulation and tie constraint between fibre and matrix..

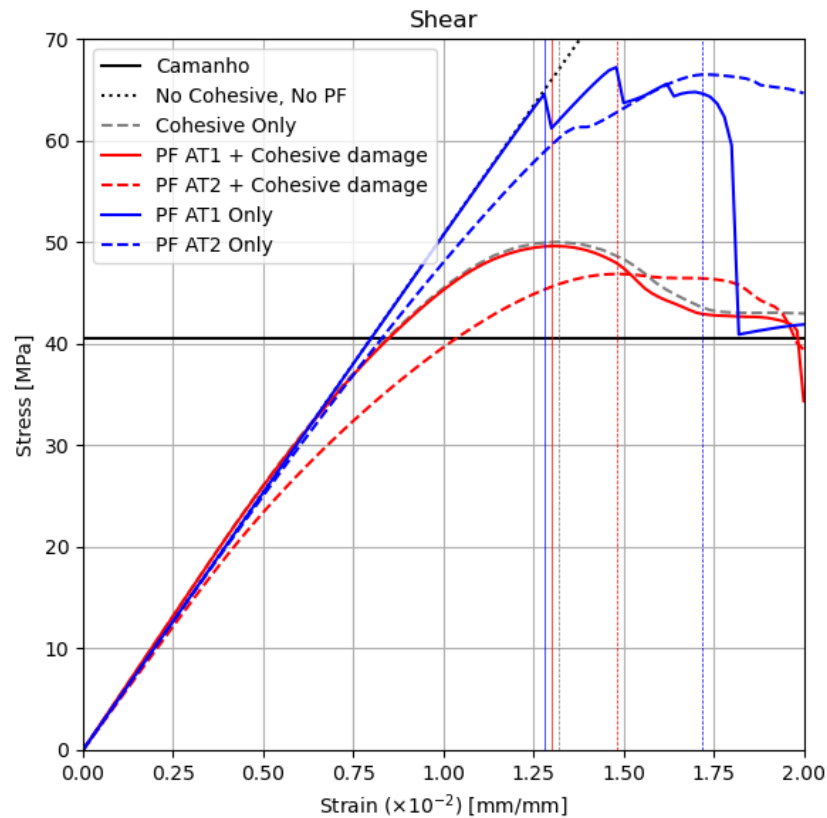


Figure 7.35: Stress-strain curves for shear loading comparing: (i) strength according to Camanho et al. [18], (ii) RVE with perfect interface connection (No Cohesive, No PF), (iii) RVE with linear elastic materials and damageable interface (Cohesive only), (iv) RVE with PF damage using Miehe's split, AT1 formulation and interface cohesive damage, (v) RVE with PF damage using Miehe's split, AT2 formulation and interface cohesive damage, (vi) RVE with PF damage using Miehe's split, AT1 formulation and tie constraint between fibre and matrix, (vii) RVE with PF damage using Miehe's split, AT2 formulation and tie constraint between fibre and matrix..

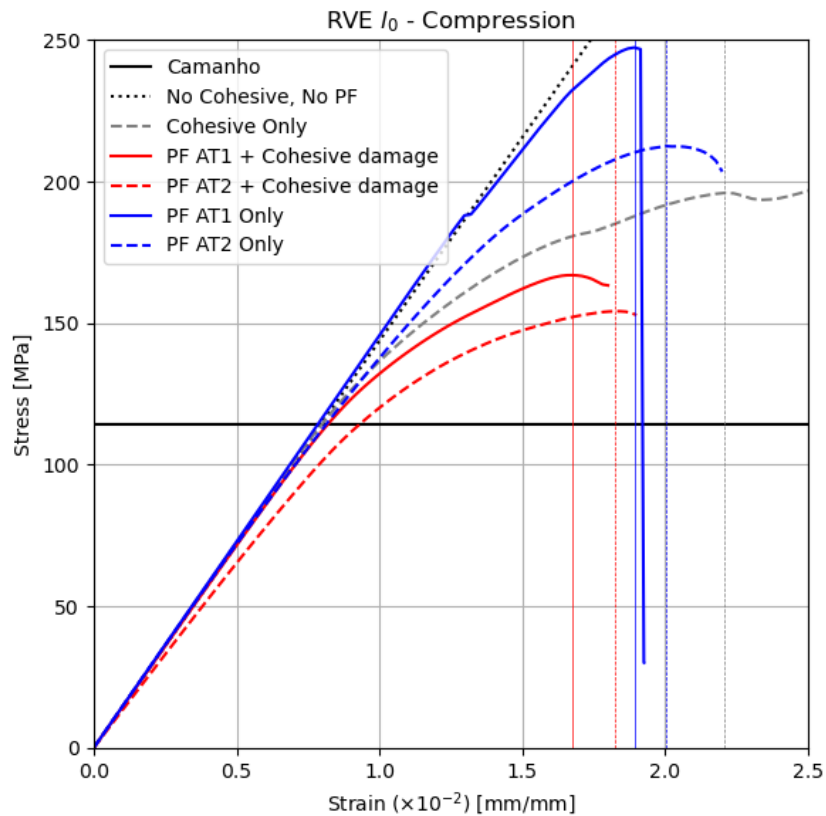


Figure 7.36: Stress-strain curves for compressive loading comparing: (i) strength according to Camanho et al. [18], (ii) RVE with perfect interface connection (No Cohesive, No PF), (iii) RVE with linear elastic materials and damageable interface (Cohesive only), (iv) RVE with PF damage using Miehe's split, AT1 formulation and interface cohesive damage, (v) RVE with PF damage using Miehe's split, AT2 formulation and interface cohesive damage, (vi) RVE with PF damage using Miehe's split, AT1 formulation and tie constraint between fibre and matrix, (vii) RVE with PF damage using Miehe's split, AT2 formulation and tie constraint between fibre and matrix..

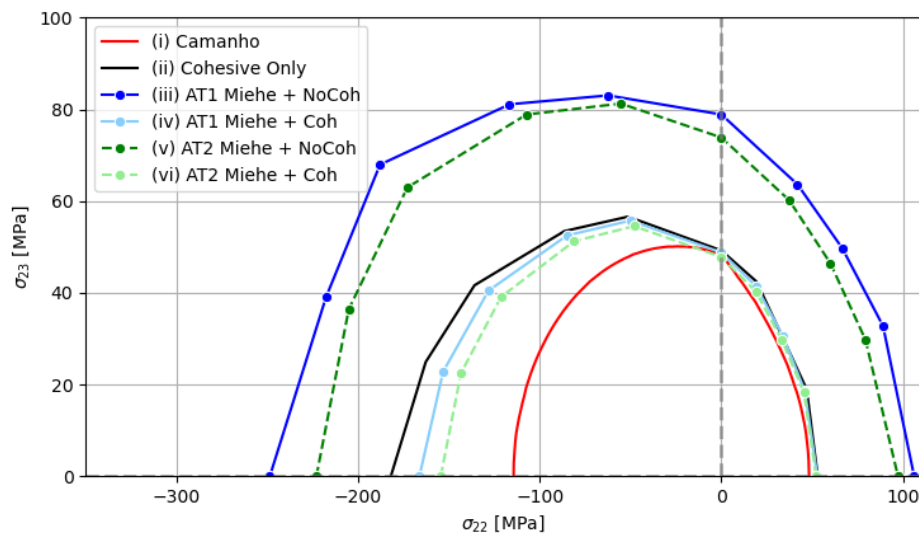


Figure 7.37: Failure envelopes computed using: (i) solution of Camanho et al. [18], (ii) linear-elastic matrix and cohesive interface damage (Cohesive Only), (iii) AT1 formulation and Miehe's split accounting for perfect interface bonding, (iv) AT1 formulation and Miehe's split accounting for interface cohesive damage, (v) AT2 formulation and Miehe's split accounting for perfect interface bonding and (vi) AT2 formulation and Miehe's split accounting for interface cohesive damage.

7.4 Concluding remarks

The feasibility of the strength prediction of classical PF formulations and energy splits was assessed using RVE analyses for different fibre distributions, RVE sizes, loading conditions, PF parameters and interaction models. Using the PF method, reasonable predictions can be obtained but the accuracy is highly dependent on the energy split, PF formulation, length scale, and loading condition. Besides, the validity of the results can be limited by the difference between the length scale parameter and the geometric dimensions of the problem, especially if the length scale is considered a strength-related property, which is the case of the formulations covered in this study¹.

It was concluded that a square RVE of 80 μm side is necessary to obtain meaningful failure strain predictions, while accurate strength analyses can be performed with much smaller RVEs. It was also found that the AT2 formulation combined with Amor's energy split gives the closest prediction when compared to an analytical failure surface, while the AT1 formulation combined with Miehe's split yields the highest overprediction. Also, it is concluded that the accuracy of PF is highly affected by the loading scenario. The best fit was found for transverse shear-dominated loading, while larger differences were found for compressive loading, whose strength predictions are strongly affected by the PF formulations and energy splits. It was demonstrated that meso-scale strength is conditioned by interface properties since interface damage is the dominant failure initiation mechanism under tensile-dominated loading. In this case, matrix failure due to the PF formulation, length scale parameter and energy split are only relevant in terms of post-peak behaviour (meso-scale toughness). On the other hand, PF parameters have a stronger influence on compressive-dominated loading. In this case, the AT2 formulation generally leads to failure envelopes closer to the analytical reference solutions. Moreover, accounting for fibre-matrix interface damage defines a threshold curve from which PF parameters stop exerting influence on meso-scale strength. Finally, it was shown that assuming a perfect fibre-matrix interface has a strong effect on the expected meso-scale strength, as failure is delayed but the apparent behaviour becomes more brittle.

This chapter thus provides useful guidance to the selection of classical PF formulations and energy splits for computational micro-mechanical analyses for general stress states considering 2D plane strain assumptions and matrix linear-elastic behaviour. Further analyses, using 3D models to assess the effects of crack tunnelling, and a nonlinear, plastic matrix behaviour, are required to complement these conclusions. In addition, more detailed analyses, incl. larger RVEs, can be explored to obtain longer crack patterns and predict in more detail the fracture angles, in particular for comparison with other ply failure criteria [184]. Finally, particularizing the Phase-Field

¹The use of the PF-CZM formulation developed by Wu and Nguyen [109] could potentially allow the reduction of the length scale to micro-scale dimensions while defining an elastic threshold based on energy criteria instead of the length scale parameter, in other words, explicitly defining the strength independently of the length scale parameter. However, the PF-CZM formulation is not assessed in this document. The current work focuses on the classical AT1 and AT2 formulations only.

formulation to specific failure surfaces, incl. pressure-dependent behaviour [185, 186], could result in interesting avenues to minimize or overcome the dependency of the solutions on the model parameters and loading condition.

Chapter 8

Micro-scale analysis of oblique cracking using Phase-Field

8.1 Introduction

Matrix dominated damage in the form of micro-cracking is one of the first failure mechanisms that takes place in the off-axis plies inside cross-ply and quasi-isotropic laminates. The onset and evolution of transverse cracks may imply changes in the mechanical behaviour of the laminate as it decreases the longitudinal stiffness and modifies the thermal expansion coefficients. It can impose complete lost of functionality if the required compliance is lost. Besides, transverse cracks can be the path through leakage or lost of pressure in liquid or pressure containers. In less severe scenarios, transverse fracture is still critical as it evolves into other, more severe, damage modes such as delamination and longitudinal splitting of the plies oriented in the load direction [187]. In this sense, the proper mechanical design of composite structures should deeply understand the initiation and evolution of transverse damage mechanisms.

The studies on transverse fracture focus mainly on the estimation of the transverse strength and the evolution of the crack density as a function of the applied load. As mentioned by Nairn et al. [187], the main difficulty on the characterization of the transverse strength properties comes from the fact that these are *in-situ* properties, thus they depend not just on the material properties but also on the layup configuration. There has been extensive work on the characterization of the *in-situ* strength and crack density evolution, from experimental approaches [48, 188, 189, 190, 191, 192], to analytic [189, 193, 194] and numerical [156, 83, 195, 14] methodologies; most studies address mainly two types of layup configurations that are defined as $[(S)/90_n]_s$ and $[90_n/(S)]_s$, where (S) is "*any non-90° ply orthotropic sub-laminate*" [21]. From these studies, there is a general agreement on the mechanical behaviour that is observed even though there are different explanations and reasoning to why such behaviour is presented. The main conclusions that are shared can be summarised as:

- The *in-situ* strength of the 90° ply increases as the thickness of this layer decreases [187].

- Inside $[(S)/90_n]_s$ layups, the *in-situ* strength of the 90° ply increases as the stiffness of the (S) sub-laminate increases [187].
- The evolution of micro-crack density is a function of the applied stress and it is affected in the same way and by the same parameters as the *in-situ* strength [187]. Namely, higher lateral constrains and lower ply thicknesses imply higher stresses to reach micro-cracking saturation. Micro-cracking saturation is defined as the maximum number of transverse cracks that an internal ply can withstand before it triggers another, maybe critical, damage mechanism such as delamination or fracture on the supporting (S) sub-laminate.
- Higher lateral constrains and lower ply thicknesses also improve the capacity to achieve higher micro-cracking densities [187].

These conclusions are mainly extracted from experimental observations and different modelling approaches. In this final chapter some of the models that were used to "explain" the experimental findings are revisited, questioned and compared in the light of experimental results and micro-scale analysis using PF.

8.2 Contextualization

Many times, micro-cracking in the 90° ply is presented in the form of a transverse fracture pattern. It is often represented as a collection of cracks oriented in the direction perpendicular to the direction of tensile loading. This is the most common situation in cross-ply laminates before crack-saturation is reached. But, tilted cracks due to tensile loading can be generated in $[(S)/90_n]_s$ laminates, where the (S) sub-laminate is composed by non- 0° and non- 90° plies [151]. Besides, once the crack saturation is reached, either a partially or fully developed curved crack can be observed. Usually, a partially developed curved crack is called an oblique crack. This type of crack pattern is present only in $[(S)/90_n]_s$ laminates and not in $[90_n/(S)]_s$ configurations. The most common definition of a curved crack is a matrix crack that forms initially as an oblique crack with an angle less than 90° with respect to the loading direction [19, 196, 20, 21, 187], see Fig. 8.1.

Oblique or curved cracks can be formed with or without the presence of delamination, both scenarios have been reported in the literature [19, 196, 20]. According to most authors, curved cracks are always found close to a perpendicular straight crack, extending from the $[(S)/90_n]_s$ interface towards the perpendicular straight crack [19]. A curved crack is always formed in between two perpendicular straight cracks when the distance between them reaches a critical value that corresponds to the state of crack saturation [21, 187]. Curved cracks are believed to originate at the $[(S)/90_n]_s$ interface in a direction dictated by the maximum principal stress [19, 196, 20, 21, 187]. Besides, they seem to grow much slower than transverse straight cracks [19, 196, 20, 21, 187]. Assuming a perfect distribution of transverse straight cracks, oblique or curved cracks are believed to be symmetric with respect to the center line of the 90° ply and the closest straight crack [19], see Fig. 8.1.

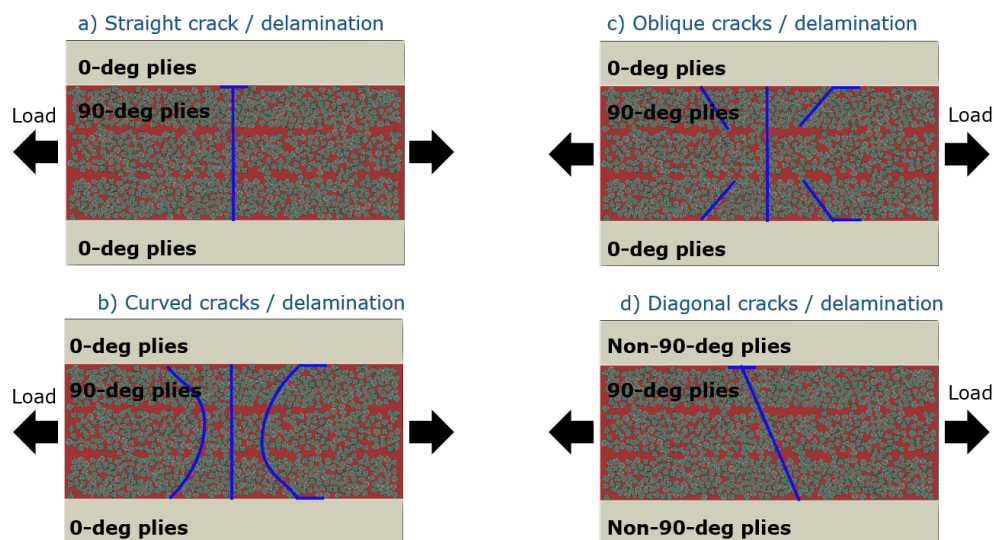


Figure 8.1: Types of transverse fracture in $[(S)/90_n]_s$ laminates: a) Straight transverse crack with/without partial delamination, b) Curved cracks around a straight transverse crack with/without partial delamination, c) Oblique cracks around a straight transverse crack with/without partial delamination, and d) diagonal crack with/without partial delamination [19].

To the author's knowledge, all the attempts to understand curved cracks have been performed using meso-scale models, assuming linear elasticity, accounting for residual stresses due to curing and in 2D analysis, where the through thickness section of the laminate is studied under plane-strain condition [19, 20, 21, 187]. Both (S) and 90_n sub-laminates are considered as homogeneous and thanks to the plane-elasticity assumption, anisotropic behaviour is considered only in the (S) layers, while the 90_n sub-laminate is considered to be isotropic in the given plane. There is a general belief that oblique cracks originate from the $[(S)/90_n]_s$ interface, and their orientation as well as their location is related to the distribution of principal stresses close to the $[(S)/90_n]_s$ interface and in the proximity of the straight cracks [19, 20, 21, 187].

Therefore, this phenomena has been studied by analysing the stress distribution in the central 90_n sub-laminate between two straight cracks in a representative section of a cross-ply laminate, see Fig. 8.2. The initial straight transverse cracks are modelled by imposing either surface tractions or displacements on the 0_n sub-laminates, while leaving the lateral surfaces of the 90_n in a stress free condition. The stress analysis has been performed with different approaches which have not been yet properly compared but are significantly different:

- First, the work of [21, 187] use the stress distribution at the $[(S)/90_n]_s$ interface from the analytical solution derived by Hashin in [22] assuming surface tractions as boundary conditions on the 0_n sub-laminates in the representative section depicted in Fig. 8.2.
- The work of [21, 187] define the onset of oblique cracks as the point where *"the interfacial principal stress plot makes a transition from having a single maximum halfway between two existing microcracks to having two local maxima each associated with one of the existing*

straight microcracks" [21], see Fig. 8.3. The position and orientation of the local stress maxima at the interface when the transverse straight cracks reach saturation agrees well with the experimental results shown in that work. However, as it is shown later, a surface traction boundary conditions impose unrealistic deformation patterns.

- On the other hand, the stress distribution can also be found using Finite Element Analysis (FEA), as it is the case of the work of Jalalvand et. al [20] and Groves et. al [19]. In the work of Jalalvand et. al [20], a purely linear elastic analysis is initially performed on the representative section shown in Fig. 8.2.

Jalalvand et. al [20] imposed displacement boundary conditions which lead to a completely different stress distribution when compared to the solution found by Hashin in [22]. As it is shown later, the deformation pattern seems more realistic when displacement boundary conditions are used, and the stress distribution is dominated by the singularity at the crack tips, see Fig. 8.4. In the work of Jalalvand et. al [20], the stress singularity was eliminated by using cohesive interface damage between the 90_n and 0_n layers. Such cohesive layer gradually breaks promoting the effect of stress relieve at the transverse straight crack tip due to delamination. However, even though delamination can occur simultaneously with transverse cracks [19], the modelling approach proposed by Jalalvand et. al [20] can only work if there is significant delamination. Nevertheless, in their reference experimental results there is absolutely no sign of such damage mechanisms (this fact was explicitly mentioned by the authors).

In addition to the analysis of stresses at the interface using linear elastic models and cohesive interface damage, the work of Jalalvand et. al [20] also included intralaminar damage using two cohesive surfaces, the first surface was located in the middle of the 90_n sub-laminate, oriented perpendicular to the load direction and it was meant to capture the occurrence of another straight transverse crack, and the second cohesive surface was located at an apparent arbitrary location and oriented according to the average results found in the oblique cracks that were measured in the experimental campaign. The analysis mainly compares which cohesive interface breaks first depending on the length of the representative section shown in Fig. 8.2.

Jalalvand et. al [20] found that if the distance between two straight cracks is close to 4 mm ($4 \times$ inner layer thickness) another straight cracks is more likely to appear. But if the distance is reduced to 2 mm ($2 \times$ inner layer thickness) the oblique cohesive crack is triggered instead. This numerical study still leaves many questions unsolved, such as the origin of the oblique cracks and the reasons of their orientation and position. One particular aspect is the fact that the position of the cohesive surface, that was meant to model the oblique crack, was located at 0.6 mm from the transverse crack, which is far from the average distance found according to the experimental observations (0.4 mm). In fact, in the experimental observation only one crack was found located at that distance. Jalalvand et. al [20] provides no reasoning or explanation for the selection of such primal parameter.

A different approach to perform numerical stress analysis was the methodology used by Groves et. al [19]. In this work, the resin rich region was explicitly taken into account, then the analyses

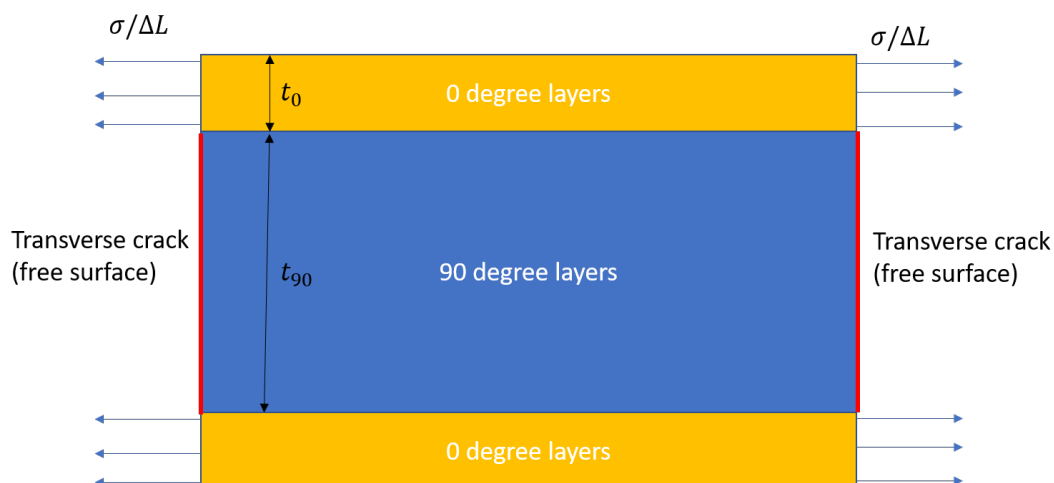


Figure 8.2: Traditional modelling approach to study transverse fracture [20, 21].

focused on finding the maximum principal stresses in the area right above such region. The main limitation of this analysis is that both the material properties as well as the thickness of the resin rich region were assumed based on the laminate dimensions and not on material characterization or microscopic observations. Besides, the location of the peak of the maximum principal stress as well as its orientation do not correspond to what was found in their reference experimental results.

In this chapter, new findings and additional explanations to the origin and evolution of curved cracks are given. In addition the first section focuses on explaining the differences and contradictions found in the previous work, it uses meso-scale FEA to compare and assess the accuracy of the stress distribution with surface tractions and displacement boundary conditions, and the analytical stress field derived by Hashin in [22]. It also questions and assesses the accuracy of the cohesive surface approach of Jalalvand et. al [20]. Later on, micro-mechanical numerical analysis are performed in order to capture the origin and evolution of such curved cracks but without the need of deliberately promoting damage or pre-cracks in the areas where damage is expected, this is to the authors perspective a less biased (more objective) analysis of the problem. Micro-scale analysis shows that additional parameters such as the size of the resin rich region can play an important role on the suppression of oblique-like fracture and instead promote delamination-like damage patterns.

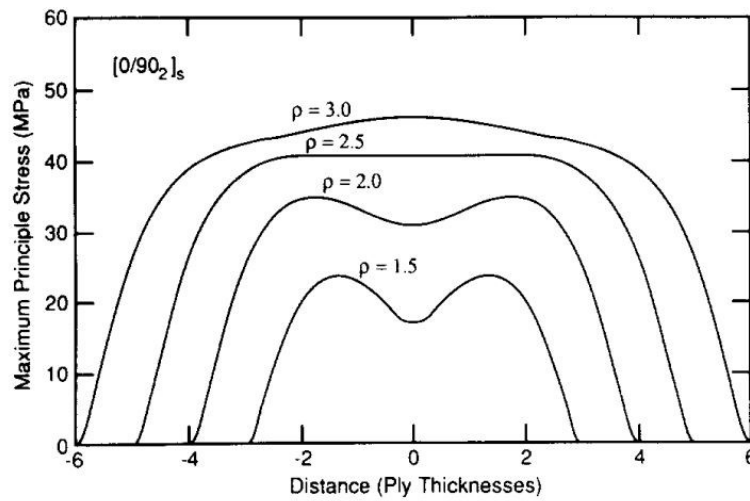


Figure 8.3: The first principal stress along the 0/90 interface in a typical $[0/90_2]_s$ carbon/epoxy laminate for four values of microcrack spacing, ρ is a dimensionless microcrack spacing, defined by $\rho = L/th_{90}$. The critical value of ρ is approximately 2.5 [21]. Reprinted from *Composites Science and Technology*, Volume 47 /Issue 4, Shoufeng Hu, Jong S. Bark, John A. Nairn, *On the phenomenon of curved microcracks in $[(S)/90n]_s$ laminates: Their shapes, initiation angles and locations*, Pages No. 321 -329, Copyright (1993), with permission from Elsevier.

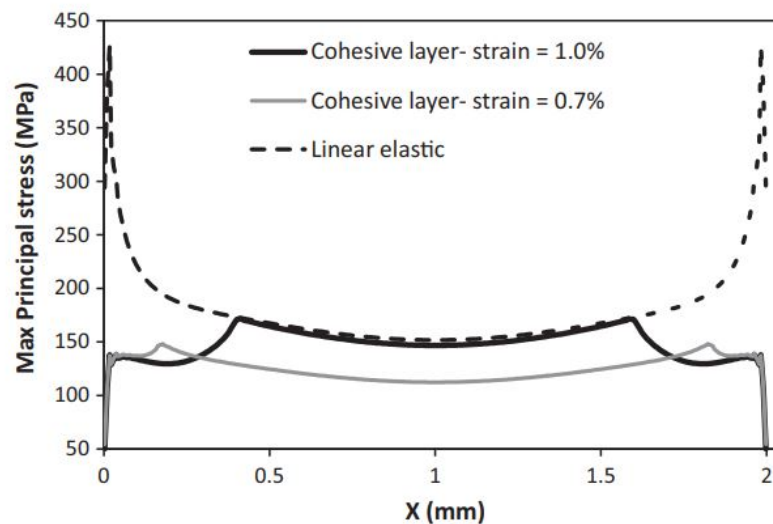


Figure 8.4: Maximum principal stress (S1) at the 0/90 interface [20] with cohesive elements at the interface at 1% longitudinal deformation (Cohesive layer - strain = 1.0%), with cohesive elements at the interface at 0.7% longitudinal deformation (Cohesive layer - strain = 0.7%) and using a tie constraint at the interface (Linear elastic). Reprinted from *Publication Composites Part A*, Vol 67, Meisam Jalalvand, Michael R. Wisnom, Hossein Hosseini-Toudeshky, Bijan Mohammadi, *Experimental and numerical study of oblique transverse cracking in cross-ply laminates under tension*, Pages No. 140 - 148, Copyright (2014), with permission from Elsevier.

Table 8.1: Meso-scale material properties of the IM7/8552 thermoset pre-preg.

Elastic properties					
E_{11}	$E_{22} \text{ \& } E_{33}$	$G_{12} \text{ \& } G_{13}$	G_{23}	$\nu_{12} \text{ \& } \nu_{13}$	ν_{23}
[MPa]	[MPa]	[MPa]	[MPa]	[-]	[-]
171420	9080	5290	3053	0.32	0.44
Fracture properties					
σ_I	σ_{II}	G_{Ic}	G_{IIc}	$B.K$	$K_I \text{ \& } K_{II}$
[MPa]	[MPa]	[N/mm]	[N/mm]	[-]	[N/mm ³]
62.3	92.3	0.28	0.79	1.45	10 ⁶

8.3 Meso-scale analysis

The meso-scale analysis refers to the modelling approach where the 0_n and 90_n sub-laminates are considered as homogeneous materials with orthotropic mechanical properties considering infinitesimal deformations and linear elasticity. The first part of this section is limited to linear elastic studies to evaluate the accuracy of the analytic solution found by Hashin in [22] and the 2D plane-strain assumption of Jalalvand et. al [20] in the first part of their analysis. The second part includes cohesive as well as Micro-scale Phase-Field damage. The idea is to evaluate the predictive capabilities of the cohesive approach of Jalalvand et. al [20] and compare it to the analytical solution and the micromechanical analysis using PF.

For the sake of having a meaningful base-line and reference data for comparison; all the meso-scale models in this section are compared with the experimental results found in the work of Jalalvand et. al [20]. The layup dimensions in Fig. 8.2 correspond to $t_0 = 0.125$ mm and $t_{90} = 1$ mm and the material properties are presented in Table 8.1.

8.3.1 Linear elastic stress analysis

As mentioned previously, the analytical derivation of Hashin et. al [22] provides the stress distribution in a cracked laminated section as the one depicted in Fig. 8.2 where surface tractions are imposed on the vertical edges of the 0_n sub-laminate and a stress-free conditions is assumed on the vertical edges of the 90_n sub-laminate. The stress distribution in the interface of the 0/90 layers can also be found using FEA. For the sake of comparison, two linear elastic models have been set using a 2D plane-strain formulation imposing stress (following Hashin and Hu in [22, 21]) and displacement (following Jalalvand et. al [20]) BC. In the following, the results of the models are presented, analysed and compared focusing mainly on the limitations of the analytical solution of Hashin in [22].

The most evident issue with Hashin's approach is related to the deformation pattern that results from defining a cracked surface through the way BC are imposed. In Fig 8.5 a), it can be seen that a central crack modelled using surface traction BC on the 0_n sub-laminates create rotation, which should not occur if and actual central crack is modeled as shown in Fig 8.5, c). On the other hand, displacement BC accurately capture the expected deformation pattern; see Fig 8.5, b).

Table 8.2: Distance between the transverse and oblique crack, and angle of the oblique crack according to different methodologies for a section of $L = 2$ mm.

Method	Distance	Angle
[-]	[mm]	[degrees]
Jalalvand et. al [20]	0.6	61.1
Nairn and Hu [187, 21]	0.62	58.64
Linear elastic FEA + Surface traction BC	0.36	68.05

The selection of either modelling approach heavily affects the stress analysis. For instance, if surface tractions are used, there is no singularity in the stress field. However if the crack is modelled explicitly or displacement BC are used, the singularity is present at the tip of the transversal crack; see Fig. 8.6. In this section we focused on the stress distribution on the 90_n sub-laminate, right at the interface with the 0_n sub-laminate. The reason is because as explained by Groves et al. [19] and supported by Nairn and Hu [187, 21], this is the area where the oblique cracks are believed to initiate.

From Fig. 8.6 it can be seen that σ_{yy} and σ_{xy} look rather similar regardless of the BC used. However σ_{xx} and σ_{Max} considerably deviate in the region close to the crack tip due to the effect of the singularity in the displacement BC and explicit crack cases. An analysis similar to the one performed by Nairn and Hu [187, 21] could be done using the FEA model of surface tractions BC. In this case, the peak of the maximum principal stress (σ_{Max}) is located at a distance of 0.356 mm from the transversal crack, this value is in deed very close to the average distance found in the experimental results of Jalalvand et. al [20], which is 0.4 mm. An equivalent analysis cannot be done if the other type of BC are used, as the peak of σ_{Max} is located right at the tip of the transversal cracks.

The other limitation of the approach followed by Nairn and Hu [187, 21], using the analytical stress distribution of Hashin in [22], is related to the apparent inaccuracy of the analytical solution when compared to FEA, this difference is stronger in the cases of σ_{xx} and σ_{Max} , see Fig 8.7. On top of that, according to the analytical solution, the location of the oblique crack should be 0.62 mm, which is out of the range found in [20]. In the experimental observations, the distance between oblique and transversal cracks took values from 0.2 to 0.6 mm.

8.3.2 Finite element analysis using cohesive interface damage

In the case of a purely qualitative analysis, the methodology of Jalalvand et. al [20], Nairn and Hu [187, 21], a linear elastic stress analysis using surface traction BC agree that for the two cases studied by Jalalvand et. al [20]. Namely, tension loading of a section of 2 mm length yields an oblique crack, see Fig 8.8 b). While increasing the length up to 4 mm yields a transversal central crack, see Fig 8.8 a). The main differences are in fact the distance between the tip of the oblique and the transversal crack, and the angle of the oblique crack, see Table 8.2 for a summary of the results.

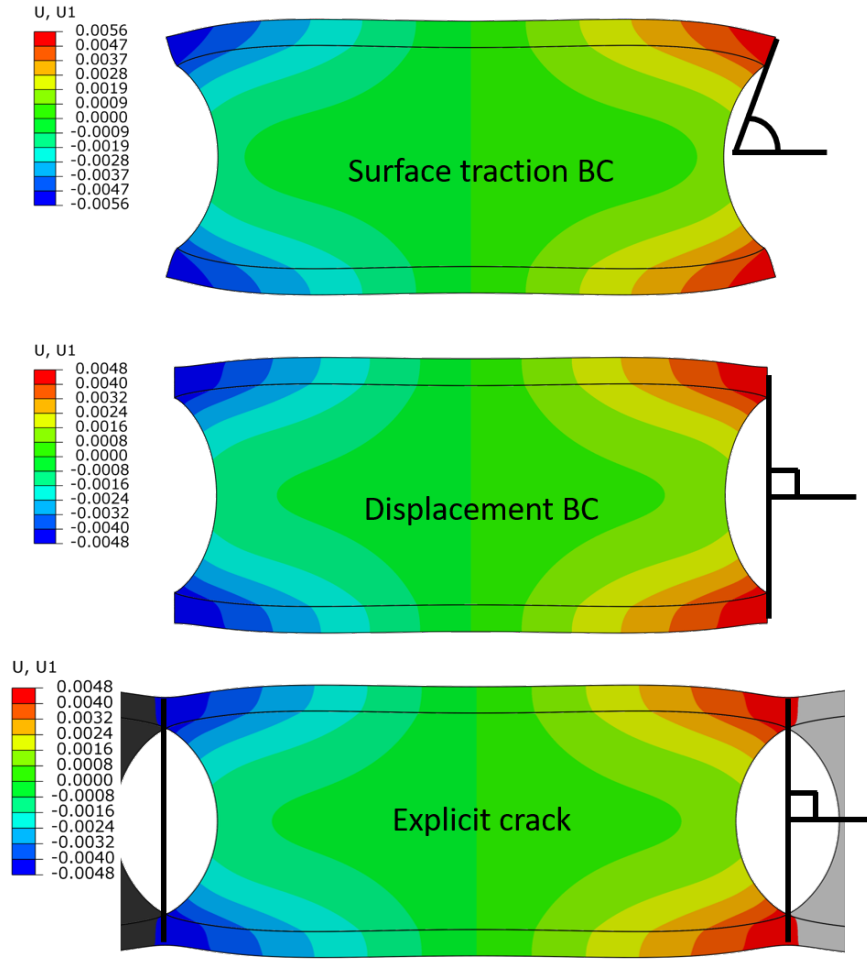


Figure 8.5: Deformation patterns of cracked specimens defined implicitly: a) Using surface traction BC, b) Displacement BC and c) explicit crack for a representative section of 2 mm length.

According to the methodology of Nairn and Hu [187, 21], for the layup of Jalalvand et. al [20] the maximum section length where an oblique crack can be obtained is 2.75 mm. The methodology of Nairn and Hu [187, 21] yields distances that correspond to the range found in the experimental campaign for length sections lower than 2 mm. A transition length could also be found using Jalalvand's methodology but the process would be iterative and thus falls out of the scope of this work.

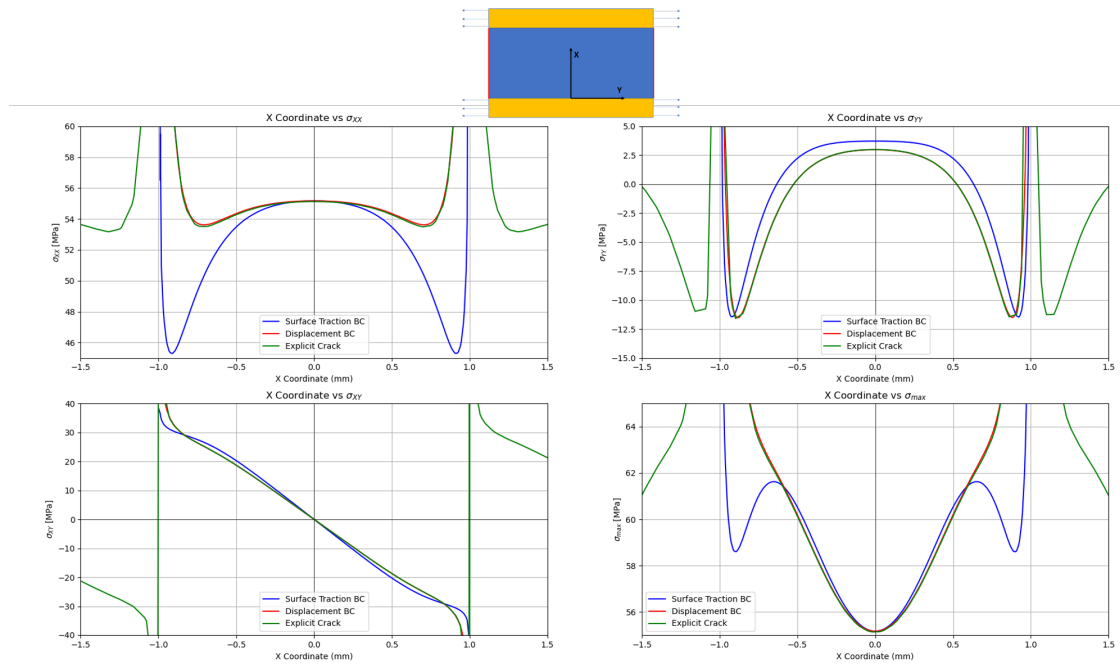


Figure 8.6: Stress distribution at the interface between the 90_n and 0_n sub-laminates for a representative section of 2 mm length. It compares different stress measures for different boundary conditions.

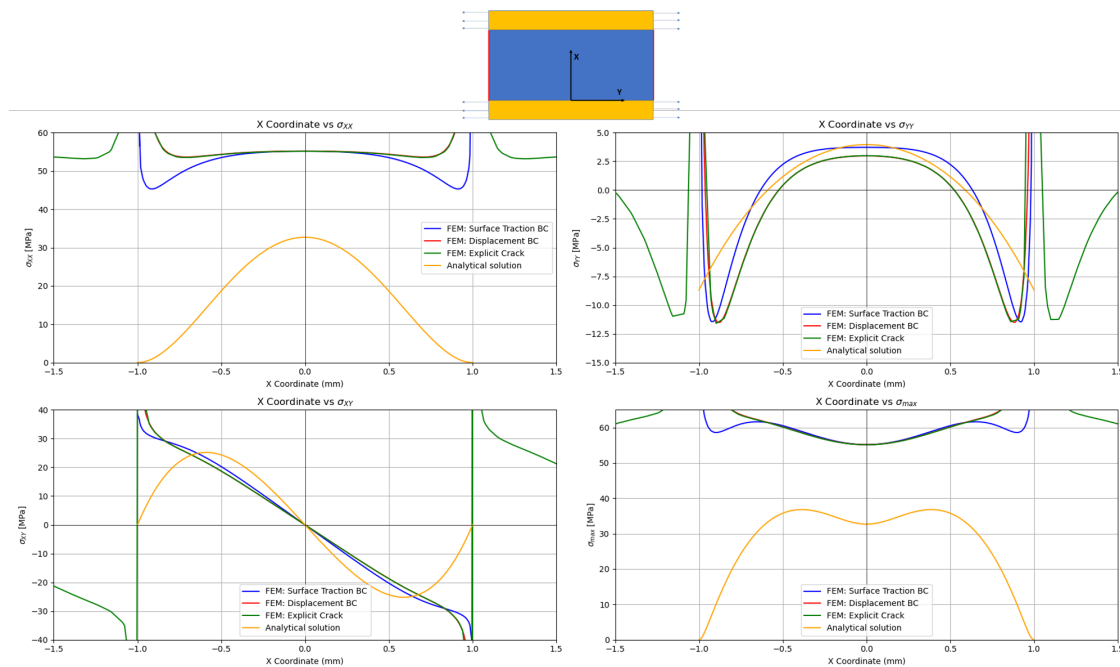


Figure 8.7: Stress distribution at the interface between the 90_n and 0_n sub-laminates for a representative section of 2 mm length. It compares different stress measures for different boundary conditions in FEA and the analytical stress distribution of Hashin in [22].

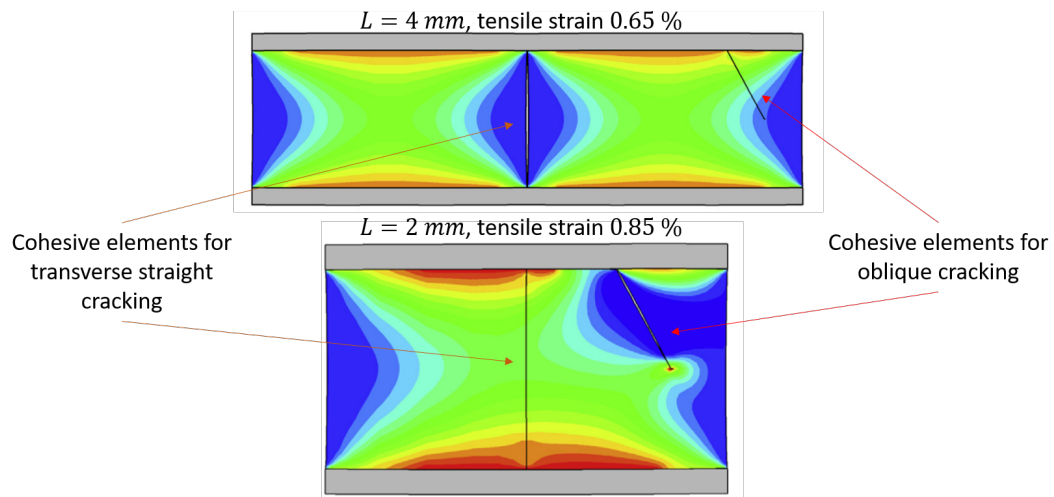


Figure 8.8: Cohesive modelling approach of Jalalvand et. al [20] for a) section length of 4 mm and b) section length of 2 mm. Reprinted from *Publication Composites Part A, Vol 67, Meisam Jalalvand, Michael R. Wisnom, Hossein Hosseini-Toudeshky, Bijan Mohammadi, Experimental and numerical study of oblique transverse cracking in cross-ply laminates under tension, Pages No. 140 - 148, Copyright (2014), with permission from Elsevier.*

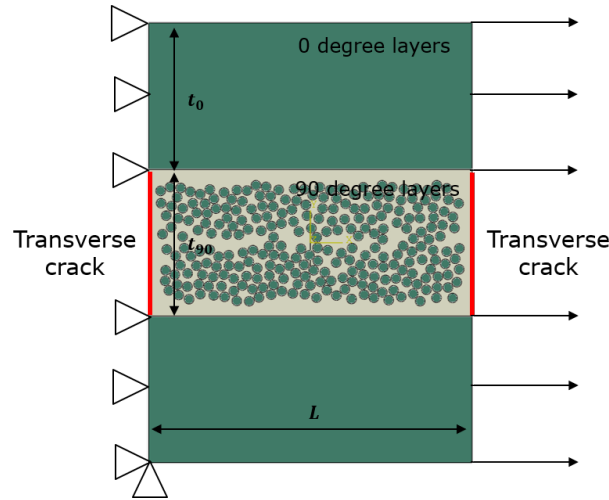


Figure 8.9: Micro-scale embedded section in a cross-ply laminate. Boundary conditions and model explanation.

8.4 Micro-scale analysis

This section presents a more detailed study of the origin and evolution of competing oblique and transverse cracks in cross-ply laminates. The reader must keep in mind that there is a large uncertainty in the material properties that have been used and the fact that no validation has been conducted for the ply thickness studied in embedded cell models.

8.4.1 Modelling approach

For the micro-scale approach, displacement boundary conditions similar to Jalalvand et. al [20] are used. The modelling approach is sketched in Fig. 8.9. The 0° plies are represented using a linear elastic anisotropic material. However, this time the 90° layers are modelled using an explicit representation of the fibre, matrix and their interface. The interface of the two plies is assumed to be perfectly bonded (Tie constraint in Abaqus). The material properties of the 0° layer are shown in Table 8.1, the properties for the matrix, fibre and interface are shown in Table 5.1.

The mesh size used was based on the mesh convergence analysis of the previous chapter, for this reason it would not be practical to model the specimen dimensions in Jalalvand et. al [20] due to the large amount of elements that would be needed. In this analysis, the thickness of the embedded sections are defined to go from one layer of known thin ply commercial material (0.04 mm) up to three layers (0.12 mm). In order to reduce the amount of variables to study, the number of supporting layers (0° plies) has been increased in the same proportion of the transversal plies, see Fig. 8.10. For each of the representative thicknesses, several specimens are tested using different lengths in order to find the transition length where oblique cracks start to appear. In order to have a meaningful comparison, the specimen length is defined in terms of the proportion to the specimen thickness. In this work, such dimension is called "*normalized length*"

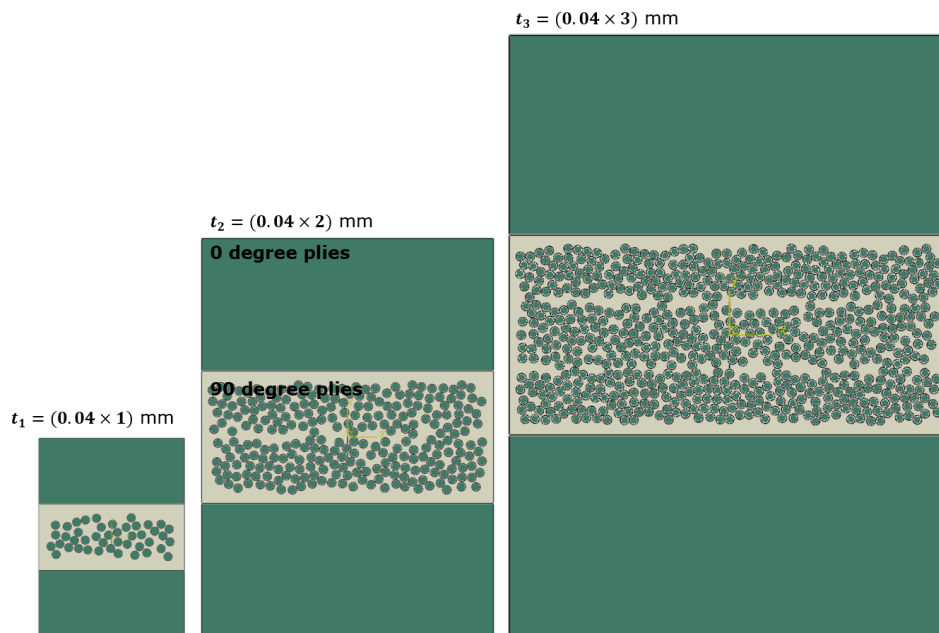


Figure 8.10: Micro-scale embedded sections in cross-ply laminates. Fibre distributions for different ply thicknesses.

8.4.2 Results and discussion

It was found that as the thickness of the inner ply decreases, the transition of the normalized length necessary to observe an oblique crack instead of a transverse crack also decreases, see Fig. 8.11. For the sake of better visualization, this figure depicts only the PF distribution and cohesive interface separation in the inner 90° layers as there is no damage modelling in the 0° plies. One interesting observation comes from the fact that the singularity at the initial transverse cracks imposed by the boundary conditions are smoothed out by PF damage in the form of cracks running at the ply interfaces. This type of damage could be a sign of the potential delamination between plies as a result of the stress concentration created by the initial transverse cracks. In general, oblique crack patterns come with larger areas of potential delamination.

The strain at which either type of crack appears is also a function of the specimen thickness. Fig. 8.12 shows the maximum strain at which oblique and transverse cracks appeared in the layouts shown in Fig. 8.11. It can be seen that fracture in thinner layers requires higher strains regardless of the type of crack that is formed. It is also shown that oblique cracks require a larger strain compared to transverse cracks.

In general, the normalized length required to obtain an oblique crack gradually decreases as the specimen thickness decreases. This dimension refers to the smallest distance that can exist between two transverse cracks, which has been studied in the literature with the aim of identifying the crack saturation capacity of a specific layup configuration. In this work, the micro-scale analysis already allows to see how smaller ply thicknesses can reach higher crack saturations, which

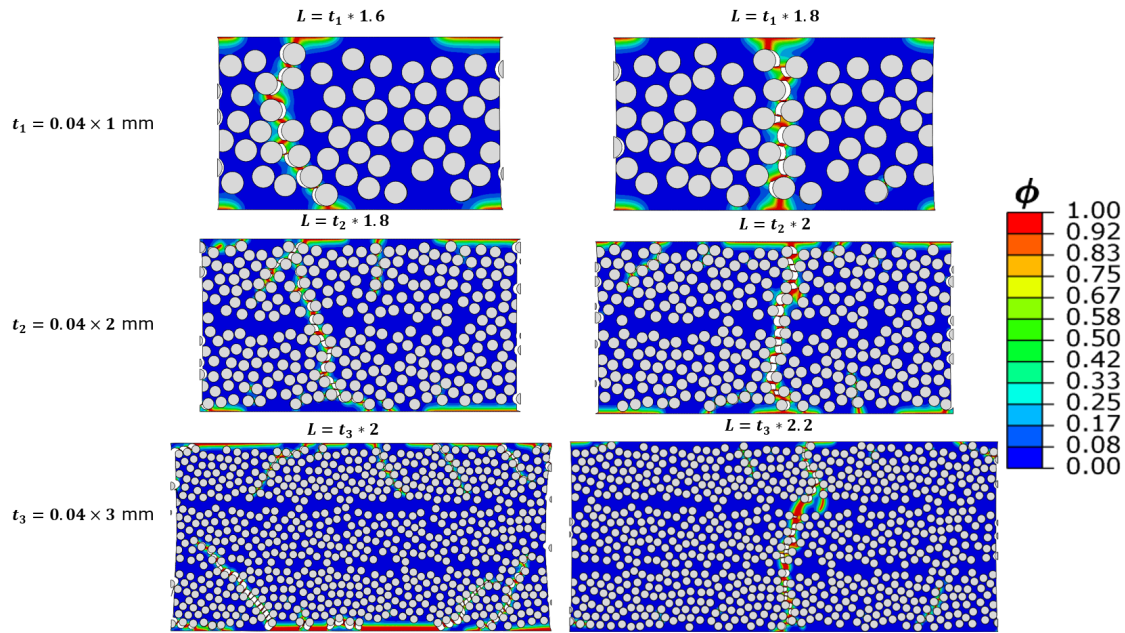


Figure 8.11: PF damage and cohesive interface separation in the micro-scale embedded sections in cross-ply laminates of different normalized lengths and thicknesses. The results in the left-hand side show the formation of curved or oblique cracks, while the results in the right-hand side show the formation of a straight transverse crack.

means, lower minimum distance between transverse cracks, see Fig. 8.13. This observation can help to explain why oblique cracks are usually observed in thick inner layers of cross-ply and angle ply laminates. Thicker inner layers reach crack saturation much faster, before other failure mechanisms are triggered, such as sudden delamination or fracture of the supporting layers.

A final observation, one that was not possible to visualize using meso-scale models is related to the location of area where the oblique cracks initiate. In the laminate with three thin-ply layers and the representative section whose length is equal to two times the inner layup thickness ($t_3 = 0.04 \times 3$ mm, $L = t_3 \times 2$) the evolution of the upper left oblique crack is studied for different strain levels; see Fig. 8.14. According to this model, the oblique crack is created not at the ply-interface but at the location where several fibre-matrix decohesions merge to form a crack. The oblique crack appears to travel inside of the laminate first and only after it reaches certain length it actually propagates towards the ply-interface. This implies that a meso-scale approach where stiffness transition between the two plies happens at a single line, cannot truly capture initiation effects that are micro-mechanic by nature.

Another way one can understand the major role of the fibres close to the interface is by observing the way the failure mechanisms change by varying the size of the resin rich region. Namely, the region between the last fibre in the cross-ply laminate and the ply-interface. Fig. 8.15 shows the damage distribution in the inner 90° layers for three representative sections of thickness ($t_1 = 0.04$ mm) and lengths ($L = 1.2 \times t_1$, $L = 1.4 \times t_1$ and $L = 1.6 \times t_1$) for different sizes of the resin rich

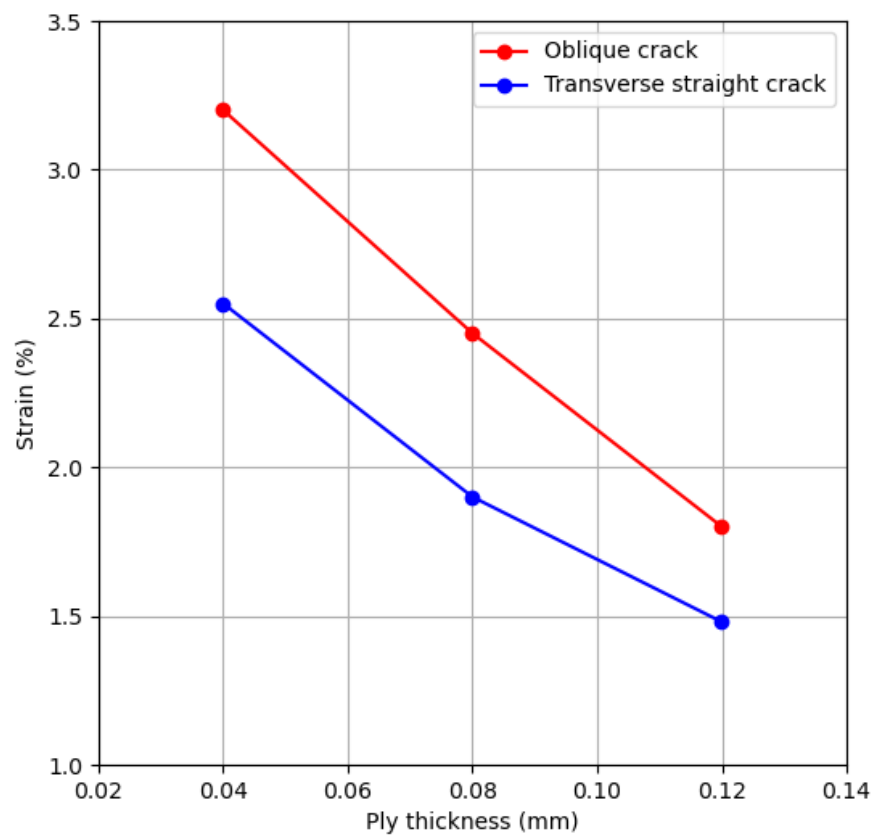


Figure 8.12: Maximum strain to create and oblique or transverse straight crack in layups of different thickness.

region ($1.1 \times$ fibre radius and $2.1 \times$ fibre radius). It can be seen that as the size of the resin rich region increases, the creation of oblique cracks is suppressed and even replaced by transverse straight cracks.

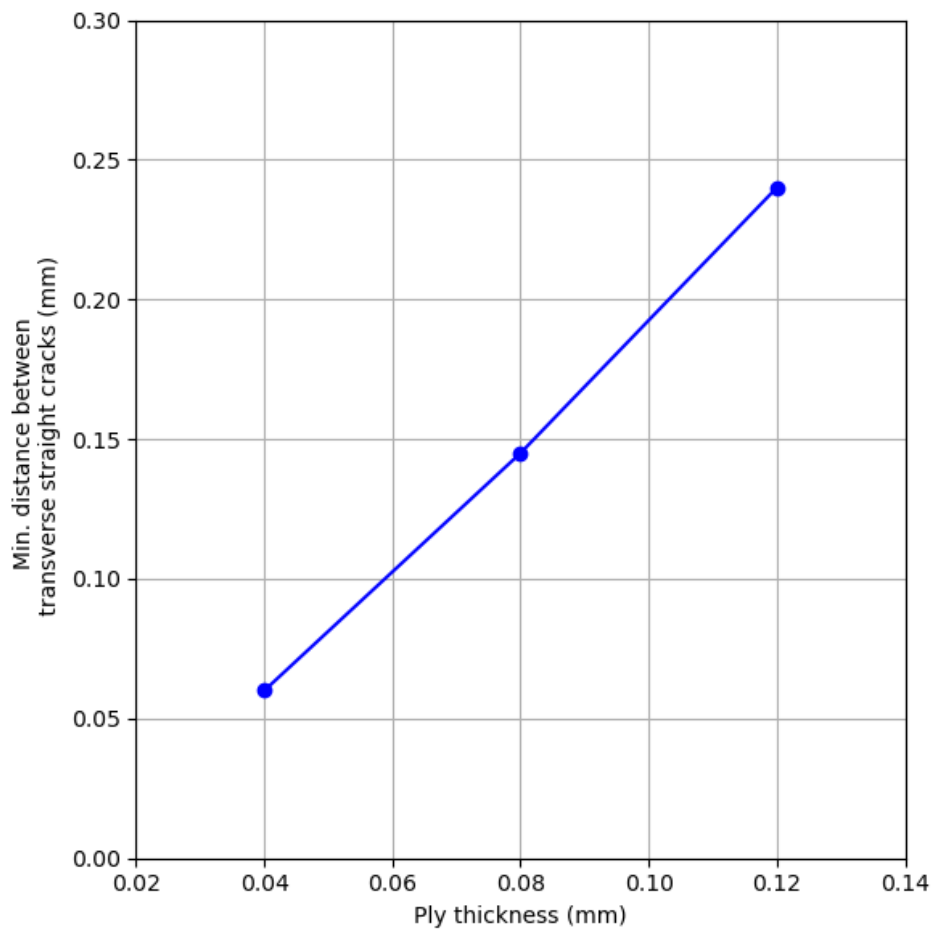


Figure 8.13: Minimum absolute distance between transverse cracks necessary to observe an oblique crack as a function of different inner layer thickness.

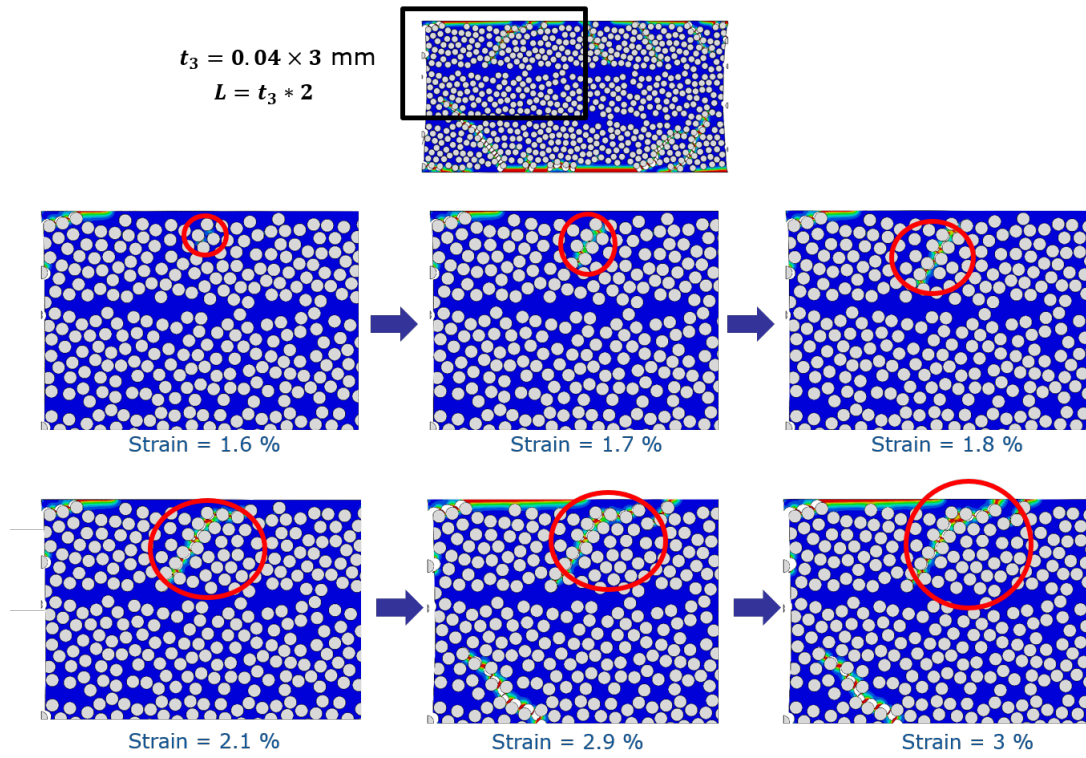


Figure 8.14: Evolution of the upper left oblique crack in the representative section of the layup $t_3 = 0.04 \times 3 \text{ mm}$, $L = t_3 \times 2$.

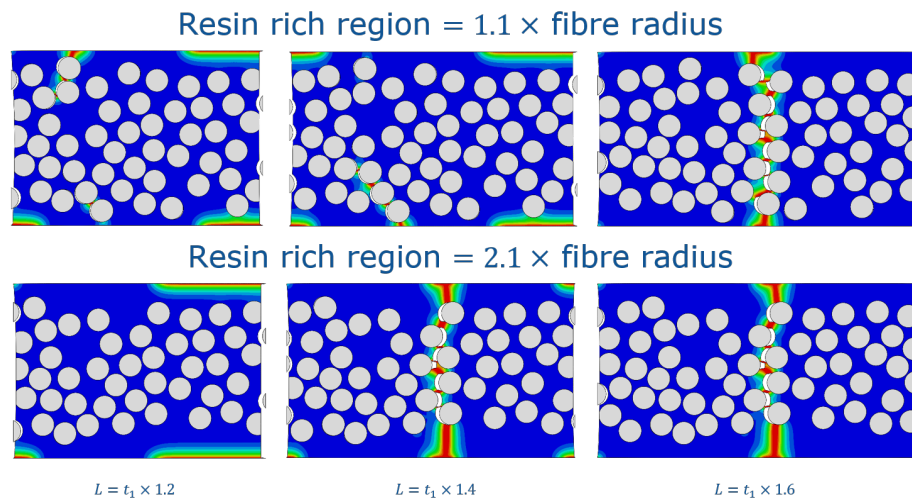


Figure 8.15: Damage distribution in the inner 90° layers for three representative sections of thickness ($t_1 = 0.04 \text{ mm}$) and lengths ($L = 1.2 \times t_1$, $L = 1.4 \times t_1$ and $L = 1.6 \times t_1$) for different sizes of the resin rich region ($1.1 \times \text{fibre radius}$ and $2.1 \times \text{fibre radius}$).

8.5 Concluding remarks

In this chapter, several approaches have been used to study the creation and evolution of transverse and oblique cracks in cross-ply laminates. From this study, several conclusions can be drawn:

- Analyses based purely on the stress distribution are highly polluted by the singularity created at the tip of the transverse cracks and may yield very different results depending on the type of BC and assumptions used.
- Previously proposed analytical solutions can be inaccurate in terms of deformations and stress distributions.
- Although meso-scale damage models can bring additional insight into the problem, these still require significant assumptions.
- Although micro-scale RVEs give more detailed information and account for the effect of additional variables, the increased computational cost can be significant, creating strong limitations in its applicability.
- The initiation and evolution of the oblique cracks is dominated by micro-scale parameters such as fibre distribution close to the ply interface and size of the resin rich region. Thus, accounting for these parameters requires the use of a micro-scale approach.

Chapter 9

Conclusions and future work

This work has extensively examined the numerical and experimental studies of fracture behaviour in thermoset and thermoplastic based UD FRPs using a micro-scale approach, focusing mainly in the role of the Phase-Field (PF) method as an emergent tool. The study highlights the advantages of the PF method over traditional approaches like cohesive zone models (CZM) and continuum damage mechanics (CDM) models, particularly its ability to model crack nucleation and propagation without predefined paths or strong mesh dependency. However, its application to micro-scale phenomena remains limited, with most studies relying on assumptions that may not fully represent the complex behaviour of composites.

The research revealed several knowledge gaps and contradictions in the existing literature. From here, there is questionable reliability of experimental techniques, such as micro-scale strain measurement. Besides, the variability in material property values poses major challenges and concerns. Experimental observations, often limited by high gradients or the methods themselves, raise questions about the representativeness of micro-scale data. Additionally, fibre-matrix and matrix strength, shown to influence fracture behaviour, have been inconsistently accounted for, further complicating the validation of numerical models.

This thesis explored the implementation of PF in finite element software Abaqus, contrasting the use of User Element (UEL) and User Material (UMAT) subroutines. UEL offered superior control and numerical performance but posed challenges in post-processing, while UMAT provided ease of visualization at the cost of computational flexibility. These findings suggest that the choice of implementation should balance computational efficiency with the intended level of analysis, particularly for studies requiring micro-scale fidelity.

Coupling PF with plasticity models was another focal point, with methodologies ranging from simultaneous degradation of elastic and plastic energies to more nuanced approaches incorporating plasticity-driven fracture toughness reduction. The findings show the limitations of existing formulations, particularly under complex loading conditions or in the presence of significant plasticity. Importantly, the study highlighted the need for additional parameters in some models, which adds complexity but may provide a closer approximation to physical phenomena.

A recurring theme across the work is the critical role of boundary conditions and size of RVEs

in fracture modelling. The imposed conditions can significantly influence predictions, particularly in the presence of localization phenomena such as fracture. Similarly, fibre distribution and RVE loading were found to contribute to the variability in fracture predictions. This highlights the need of systematic methodologies to establish robust guidelines for their selection.

Perhaps the most striking conclusion is the recognition of a broader issue: the absence of reliable experimental benchmarks to validate numerical models objectively. The inconsistencies in material properties and fracture predictions across studies reflect a deeper need to revisit experimental methodologies. Without rigorous, repeatable, and unbiased experimental data, the advancement of numerical techniques like PF remains speculative, limiting their utility for real-world applications.

The numerical studies conducted as part of this thesis provide valuable insights into the application of PF methods to UD FRPs, particularly at the micro-scale. Initial simulations focused on open-hole structures subjected to various loading conditions, revealing the influence of PF parameters such as the length scale, formulation type, and energy split. These parameters were shown to significantly affect the localization and propagation of damage, as well as the brittle versus gradual nature of fracture responses.

Subsequent studies incorporated more complex features, such as fibre-matrix interfaces with cohesive damage. By systematically adding complexity, including varying fibre arrangements and cohesive interactions, the analysis highlighted how these factors interact with PF parameters to influence crack initiation and propagation. For instance, cohesive interface damage was found to dominate fracture behaviour in regions with weak fibre-matrix bonding and tensile loading, whereas matrix-driven PF damage played a larger role in systems with strong interfacial properties and compressive loading.

The study of damage in RVEs and embedded cell models revealed the significant impact of fibre distribution, thickness of the resin rich regions, and RVE dimensions on fracture predictions. Variability in RVE distributions resulted in substantial differences in predicted failure mechanisms, emphasizing the need for rigorous criteria to define RVE size and fibre distribution. Additionally, while traditional PF formulations may seem accurate at predicting tensile failure, their accuracy under compressive, shear, and multi-axial loading remains uncertain. This underscores the importance of developing more sophisticated models that incorporate pressure-dependent plasticity and residual stress effects to better simulate real-world loading scenarios.

The findings of this thesis highlight the critical need for a more experimental-numerical combined approach for advancing this emerging field. On one hand, experimental methodologies must be refined to provide accurate, representative measurements of micro-scale properties. Efforts should focus on minimizing measurement artefacts and ensuring that strain fields and gradients are accurately captured. On the other hand, numerical studies must adopt more systematic approaches to select the right parameter that must be assessed and compared; emphasizing transparency and repeatability. This includes exploring a wider range of boundary conditions, material properties, and geometries to better understand their influence on fracture predictions.

Future research should also investigate the integration of elasto-plastic and hyper-elasto-plastic

models with PF formulations to improve predictions under complex loading scenarios. Additionally, exploring alternative PF formulations that allow for micro-scale length scale parameters which are not directly linked to mechanical properties could enhance the fidelity of fracture predictions at smaller scales.

In conclusion, while the Phase-Field method holds significant promise for modeling fracture across scales, its full potential can only be realized through a concerted effort to bridge the gap between experimental and numerical studies. By addressing the fundamental challenges identified in this work, researchers can unlock new possibilities for the design and optimization of composite materials, paving the way for more reliable and resilient engineering applications.

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