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Study of the Turbulent Mixing of Confined Coaxial Jets

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Abstract

In the present work the turbulent mixing of coaxial confined jets was studied, using measurements that were compared with numerical solutions of the Navier-Stokes equations by the Large-Eddy simulation method (LES). The passive scalar transport equation was solved, using flux limited schemes in the convective terms and dynamic modelling of the subgrid quantities. Numerical and modelling tests were performed, with the effects on the profiles compared against the measurements. The main contribution of this work is the focus on the passive scalar turbulent quantities, both in experimental measurements and in LES simulations. The velocity ratio r , between the bulk velocities of the outer and inner jets, had an impact on the uncertainty. High velocity ratio conditions had lower uncertainty in turbulent scalar statistics and fair agreement with LES for the scalar fluctuation. The turbulent scalar flux, rarely presented in LES of complex flows, shows similar order of magnitude but different profile shapes.

The experimental database, obtained previously, was organised and stored and can now be easily accessed in full. Post-processing software was developed to analyse the database, obtaining profiles of the various statistics with uncertainty estimates and curve-fits. The statistics uncertainty was estimated using bootstrap methods and the impact of noise on the measurements was studied. The lowest velocity ratio condition, $r = 0.8$, had the smallest uncertainty on the mean scalar, whereas the highest, $r = 6.5$, had the smallest uncertainty on the fluctuation and turbulent scalar flux. A good compromise between uncertainty in the mean and turbulent scalar quantities was the $r = 3.2$ condition. The PDF evolution had a marching behaviour for low velocity ratio, indicating mixing by small-scale structures, and non-marching behaviour for high-velocity ratio, indicating mixing by large-scale structures.

The cylindrical geometry was simulated using a previously validated code. Non-orthogonal grids were used; corrections for non-orthogonality were implemented and validated in a turbulent pipe flow simulation. The scalar numerical schemes and dynamic model were tested against published LES for the plane channel flow, with agreement.

The LES numerical and modelling tests were focused on velocity ratios $r = 0.8$ and $r = 3.2$. The budgets of the transport equation terms have shown that the molecular diffusivity (*i.e.*, Sc , the Schmidt number) had negligible weight on the statistics. The

Sc^{sgs} had an effect on the budgets, but not on the statistics profiles. The convective discretization scheme had an impact, and agreement in the fluctuation and turbulent scalar flux was improved with use of a TVD scheme, showing good agreement with experiments for $r = 3.2$. The statistics were quite insensitive to changes in the diffusive terms, and we propose a connection with the diffusivity independence hypothesis: behaviour of ϕ is independent of the diffusive terms and, in LES of passive scalar, a hyperbolic equation can be used to obtain the scalar mean, $\langle \phi \rangle$.

Resumo

Neste trabalho estuda-se a mistura turbulenta de jactos coaxiais, recorrendo a medições experimentais e comparando-as com soluções numéricas das equações de Navier-Stokes pelo método da simulação das grandes escalas (LES, *Large-Eddy Simulation*). A equação de transporte do escalar passivo foi resolvida recorrendo a esquemas com limitador de fluxo para os termos convectivos e ao modelo dinâmico para a contribuição das escalas não resolvidas. Foram feitos testes dos parâmetros numéricos e de modelação sendo os seus efeitos nos perfis calculados confrontados com as medições. A principal contribuição do trabalho é o foco nas estatísticas de turbulência do escalar passivo, tanto nas medições experimentais como nas simulações LES. A razão de velocidades r , entre as velocidades médias dos jactos exterior e interior, teve influencia na incerteza. As menores incertezas nas estatísticas de turbulência do escalar foram obtidas para as razões de velocidades elevadas, nas quais houve boa concordância com LES da flutuação do escalar. O fluxo turbulento de escalar, raramente analisado em LES de escoamentos complexos, mostrou ordem de grandeza semelhante mas perfis de formas distintas.

A base de dados experimental, obtida em doutoramento anterior, foi organizada e guardada de forma a poder ser acedida na sua totalidade. Foram escritos programas para análise dessa base de dados, como sejam a obtenção de perfis de várias grandezas e respectivas estimativas da incerteza e curvas de ajuste. A incerteza foi estimada com métodos *bootstrap* e o efeito do ruído nas medições foi estudado. A razão de velocidades mais baixa, $r = 0.8$, teve a menor incerteza na média do escalar, enquanto que a mais alta, $r = 6.5$, teve a menor incerteza na flutuação e no fluxo turbulento de escalar. Um bom compromisso entre incerteza na média, flutuação e fluxo turbulento de escalar foi a condição com $r = 3.2$. A evolução das funções densidade de probabilidade mostrou picos móveis (*marching behavior*) para as razões de velocidades baixas, indicando mistura por estruturas de pequena escala, e picos imóveis (*non-marching*) para razões de velocidades altas, indicando mistura por estruturas de larga escala.

A geometria cilíndrica foi simulada utilizando um código validado anteriormente. Usaram-se malhas não ortogonais, tendo sido implementadas correcções para a não ortogonalidade e feita a sua validação no escoamento no interior de um tubo. Os esquemas numéricos e modelo dinâmico para o escalar passivo foram validados num escoamento em canal plano.

Os testes numéricos e de modelação em LES focaram-se nas razões de velocidades $r = 0.8$ e $r = 3.2$. O balanço dos termos das equações de transporte permitiu concluir que a difusividade molecular (*i.e.*, Sc , o número de Schmidt) não tinha efeito nas quantidades calculadas. O número de Schmidt turbulento, Sc^{sgs} , tinha efeito no balanço mas não nos perfis das quantidades. O esquema de discretização dos termos convectivos teve impacto nos resultados, tendo a concordância da flutuação e do fluxo turbulento de escalar melhorado com o uso de um esquema TVD, com boa aproximação aos dados experimentais para $r = 3.2$. As estatísticas do escalar passivo foram insensíveis a mudanças nos termos difusivos das equações e é proposta uma ligação com a hipótese de independência da difusividade: o comportamento do escalar passivo ϕ é independente dos termos difusivos e, no LES de um escalar passivo, a média $\langle \phi \rangle$ pode obter-se usando uma equação hiperbólica.

Résumé

Dans ce travail le mélange turbulent de jets coaxiaux confinés a été étudié, en utilisant les mesures qui ont été comparées avec les solutions numériques des équations de Navier-Stokes, obtenues avec la méthode de Simulation des Grandes Echelles (LES, de l'anglais *Large-Eddy Simulation*). L'équation de transport scalaire a été discrétisée en utilisant des schémas du type limiteur (TVD) dans les termes d'advection et un modèle dynamique de sous-maille. Des tests numériques et de modélisation ont été effectués et les effets sur les profils comparés avec les mesures. La contribution principale de ce travail est l'accent mis sur les quantités turbulentes du scalaire passif, à la fois sur les mesures et sur les simulations LES. Le rapport de vitesse, r , entre les vitesses moyennes des jets centraux et annulaires, a accentué l'incertitude. Les régimes avec un fort rapport de vitesse ont eu moins d'incertitude dans les statistiques turbulentes du scalaire et le même ordre de grandeur que LES pour les fluctuations de ce dernier. Le flux turbulent du scalaire, rarement présenté dans LES des écoulements complexes, montre le même ordre de grandeur mais différentes formes de profil.

La base de données expérimentale, obtenue précédemment, a été organisée et stockée et est maintenant facilement accessible. Les logiciels de post-traitement ont été développés pour analyser la base de données, *e.g.*, l'obtention des différents profils statistiques, l'incertitude des estimations et la courbe de *fitting*. L'incertitude des statistiques a été analysée avec les méthodes *bootstrap* et l'impact du bruit sur les statistiques turbulentes du scalaire a été étudié. Le plus faible rapport, $r = 0.8$, a eu la plus petite incertitude sur la moyenne scalaire, tandis que le plus fort, $r = 6.5$, a eu la plus petite incertitude sur la fluctuation et le flux turbulent du scalaire. Un bon compromis entre l'incertitude de la moyenne et des quantités turbulentes a été le régime avec $r = 3.2$. L'évolution des fonctions de densité de probabilité a eu un comportement de marche à faible rapport de vitesse, en indiquant le mélange des petites structures, et un comportement de non marche avec des rapports de vitesse élevées, indiquant le mélange de structures de grande envergure.

La géométrie a été simulée avec un logiciel validé précédemment. Des grilles non-orthogonales ont été utilisées avec des corrections pour la non-orthogonalité, validées dans l'écoulement turbulent développé dans un tube. Les schémas numériques et le modèle dynamique pour le scalaire ont été testés dans l'écoulement turbulent de canal plan.

Les essais numériques, et ceux de la modélisation ont porté sur les rapports de vitesse $r = 0.8$ et $r = 3.2$. Le balance de l'équation de transport a constaté que la diffusivité moléculaire (c'est-à-dire Sc , le nombre de Schmidt) avait peu de poids sur les statistiques. Le numéro de Schmidt turbulent Sc^{sgs} , du modèle de sous-maille, a modifié le balance, mais n'a eu aucun effet sur les statistiques des profils. La discrétisation du terme advectif a eu un impact positif sur les profils; la fluctuation et le flux turbulent de scalaire montrent un meilleur accord avec les mesures avec l'utilisation d'un schéma TVD, surtout pour $r = 3.2$. Les statistiques sont tout à fait insensibles aux changements de la diffusion, et nous proposons un lien avec l'hypothèse de l'indépendance de diffusion : le comportement de ϕ est indépendant de la diffusivité et, dans LES de scalaire passif, une équation hyperbolique peut être utilisée pour obtenir la moyenne scalaire, $\langle \phi \rangle$.

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Nomenclature

Roman Symbols

a	Coefficient of the discretized linear equation system
A_i	Inner pipe diameter
A_o	Outer pipe diameter
$\mathcal{B}$	Budget (out-of) balance term
$\mathcal{C}$	Budget convective term
C_f	Friction coefficient
C_{ev}	Smagorinsky constant
C_{ed}	Passive scalar Smagorinsky constant
D_a	Annulus hydraulic diameter
$\mathcal{D}$	Budget diffusive term
D_c	Converging nozzle inlet diameter
D_i	Inner pipe average diameter
$D_{i,i}$	Inner pipe inside diameter
$D_{i,o}$	Inner pipe outside diameter, <i>i.e.</i> , annulus interior diameter
D_o	Outer pipe diameter
F	Momentum or passive scalar flux in the cell face
f	Grid expansion factor
F^c	Convective flux in the cell face
F^d	Diffusive flux in the cell face

$\mathcal{F}_j$	Tensor for the passive scalar dynamic model
$\mathbf{i}$	Unit vector in Cartesian direction i
L	Domain length
L_{ann}	Annulus length
L_c	Converging nozzle length
$\mathcal{L}_{ij}$	Turbulent stress tensor
L_{trans}	Development length
$\dot{m}$	Water mass flux
M_{ij}	Tensor for the momentum dynamic model
$\dot{m}'$	Mass correction
$\dot{m}_\phi$	Scalar mass flux
$\mathbf{n}$	Cell face unit vector
N_{boot}	Number of bootstrap samples
N_j	Tensor for the passive scalar dynamic model
p	Pressure
p'	Pressure correction
Pe	Peclet number
Q	Volume flow rate
q_j	Passive scalar flux
$\bar{q}_j$	Resolved passive scalar flux
q_j^{sgs}	Subgrid-scale passive scalar flux
r	Radius, measured from pipe or nozzle axis
r	Velocity ratio
r^+	Radius, expressed in λ_ν units
r	Ratio of consecutive gradients
Re	Reynolds number

Re_i	Inner flow Reynolds number
Re_o	Outer flow Reynolds number
res	Mass flux balance residual value in a cell
S	Face section
S	Strain rate tensor norm
Sc	Schmidt number
S_c^i	Projection of face c section S in direction i
Sc^{sgs}	Turbulent Schmidt number
S_{ij}	Strain rate tensor
T_{ij}	Tensor for the momentum dynamic model
u_τ	Friction velocity
U	Uncertainty
$\langle u \rangle$	Time averaged velocity
$\langle u \rangle_b$	Bulk velocity
$\langle u \rangle_{bi}$	Inner bulk velocity, in pipe
$\langle u \rangle_{bo}$	Outer bulk velocity, in annulus
u_{cl}	Axial velocity mean value at the inlet centre
u_i	The i component of the velocity vector, in Cartesian coordinates
$\langle u' \phi' \rangle$	Time averaged turbulent streamwise passive scalar flux
$\langle u' u' \rangle^{1/2}$	Time averaged velocity fluctuation
$\mathbf{v}$	Velocity vector
v^*	Velocity at cell face after projection step
W	Wedge length
x_i	Cartesian coordinates, $x_1 = x$, $x_2 = y$, $x_3 = z$

Greek Symbols

α	Passive scalar diffusivity
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α^{sgs}	Turbulent mass diffusivity
β	Diameter ratio
$\overline{\Delta}$	Filter width (grid)
$\widehat{\Delta}$	Filter width (test)
δ_{ij}	Kronecker delta
Δt	Time step
ϕ	Passive scalar, or generic variable, to define numerical procedures
$\langle \phi \rangle_d$	Passive scalar mean value at the inlet centre
ϕ_{dil}	Fully diluted concentration
ϕ_{in}	Inlet (maximum) concentration
$\langle \phi' \phi' \rangle^{1/2}$	Time averaged passive scalar fluctuation
$\langle \phi \rangle$	Time averaged passive scalar
λ	Linear interpolation coefficient
λ_ν	Viscous length
μ	Fluid dynamic viscosity
ν	Fluid kinematic viscosity
Ω	Cell volume
Π	Budget pressure gradient term
Ψ	Flux limiting function
ρ	Fluid density
σ	Standard deviation
τ_{ij}	Shear stress tensor ij component
τ_w	Wall shear stress

Superscripts and subscripts

$\bullet_D$	Downstream node
$\bullet_E$	Variable in the east cell centre

$\bullet_{E'}$	Variable in position E' (figure 3.3)
$\bullet_e$	Variable in the cell face centre
$\bullet_{e'}$	Variable in the estimated cell face centre
$\bullet_{min}$	Minimum value
$\bullet_{max}$	Maximum value
n	Direction normal to the cell face
$\bullet_P$	Variable in the cell centre
$\bullet_{E'}$	Variable in position P' (figure 3.3)
$\bullet_U$	Upstream node

Operators

$\langle \bullet \rangle$	Time or ensemble average
$\bullet'$	Fluctuation from the mean
$\hat{\bullet}$	Test-filtered quantity
$\bar{\bullet}$	Resolved, grid filtered, quantity
$\bullet^{sgs}$	Subgrid-scale quantity

Abbreviations

DNS	<i>Direct Numerical Simulation</i>
LDV	<i>Laser-Doppler Velocimetry</i>
LES	<i>Large-eddy simulation</i>
LIF	<i>Laser-induced Fluorescence</i>
PDF	<i>Probability density function</i>
RANS	<i>Reynolds-averaged Navier-Stokes simulations</i>

Chapter 1

Introduction

Mainly because it requires a three-dimensional and time-dependent high-resolution simulation LES was for a long time confined to research and simple, ideal flows, due to lack of computational power. However, the availability of both cheaper and more powerful computers now allows LES to be applied to more realistic cases, that resemble industrial flows. The present work deals with turbulence in fluids, focusing on the mixing of a high Sc passive scalar in the entry region of a confined coaxial jet flow. An experimental database on the same flow was reviewed and matching LES simulations were run.

1.1 Motivation and importance

The flow configuration being studied, a circular jet transporting a passive scalar enclosed by an annular one, mimics flows of industrial interest, relating to combustion chambers and injection systems, and of environmental interest, relating to jet discharges. It is also the model for confined mixing in more complex geometries and has been studied previously in considerable extent, either by numerical or experimental techniques.

Turbulent flow is the most frequent regime in industrial and environmental flows; engineers need ways to predict it and LES has become a reliable approach. The solution of the passive scalar field is important in practical applications, such as pollutant dispersion, and is a first step in the simulation of chemical reaction, *e.g.*, combustion. The availability of reliable LES of the velocity field allowed focus to shift to the solution of the passive scalar field. Although mathematically simpler than the Navier-Stokes equations, the numerical solution of the passive scalar transport equation applied on top of a turbulent velocity field proved harder than first imagined.

The passive scalar transport equation does not have the pressure gradient term, that in the Navier-Stokes equations regularises the velocity field. This means that local variations

are sharper in the passive scalar field. The fractional-step pressure correction ensures accurate mass conservation of the main fluid. No such mechanism is in place for the passive scalar contaminant. Finally, the passive scalar must respect a boundedness property, that requires upwind biased convective term discretization to be observed in numerical simulations.

Most simulations of the passive scalar field focus on the mean field only. This is in part explained by the absence of experimental measurements of the passive scalar turbulent quantities with uncertainty estimates: neither Johnson and Bennet (1981) nor Lima (2000) included uncertainty estimates for those quantities. The accuracy of the fluctuation, $\langle \phi' \phi' \rangle^{1/2}$, is a necessary first step to access the stochastic variability of a passive scalar (*e.g.*, a harmful pollutant) in order to estimate peak concentration and even mixing rate. The accuracy of the turbulent scalar flux, $\langle u' \phi' \rangle$ is essential for LES to be used in the improvement of RANS passive scalar models, as $\langle u' \phi' \rangle$ is the term modelled in the RANS closure.

The goal of this work was to analyse the agreement between experiment and LES simulations and the influence and interplay of modelling and numerical choices, using experiments with uncertainty information. This involved a series of LES simulations, where modelling (*i.e.*, the Sc^{sgs}) and numerical parameters (*i.e.*, the discretization of the convective terms) were modified and compared against the experiments. The experimental database of Lima (2000) was reviewed in order to compute estimates of uncertainty for the passive scalar turbulent statistics, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, and to choose the conditions most appropriate for comparison with numerical experiments.

1.2 Brief bibliographic review

In the present work we study turbulent flow. The following quote from Lumley and Yaglom (2001) shows why it is still important to study turbulence:

”The field [turbulence] does not appear to have a pyramidal structure, like the best of physics. We have very few great hypotheses. Most of our experiments are exploratory experiments. What does this mean? We believe it means that, even after 100 years, turbulence studies are still in their infancy. [...] We do have a crude, practical, working understanding of many turbulence phenomena but certainly nothing approaching a comprehensive theory, and nothing that will provide predictions of an accuracy demanded by designers. [...] Each [engineering approach] represents a kind of experiment, that can tell us something about turbulence”

The present work uses LES and measurement *experiments*, in the Lumley and Yaglom (2001) sense, to study the confined mixing of coaxial jets, particularly the behaviour of passive scalar turbulent quantities. In this section the work is placed in connection to the state of the art on free and confined mixing in coaxial jets by the time the thesis work

started, *circa* 2002; relevant later works are also quoted.

Unconfined coaxial jets can be seen either as a superposition of two jets (Ko and Kwan, 1976) for low velocity ratio or as a superposition of a mixing layer and a wake (Dahm et al., 1992). Coaxial confined jets add a pressure gradient and the interaction of boundary layers from the external wall with the shear layer, whose effect is small in the entry region.

Unconfined jets have been studied for a long time, with older works focusing on mean profiles. Ko and Kwan (1976) seem to be the first to analyse coherent structures, inferred from mean velocity and pressure fields and from spectral analysis. They identify two shear regions, connected to two peaks in the velocity spectra, corresponding to vortices originating in each shear layer. They also identify two potential cores associated with the inner and outer jets. Dahm et al. (1992) made a study based on LIF visualisation, that allowed direct observation of coherent structures and underlined the importance of the velocity ratio r in the selection of flow regimes. This work was the first to detect a locking mechanism between the vortices from each shear layer. The importance of the velocity ratio was analysed in Rehab (1997) that identified a critical velocity ratio above which recirculation occurs. It was found that this critical velocity ratio is affected by β , the diameter ratio: an higher diameter ratio results in higher critical velocity ratio.

This focus on the physics of coherent structures was followed in a preliminary work presented in appendix D and is also seen on recent LES and DNS studies such as Balarac and Métais (2005) and Balarac et al. (2007b).

Being a model of industrial flow (*e.g.*, combustion chambers), the confined case has more often been the target in validation exercises. The most cited experimental work on confined coaxial jets is Johnson and Bennet (1981), where the coaxial jets exit into a sudden expansion. A passive scalar, fluorescein in water, with Sc about 2000, is measured. The uncertainty analysis is made only for the mean values, but fluctuation and turbulent scalar flux are presented. The geometry of Johnson and Bennet (1981) is simulated using LES in Akselvoll and Moin (1996). In this work, the passive scalar is seen as a turbulent flow tracer and analysis is based on $\langle\phi\rangle$, where fair agreement is shown, and on visualisation of instantaneous fields. Neither the Sc used nor $\langle\phi'\phi'\rangle^{1/2}$ or $\langle u'\phi'\rangle$ are reported. Those were the main references at the beginning of the present work.

The work of Lima (2000) is an improvement over Johnson and Bennet (1981) and focuses on the coaxial jet mixing; there is no sudden expansion. The uncertainty analysis also focus on the mean value but the availability of the experimental database allows the determination of uncertainty estimates for higher-order statistics.

Recently, other LES simulations of confined coaxial jets have been published. The work by Dianat et al. (2006) simulates Lima (2000) measurements of $r = 3.2$. Fair agreement is shown for $\langle\phi\rangle$ and $\langle\phi'\phi'\rangle^{1/2}$, but $\langle u'\phi'\rangle$ is not presented. A set of papers about coaxial jets of very low velocity ratio $r \approx 0.2$, related to a jet with co-flow or to a coaxial sudden expansion, have been recently reported. Zhdanov et al. (2006) presents the experimental

measurements, $\langle u'\phi' \rangle$ is not reported; in Jahnke et al. (2004, 2005) LES simulations on the same geometry are presented and a comparison is made at Hassel et al. (2006). The LES work from Jahnke et al. (2005) uses a fixed $Sc^{sgs} = .7$ and focus on the degree of mixedness, a quantity derived from $\langle \phi \rangle$. The influence of Sc is studied, comparing a test with air ($Sc = 0.7$) with a test with water ($Sc = 1000$), concluding that the influence of the Sc number itself is very weak and comparable with magnitudes of errors of the numerical method.

While it is well known that reproducing passive scalar fluctuation and turbulent scalar flux is a hard problem (*e.g.*, rigorous DNS studies of $O(1000)$ Sc have only been completed recently and for low Re Yeung et al., 2004), earlier works did not report the problem (*e.g.*, Akselvoll and Moin, 1996). Mistrust on the reliability of measurements of these quantities might be the cause, as even the mean values consistency of Johnson and Bennet (1981) is questioned in Akselvoll (1995), who recommends the use of a different experiment to verify the computational results. A recent study of coherent structures in a confined jet (Akihiko et al., 2007) compares against experiment for the $\langle \phi \rangle$ field only.

In the review by Dimotakis (2005) the fundamental problems of passive scalar mixing measurement and simulation are outlined and the most promising approaches to solve those problems are pointed out: improved experiments and large-eddy simulation. The validation of turbulence simulations not constrained to simple average profiles is recommended. The present work goes in that direction, using LES with dynamic models and LIF based measurements to compare measured passive scalar turbulent quantities against LES simulations.

1.3 The contributions of this work

The measurements from Lima (2000) were post-processed in order to analyse $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ in more depth than was done in Johnson and Bennet (1981) and adapted the code of Silva Lopes (2000) to improve upon Akselvoll (1995) by including analysis of the passive scalar turbulent quantities, compared against the experimental measurements. The main contributions are now summarised:

- Gathering, preservation and synthesis of the database of experimental measurements from Lima (2000). Analysis of the probability density functions of u and ϕ . Evaluation of the results quality using a variety of methods, concluded with a choice of the conditions most appropriate for numerical simulation. Determination of confidence intervals and of typical uncertainties for $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, using the bootstrap method and analysis of the effect of noise.
- Developments in VISCT, the LES code of Silva Lopes (2000): Second order discretization for highly orthogonal grids was added, including an improvement on the continu-

ity enforcing procedure from Ferziger and Peric (2002); passive scalar transport has been included, using a TVD method and a bounded convection scheme (Herrmann et al., 2004); a dynamic model for subgrid scale passive scalar transport (Keating, 2004) has been implemented and tested. Budgets of the transport equation of passive scalar statistics, focusing on the numerical origin, have been computed and analysed.

- LES simulation of confined coaxial jets, showing good results in a simulation that could be part of an industrial multiblock code. The velocity field is validated, with good agreement in the mean and fluctuating fields.
- An investigation of passive scalar mixing in LES of coaxial jets. A dynamic subgrid scale model for the passive scalar was implemented along with computation of the budgets of numerical terms. The reproduction of $\langle \phi \rangle$ was good and $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ are presented. A link between the results and the diffusivity independence hypothesis is proposed.

1.4 Outline of this thesis

The thesis starts with the analysis and improvement of the experimental database of Lima (2000) in Chapter 2. This is achieved by preserving the database in a much more accessible format, by increasing the detail in the geometry description and, most importantly, by reviewing the post-processing and adding uncertainty analysis of higher order statistics, using resampling methods and noise analysis.

In Chapter 3, the mathematical and numerical tools used in the LES simulations are presented, including the passive scalar transport solver and the passive scalar subgrid scale model; the details of the equations for budget analysis appear in Appendix A. The connection between the mathematical model and the LES simulation, through validation exercises, is in Appendix B.

Chapter 4 is concerned with the simulations, presented and compared to the experiments in order to get physical and numerical knowledge.

Conclusions are summarised in Chapter 5. A RANS based analysis of the confined coaxial jets flow (Appendix C) was made to verify the potential and limitations of this approach and a simulation of the hydrodynamic field based on experimental inlet profiles and using a sixth-order code (Appendix D) was made to analyse the transition and compare the preferential frequencies with experimental results.

Chapter 2

Post-processing of LDV/LIF Measurements of Passive Scalar Mixing in Confined Coaxial Jets

Abstract

The experimental database was classified, analysed and stored in modern media, in an universally readable format. The details of the flow upstream of the test section and all the geometric details needed to set-up a numerical simulation are included. The post-processing was redone, and confirmed the analysis by Lima (2000). The uncertainty of the experiments was assessed by a variety of techniques, including bootstrap analysis. Condition with $r = 0.8$ had more accurate mean values, whereas $r = 3.2$ was a good compromise between accuracy on the mean values and on turbulent quantities. Accordingly, the two conditions were chosen for use in validation of numerical simulations.

2.1 Introduction

Verification and validation The discrepancies between measured and calculated flow properties are due to model inaccuracies, numerical error, measurement uncertainty and discrepancies in the boundary conditions (Pope, 2000, pg. 342). The last two are related to the measurements and need to be smaller than the numerical error, if conclusions about the model accuracy are to be established. Uncertainty determination is a pre-requisite of a good experimental database, namely if the aim is the usage of that database in flow model development and appraisal. This has been recognised for some time now, and is part of the author's instructions in many scientific journals (*e.g.*, Roache et al., 1986);

however, experimental databases without uncertainty analysis are still common. The need for an accurate determination of experimental uncertainty is closely related to the concepts of Verification and Validation (V&V) in computer modelling (Roache, 1998; AIAA, 1998; AGARD, 1998), which in addition require experiments designed in accordance, or guided by the requirements of V&V, as was the case of the experiments in Lima (2000).

Database size and format The time series database, scattered in about three hundred 1.44 MBytes floppy disks, and in a proprietary binary format, was copied to one compact disk, after conversion to universally readable text files. The measurements were all made in Lima (2000) but all the profiles presented here have been made from the stored timeseries and can be viewed as a verification of the post processing, as no major inaccuracies have been found.

PDF analysis The behaviour of probability density functions matched the general conclusions from recent works (*e.g.*, Balarac et al., 2007b): non-marching behaviour is observed when very large scale mixing is present, whereas when structures are smaller, marching PDF's have been found.

Uncertainty appraisal The uncertainty of the measurements was evaluated by classical methods, by bootstrap methods, by mass flux uncertainty analysis and computation from mean profiles and by studying the effect of optical and electronic noise on the passive scalar measurements of turbulent quantities. It was found that mean quantities are best reproduced for velocity ratio $r = 0.8$, whereas $r = 3.2$ was the best compromise between accuracy on the mean values and on the turbulent quantities. The effect of noise was found to be important on the measurement of passive scalar turbulent quantities leading to overevaluation of $\langle \phi' \phi' \rangle^{1/2}$ and underevaluation of $\langle u' \phi' \rangle$.

In the present chapter and before embarking on the computer simulations, the database of Lima (2000) is revisited, including its reorganisation, production of software tools for its analysis and uncertainty analysis by a variety of techniques in order to choose the most appropriate conditions for comparison with numerical simulations. Analysis new to this work, comparing to Lima (2000), are the survey of Rhodamine-B Sc number, the smooth curve fits that take into account both halves measured, the bootstrap based confidence intervals and typical uncertainties, the analysis of the effects of noise on the uncertainty of higher order statistics and the analysis of behaviour of probability density functions.

Chapter outline The chapter starts with a detailed description of the flow, section 2.2, followed by a presentation of the post-processing and verification techniques, section 2.3. Results and discussion are presented in section 2.4 and the conclusions are summarised in section 2.5.

2.2 Detailed flow description

In this section, the details of geometry and flow conditions required to set up a simulation are described, sections 2.2.1 and 2.2.2. This adds extra detail in the test section inlet and in the flow upstream of the test section, compared to that available in Lima (2000). In section 2.2.3 a discussion on the Schmidt number value is made.

2.2.1 The geometry

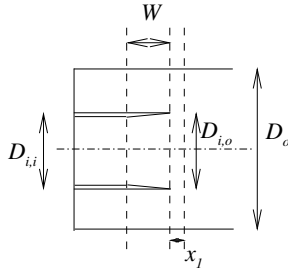


Figure 2.1: Test section geometry

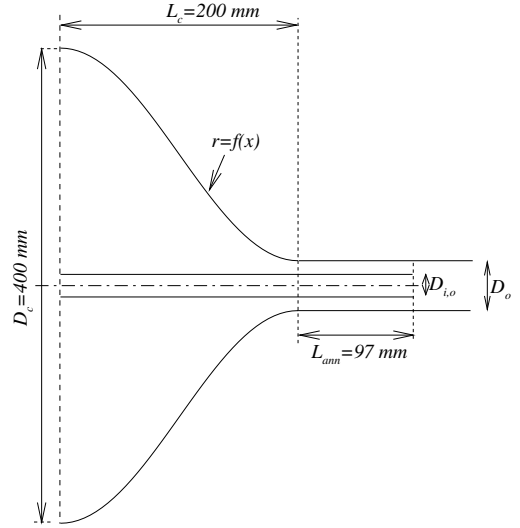


Figure 2.2: Upstream region geometry

The flow studied is the coaxial confined jet flow, shown schematically in figure 2.1. At the inlet section of a pipe ($D_o = 42$ mm) there was an inner flow, coming from the inner pipe, with internal diameter $D_{i,i} = 17$ mm, carrying a mixture of water and Rhodamine-B, the fluorescent tracer, a passive conserved scalar, surrounded by a flow of water; the annulus flow, with internal diameter $D_{i,o} = 19$ mm and external diameter $D_o = 42$ mm. Both the inner pipe flow and annular jet flow are then discharged into the large pipe and mixing occurs along a 2 m length. The inner pipe wall, with 2 mm thickness ($D_{i,o} - D_{i,i} = 19 - 17 = 2$ mm) ends in a smooth wedge, with length $W = 7.1$ mm and 8° angle. The average internal diameter, $D_i = 0.5(D_{i,i} + D_{i,o})$, is used to compute the diameter ratio $\beta = D_o/D_i = 2.33$. The first measurement station is located at $x = 2.38$ mm, corresponding to $x/D_{i,i} = 0.14$. The annulus hydraulic diameter is defined as

$$Da = \pi(D_o^2 - D_i^2)/\pi(D_o + D_i) = D_o - D_i.$$

The annular jet was preceded by a converging nozzle and stabilising panels, designed to ensure a flat profile at the inlet of the annulus section with low turbulence intensity, according to Bradshaw (1965) criteria. A scheme of the upstream region is presented in figure 2.2. The converging nozzle starts with a diameter $D_c = 400$ mm and reduces to D_o in a length $L_c = 200$ mm, *i.e.*, a contraction ratio $(D_c - D_o)/D_a$ of about 15. The radius along the nozzle follows the function

$$r = f(x) = 0.5D_c - 0.5(D_c - D_o)(1 - \cos(\pi x/L_c)).$$

The annulus length is $L_{ann} = 97$ mm.

2.2.2 The flow conditions

Five flow conditions, table 2.1, were measured by Lima (2000), defined by the inner and outer bulk velocities, $\langle u \rangle_{bi}$ and $\langle u \rangle_{bo}$, and thus with various velocity ratios, $r = \langle u \rangle_{bo}/\langle u \rangle_{bi}$. The inner bulk velocity was computed with the pipe inner diameter, $D_{i,i}$.

	$r = 3.2$	$r = 2.0$	$r = 1.1$	$r = 0.8$	$r = 6.5$
Condition N.	1	2	3	4	5
Re	29390	30452	29898	34993	28478
Re_o	9450	9450	8653	9450	9450
$\langle u \rangle_{bo}$ [m/s]	0.83	0.83	0.76	0.83	0.83
Re_i	4376	7069	11614	17673	2134
$\langle u \rangle_{bi}$ [m/s]	0.26	0.42	0.69	1.08	0.13

Table 2.1: Flow conditions

The interior jet was at the outlet of a 2 m, or $48D_i$, pipe. This is larger than the criteria for fully developed flow quoted in White (1988), $L_{trans} = 4.4Re_i^{1/6}D_i$, that is about 25 D_i for all conditions. A mean velocity fully developed profile occurs in the interior jet. The passive scalar is fully mixed in $\langle \phi \rangle$ but fluctuations $\langle \phi' \phi' \rangle^{1/2}$ may still be present (see section 2.4.5 for a discussion).

The annulus length was $L_{ann} = 0.097$ m, or 4.2 D_a . The development length is for the annulus $L_{trans} = 4.4Re_o^{1/6}D_a$, about 20 D_a in all conditions. Therefore, the annulus jet mean velocity profile is far from developed, being close to a flat profile with little turbulence, as intended in the experiment design.

The interior pipe jet transported the fluorescent tracer, with a constant concentration of 0.04 mg/l. There is no chemical reaction between the water and the Rhodamine-B, which retains its properties in the course of the experiment (*cf.* Lima, 2000, pg. 72–74), and there are no sources or sinks; this is the case of passive scalar conservation.

2.2.3 The Schmidt number

The fluorescent tracer was Rhodamine-B ($\text{C}_{28}\text{H}_{31}\text{ClN}_2\text{O}_3$). Assuming infinite dilution, defined as an environment where the solute is both highly dense and far from pure component, the diffusivity coefficient was $\alpha = 2 \times 10^{-9} \text{ m}^2\text{s}^{-1}$ (Reid et al., 1988). The reason for the much lower diffusivity of liquid mixtures compared to gaseous ones has to do with the fact that, in liquids, molecules are densely packed and strongly affected by force fields of neighbouring molecules (Poling et al., 2004). In the case of standard values of water kinematic viscosity (*e.g.*, $\nu = 1 \times 10^{-6} \text{ m}^2\text{s}^{-1}$ at 20 °C, from White (1988)) yields a Schmidt number of $Sc = \frac{\nu}{\alpha} \approx 500$.

There is no established method to compute Sc , particularly accounting for the concentration, and the estimate has a large and unknown uncertainty. The work by Vincont et al. (2000) gives a value of $Sc \approx 2500$, while dyes in water in general are known to have Sc of the order 1000 (*cf.* Pope, 2000, pg. 165, where 1500 is quoted) The absence of a reference value in the published literature can be understood from Poling et al. (2004), an updated version of Reid et al. (1988): many methods and ways to correct for the effect of concentration are presented. I have used an estimate of $Sc = 1000$ simply because it is between the Lima (2000) and Vincont et al. (2000) estimates and is the generally accepted order of magnitude value. For safety, two preliminary simulations with $Sc = 500$ and $Sc = 2500$ should also be made.

2.3 Techniques for verification and post-processing of experimental results

In this section we present the methods used in the verification and post-processing of Lima (2000) measurements. We start with a review of the measurement details, section 2.3.1, then the storage procedure is described (section 2.3.2) and the post-processing library that includes a method for PDF estimation from small timeseries is presented, section 2.3.3. The section concludes with a presentation of the various techniques used for estimating the results uncertainty, section 2.3.4.

2.3.1 Measurement details

Measurements for axial and radial velocity, using LDV, Laser-Doppler Velocimetry, and concentration of Rhodamine-B, using LIF, Laser Induced Fluorescence, have been made (Lima, 2000) and are post-processed. The database includes the time series for axial and radial velocity, and concentration of Rhodamine B at 9 axial locations, table 2.2, over 32, sometimes more, radial locations, covering one full diameter. For every 32 radial locations

there is one time series containing as a rule 2000 measurements; a few have 5000 and 20000 measurements.

Position	1	2	3	4	5	6	7	8	9
$x/D_{i,i}$	0.14	1	2	4	8	16	32	64	100
x/D_o	0.06	0.40	0.81	1.62	2.24	6.48	12.95	25.90	47.62

Table 2.2: Axial positions measured

The radial location uncertainty is about 0.5 mm: Although the spatial resolution is $5\ \mu\text{m}$, the control volume size is $0.97 \cdot 0.075\text{ mm}^2$; taking half of the largest ellipses length leads to the radial location uncertainty of 0.485 mm, *i.e.*, $0.06(D_i/2)$ (*cf.* Lima, 2000). The geometry dimensions have an uncertainty estimated in 0.1 mm ($0.01(D_i/2)$), typical of the material used (perspex). The measurement equipment was not prepared for measurements near the wall, and it was determined that passive scalar measurements required a distance from the wall higher than 2 mm, *i.e.*, up to $2r/D_i = 2.24$.

2.3.2 Storing the measurements

At the start, data post-processed using Fortran and Excel was available but to check and improve this analysis was a goal of our work. To improve the previous work, access to the original measurement timeseries was required. About three hundred timeseries had been stored in floppy disks, in a binary format, proprietary of the Fortran compiler used. The timeseries were recovered to check the original analysis and to apply additional software treatments.

After deciding to recover the full experimental database, the question of how to store it arose. An investigation of the methods and software available was made and is reviewed in section 2.3.2.1. The decision was made to store the timeseries in ASCII text, readable on any computer, and to organise them in a tree-like directory structure, stored on a data CD.

The first step was to copy the original binary format timeseries to a data CD, organised by the floppy disk labels used in the lab notebooks of Lima (2000). Then the whole set of timeseries was converted to ASCII text using the original Fortran compiler. Finally, the timeseries were organised by variable, flow condition and axial location (see section 2.3.2.2 for a detailed description). The dataset was ready for post-processing using powerful tools, such as Matlab and Tecplot.

2.3.2.1 Storage of scientific data

Both experimental measurements and numerical simulations generate data that must be stored in convenient format. The format should be portable, *i.e.*, readable in various computers, fast to read and write and compact. The following methods, with advantages and disadvantages, have been identified:

- ASCII text: Appropriate for small datasets. The files can be read on any computer and documenting info can be added with any text editor. However the files can become inadequately large, particularly if three-dimensional fields are being analysed, as is the case with LES simulations.
- Binary files: This is the simplest method; the files produced by the computer program, using the proprietary format defined by the compiler are used. This is fastest, both for file reading and writing and produces the smallest files. However, reading the files without the compiler that generated them may require access to the original source code and some knowledge about the compiler internal definitions. A mixed solution is to store in binary format and add a text header with content description and code fragments to ease reading. This is done in AGARD (1998), that also provided a conversion utility to allow conversion of files between the big-endian and little-endian storage schemes.
- Scientific data packages: combine small size and portability, and have facilities to introduce scientific data, such as boundary condition information. Hierarchical file formats are used, where various types of scientific data and documentation can be stored. This includes NetCDF (Brown et al., 1993), HDF (Group, 2008) and CGNS (Group, 2001), a solution targeted at CFD data files. The files are binary, but C and Fortran software libraries are provided that allow data to be read on any computer, but this requires the installation and use of new software and programming libraries. Some of the packages, such as CGNS, allow the storage of boundary condition information, thus avoiding errors in the reproduction of boundary conditions.

It was decided to keep the results in ASCII text files. These text files can easily become impracticably large but not in this experiment: after conversion to ASCII format, the database of measurements occupied 300 MBytes. This is well below the 600 MBytes storage capacity of a data CD. The files can be used in any operating system and with any data processing or visualisation software. Mac-OS, Linux and Windows have been tested and Matlab, Tecplot and Excel have been used. Meta-Data, *i.e.*, documentation, can be simply appended to the files, if so desired.

2.3.2.2 Guide to the data on the CD

The data CD is divided in four subdirectories, with names **Uaxial**, **Vradial** and **Wtang** where u , v and w velocity components are stored. A fourth directory, **Ucl**, contains axial velocity measurements along the centreline. All these timeseries contain passive scalar measurements.

Focus has been on the axial measurements, u , because according to Lima (2000) the accuracy of the simultaneous measurement of v and ϕ was significantly worse than u and ϕ . Only a few w measurements have been made, to check that swirl effects were of small importance. Nonetheless, the timeseries have been converted and stored.

The directory under u is the most complete. It is divided in directories **cond1** to **cond5**, corresponding to the condition numbers defined in table 2.1. Each condition directory contains nine subdirectories, **sec1** to **sec9**, corresponding to the nine axial locations defined in table 2.2. Each section directory contains 32 or more timeseries text files, with names D01, D02, etc. The correspondence between file name and radial locations can be seen in file `get_stats_zone.m`, where the Matlab `basic_analysis.m` routine is called and conversion parameters stored, with comments. By modifying the file `basic_analysis.m` different statistical procedures from the post-processing library (section 2.3.3) may be applied to the timeseries.

The timeseries file is a three-column text file of tab-separated numerical values, with the measurement time (in s) in the first column, the velocity (in m/s) in the second and the fluorescence intensity (in mV) on the third column, from which ϕ is computed.

2.3.3 The MATLAB post-processing library

The analysis of the time series was made using MATLAB, version 7.0.0.19901 (R14, 2004), running on Intel processors using the Linux operating system (Fedora Core release 4, Linux kernel 2.6.14). The MATLAB prebuilt routines have been customised to our requirements; routines were written to perform the following tasks:

- To compute the first four statistical moments (mean, fluctuation, skewness and kurtosis) and the turbulent scalar flux ($\langle u'\phi' \rangle$, $\langle v'\phi' \rangle$), with uncertainty estimates.
- To produce spline-based curve fits of the radial profiles.
- To estimate mass flow rate based on the radial profiles of $\langle u \rangle$ and $\langle \phi \rangle$.
- To plot estimates of probability density function (PDF).

The higher-order moments and the uncertainty estimates were computed using the MATLAB statistics toolbox (release 5.0).

Profile fittings were obtained by first folding the two halves of the measured profiles and then applying the smoothing spline of the MATLAB curve fitting toolbox (release 1.1.1). This is based on routine `csaps.m`, from the spline toolbox, which is a translation of `smooth.f`, the standard cubic smoothing spline from de Boor (2001). The routine can be described as a mix between a linear fit and a cubic spline designed to be close to the measurements and yet be smooth.

The timeseries had a relatively small number of samples to obtain a well resolved PDF. To allow an analysis, a smoothing algorithm was used to estimate the PDF. The routine `plotdens.m` from Stibox 1.29 (2000), by Anders Holtsberg, was used. It implements the smoothing algorithm of Silverman (1986), a kernel density estimate, where Gaussian functions are associated with each sample value and the estimate is a normalised sum of all the functions. Use of this PDF estimator leads to much smoother PDF estimates than it is possible using histograms, at the risk of smoothing out important features, which was not the case with the present datasets.

2.3.4 Uncertainty analysis

Evaluation of uncertainty in turbulence experiments is done either using uncertainty propagation analysis or applying statistical methods to the measurements. The first approach is presented in Coleman and Steele (1989) and has been used in Lima (2000); the second, resampling bootstrap method, is now a popular approach: the paper by Benedict and Gould (1996), which applied to turbulence the methods of Efron and Tibshirani (1994), is cited in many works and in some used as the main tool for uncertainty evaluation *e.g.*, Sadr and Klewicki (2003).

In the previous work (Lima, 2000) no comments were made on the uncertainty of passive scalar fluctuation $\langle \phi' \phi' \rangle^{1/2}$ and turbulent scalar flux $\langle u' \phi' \rangle$. These quantities are crucial for the study of turbulence and we combined bootstrap, noise effect and visual inspection to reach a recommendation on the best condition for comparison with numerical simulations. These methods are outlined in this subsection.

2.3.4.1 Estimates based on uncertainty propagation analysis

In the work of Lima (2000), uncertainties of the mean measurements and of the flow rates were provided, based on Coleman and Steele (1989) and on the measurement equipment data. We have taken a fresh look on this analysis. Lima (private communication) provided uncertainties for the passive scalar that took into account mass flow rate uncertainties, reaching uncertainties for $\langle \phi \rangle$ measurement that depend on the experimental condition.

The same approach has been followed to reach uncertainties for the bulk velocity, neglecting the uncertainty in $A_i = \pi D_i^2$, $A_o = \pi D_o^2$ and $A = A_i + A_o$, that is of no relevance

in the selection of the best conditions:

$$U_{\langle u \rangle_b} = U_Q/A \text{ thus } U_{\langle u \rangle_b}/\langle u \rangle_b = U_Q/Q$$

$$U_{\langle u \rangle_{bi}} = U_{Q_i}/A_i \text{ thus } U_{\langle u \rangle_{bi}}/\langle u \rangle_{bi} = U_{Q_i}/Q_i$$

$$U_{\langle u \rangle_{bo}} = U_{Q_o}/A_i \text{ thus } U_{\langle u \rangle_{bo}}/\langle u \rangle_{bo} = U_{Q_o}/Q_i$$

The bulk velocity ratio can also be computed:

$$r = (Q_o A_i)/(Q_i A_o) \text{ thus } U_r/r = \sqrt{(U_{Q_o}/Q_o)^2 + (U_{Q_i}/Q_i)^2}.$$

These uncertainties are not removed with profile normalisation, because all profiles are normalised with the same value, the centreline measurement at $x/D_{i,i} = 0.14$.

2.3.4.2 Estimates based on mass and scalar flux consistency

In a confined flow an estimate of the data quality can be obtained by verifying the mass conservation in radial profiles along the test section.

The flow rates were determined by integrating the mean axial velocity and concentration radial profiles. To evaluate the integrals, a quadrature formula was used between each pair of values, *i.e.*, trapezoids were used, instead of steps. A wall law was used for the velocity close to the wall, and an extrapolation (constant gradient) was used for the scalar. Values were normalised with the average mass flow rates for each velocity ratio.

2.3.4.3 Estimates based on the bootstrap method

The bootstrap estimate of standard uncertainty is obtained by drawing from the time series N_{boot} random samples; it is typical of the bootstrap method that some elements may appear more than once. For each sample a replicate of the statistics being studied is calculated and the uncertainty is obtained from the standard deviation of the N_{boot} replicates. It is observed that for a high number of replications, the replicates distribution shows a tendency towards a normal distribution, which allows the determination of a 95 % confidence interval.

The bootstrap method provides an uncertainty estimate without any assumptions associated to the statistics distribution which are generally not valid when dealing with turbulent results. The method has only the implicit assumption that the true distribution is similar to the sample distribution. The bootstrap method evaluates the statistical uncertainty. This represents the uncertainty connected to the finite sample size and can be thought as evaluating the sample size adequacy.

Noise, or rather the signal to noise ratio, was not critical when measuring the mean values as its effect is small upon averaging. For the turbulent quantities, with the exception

of zero-level noise on $\langle\phi'\phi'\rangle^{1/2}$, no process of eliminating the noise statistically was found. This leads to effect overevaluation of $\langle\phi'\phi'\rangle^{1/2}$ and underevaluation of $\langle u'\phi'\rangle$. The effects are analysed in parts of the flow that are fully mixed and where $\langle\phi'\phi'\rangle^{1/2}$ is expected to be zero.

Confidence intervals We present the bootstrap confidence interval for all statistics. Confidence intervals were built using the bootstrap uncertainty. To build the confidence intervals, one simply subtracts and adds the uncertainty to the mean.

Relative uncertainties The standard definition of relative uncertainty of a variable ϕ is the ratio between its absolute uncertainty U_ϕ and the reference value ϕ , after its average. However, as ϕ approaches zero this measure of uncertainty becomes unbounded. In the analysis of Lima (2000) database, only $\langle u \rangle$ was adequately described by the relative uncertainty, since mean velocity was never close to zero. All other statistics are zero in parts of the domain and normalisation must be done in some other way. We compared $\langle\phi\rangle$ uncertainty with the fully mixed values, both in the interior jet ϕ_{in} and in the test section ϕ_{dil} . For $\langle u'u' \rangle^{1/2}$, $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi' \rangle$, maximum variable and maximum uncertainty were at about the same location, so the relative uncertainty of the maximum value was the measure sought.

2.4 Results and discussion

In this section, the results of the database post-processing are presented and discussed. A review of the uncertainty propagation analysis of Lima (2000) is first made (section 2.4.1), then the consistency of mass and scalar flux based on the radial profiles is reviewed (section 2.4.2) with profiles with error bars and curve fits being shown in section 2.4.3. The bootstrap uncertainty is quantified in section 2.4.4 and the effect of noise on the passive scalar measurement is analysed in section 2.4.5. The section ends with an analysis of the evolution of probability density functions, in section 2.4.6.

2.4.1 Uncertainty propagation analysis

In this subsection, the uncertainties computed by Lima (2000) using Coleman and Steele (1989) methods are post-processed to be interpreted in terms of bulk velocity uncertainties and velocity ratios uncertainties, along with condition-dependent passive scalar uncertainties for the maximum inlet value, ϕ_{in} , and for the fully diluted value, ϕ_{dil} .

An inspection of the uncertainties in table 2.3 shows that the velocity ratio uncertainties and the passive scalar uncertainty increases with the velocity ratio. The lowest mean value

	Uncertainty Estimate				
	$r = 3.2$	$r = 2.0$	$r = 1.1$	$r = 0.8$	$r = 6.5$
ϕ_{in}	13.9	9.0	5.8	4.1	28.0
ϕ_{dil}	26.0	17.2	10.9	8.0	51.5
$\langle u \rangle_b$	4.2	4.0	4.1	3.5	4.3
$\langle u \rangle_{bo}$	4.3	4.3	4.8	4.3	4.3
$\langle u \rangle_{bi}$	13.9	8.7	5.3	3.3	28.6
r	14.6	9.7	7.1	5.5	28.8

Table 2.3: Uncertainty estimates, in %

uncertainties are for $r = 0.8$ and the highest for $r = 6.5$. This analysis indicates that $r = 0.8$ is the best low velocity-ratio condition.

The high velocity-ratio conditions are of more physical and engineering interest and the following tests will inform the choice between $r = 2.0$, $r = 3.2$ and $r = 6.5$. Furthermore, this analysis deals with mean values only and other tools are needed to analyse the uncertainty of turbulent quantities.

2.4.2 Mass and scalar flux conservation

$x/D_{i,i}$	$r = 3.2$	$r = 2.0$	$r = 1.1$	$r = 0.8$	$r = 6.5$
0.14	0.92	1.01	1.03	0.98	1.02
1	0.99	0.98	0.99	0.99	1.05
2	1.01	1.02	1.02	1.00	0.94
4	0.99	1.03	1.01	1.02	1.00
8	1.02	1.01	1.00	0.99	1.05
16	1.02	1.01	0.98	1.01	0.96
32	1.03	1.01	1.01	1.01	1.02
64	1.03	0.99	0.96	1.01	1.01
100	1.03	0.93	0.99	1.01	0.90

Table 2.4: Water mass flow rate, normalised with ensemble average ($\dot{m}_{w,i}/\langle \dot{m}_w \rangle$)

The computation of mass flow rates by integration of the $\langle u \rangle$ and $\langle \phi \rangle$ radial profiles is closely connected with the $\langle u \rangle_b$ uncertainty computed in section 2.4.1. Instead of comparing with the nominal value, or with the first measurement station we compare with

$x/D_{i,i}$	$r = 3.2$	$r = 2.0$	$r = 1.1$	$r = 0.8$	$r = 6.5$
0.14	1.34	1.14	1.06	0.89	2.27
1	1.18	1.09	0.96	0.93	1.46
2	1.11	1.22	0.99	0.94	0.99
4	0.92	1.15	0.97	0.89	0.80
8	0.88	1.16	1.03	1.05	0.82
16	1.01	1.04	1.10	1.14	0.81
32	0.93	0.82	1.09	1.17	0.58
64	0.93	0.73	0.98	1.17	0.68
100	0.93	0.66	0.79	1.17	0.49

Table 2.5: Passive scalar mass flow rates, normalised with ensemble average ($\dot{m}_{\phi,i}/\langle\dot{m}_{\phi}\rangle$)

the ensemble average. On normalised profiles it is this deviation that will appear when comparing with numerical simulation profiles, that conserve mass.

Each profile was measured in a slightly different experiment (sometimes on different days) and therefore there is nothing preventing, within experimental uncertainty, the fluxes to become higher or lower than at the inlet section.

As a rule the variations were larger than the estimated bulk velocity uncertainties from table 2.3. This is to be expected, since the process of estimating the mass flow from the profiles has a large uncertainty, related to the measurement of ϕ and u and also to the r -location uncertainty. We estimated this uncertainty in the mass flow with a classic analysis in about 20 %. Nonetheless, the global trends coincide: the passive scalar mass flux uncertainty is much larger for $r = 6.5$ and $r = 3.2$, as predicted.

Comparison with (Lima, 2000, Appendix B, pg 210) was made for the extreme values. Although the new estimate is more accurate, the results are similar, which indicates that the differences are governed by the uncertainty on measurements and flow settings and not on the details of the profile integration procedure.

The differences between $r = 0.8$ and $r = 1.1$, the low velocity-ratio conditions, are small. The behaviour of $r = 2.0$ and $r = 3.2$ is also similar. However, $r = 6.5$ showed variations higher than 100 % in the passive scalar flux, and is clearly worse. The choice of high velocity-ratio condition is therefore narrowed to $r = 2.0$ and $r = 3.2$.

2.4.3 Profiles with confidence interval and fit

The measurements over the whole diameter are folded and a spline based curve fit of both halves is presented on the same plots. Figures 2.3 to 2.8 demonstrate the availability

of experimental profiles with confidence intervals and a smooth spline fit of the folded profiles. The other conditions were not explored in the same depth and the profiles are not shown.

The profiles symmetry, which can be seen on figures 2.4 to 2.8, shows that the effects of attenuation are small, certainly smaller than other uncertainties involved. Otherwise one would notice a gradual decay in concentration with the radial distance. Deviations from symmetry can have other causes, such as low quality or ageing of the perspex pipe, misalignment of the test section itself, misalignment of the laser traversing system with respect to the test section, etc. The symmetry of the profiles is therefore an indication of the measurements quality.

A detailed analysis of the flow physics is not the focus here and has been made in Lima (2000). We focus on details that are more relevant for the validation of numerical simulations:

- The passive scalar is fully mixed at the interior pipe outlet (*i.e.*, the test section inlet), and has a square profile at $x/D_{i,i} = 0$. The shape of $\langle\phi\rangle$ profiles at $x/D_{i,i} = 0.14$, the first profile in figures 2.4 and 2.6, showed that most of the mixing has occurred between $x/D_{i,i} = 0$ and $x/D_{i,i} = 0.14$.
- A visual inspection of the profiles shows good symmetry for all conditions in terms of $\langle u \rangle$ and $\langle \phi \rangle$; exceptions are $\langle u'u' \rangle^{1/2}$ for $r = 6.5$ and $\langle u'\phi' \rangle$ for $r = 1.1$, $r = 0.8$ and $r = 6.5$.

The scales used show that the turbulent passive scalar flux is significantly higher (5 to 20 $\times$) for high velocity ratio than for velocity ratio close to 1. The relative uncertainty of $\langle u'\phi' \rangle$ is lower for higher velocity ratio, as is verified on section 2.4.4.

- For $r = 6.5$, most variation occurred up to $x/D_{i,i} = 2$. Profiles further downstream already resemble the fully mixed profiles that, in other conditions, only appear for much larger $x/D_{i,i}$; the passive scalar for $x/D_{i,i} > 4$ of $r = 6.5$ is almost fully mixed.
- Skewness and kurtosis are connected with the probability distribution and are important in the description of turbulence and profiles, with error bars, for $x/D_{i,i} = 1$ are shown in figure 2.9 for $r = 3.2$ and in figure 2.10 for $r = 0.8$. A simple inspection of the scales shows that the $r = 0.8$ condition is much closer to Gaussian, with minor deviations from the 0 skewness and 3 kurtosis that characterise Gaussian behaviour of the PDF. In contrast, $r = 3.2$ is likely to have large, fat tails. This is confirmed in the PDF estimates of section 2.4.6. The asymmetry and flatness indicated by the large values of skewness and kurtosis are signs of the "fat tails" that can be observed in the probability distributions (section 2.4.6). The fat tails can be described as "deviations from Gaussianity", but that hides the fact that the probability of large deviations (say 5σ) from the mean is many orders of magnitude higher than on a Gaussian distribution.

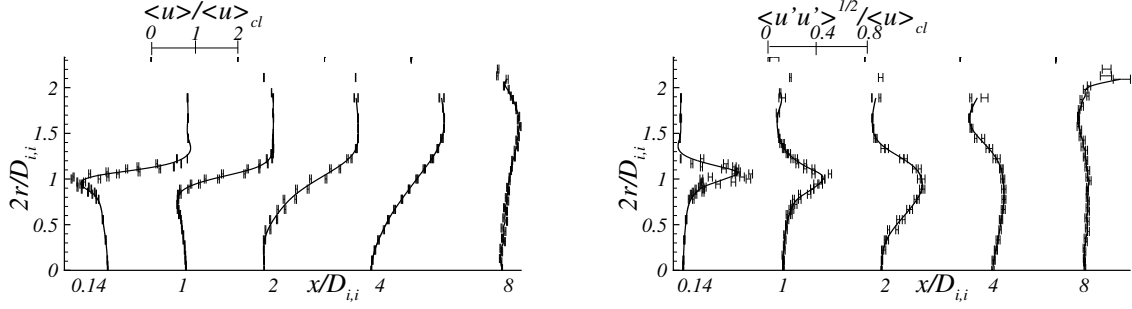


Figure 2.3: Streamwise velocity mean and fluctuation, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 3.2$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: curve fit

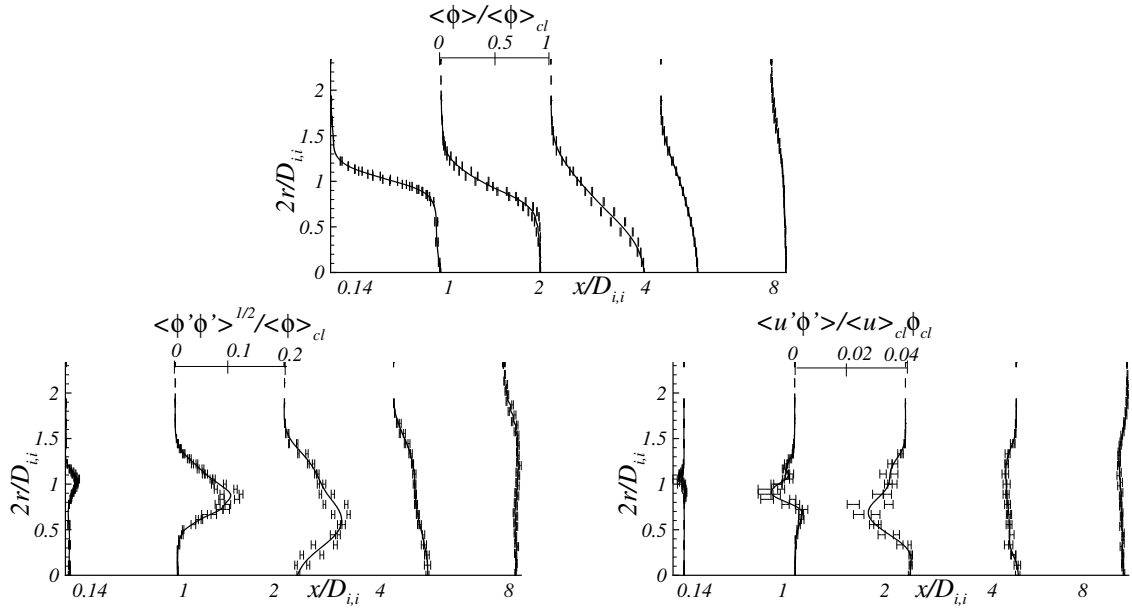


Figure 2.4: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 3.2$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: curve fit

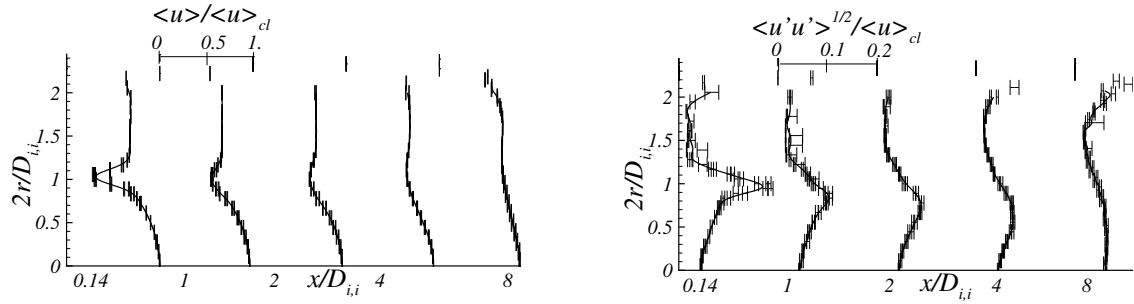


Figure 2.5: Streamwise velocity mean and fluctuation, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 0.8$ at $x/D_{i,i} = 0.14, 1, 2, 4$ and 8

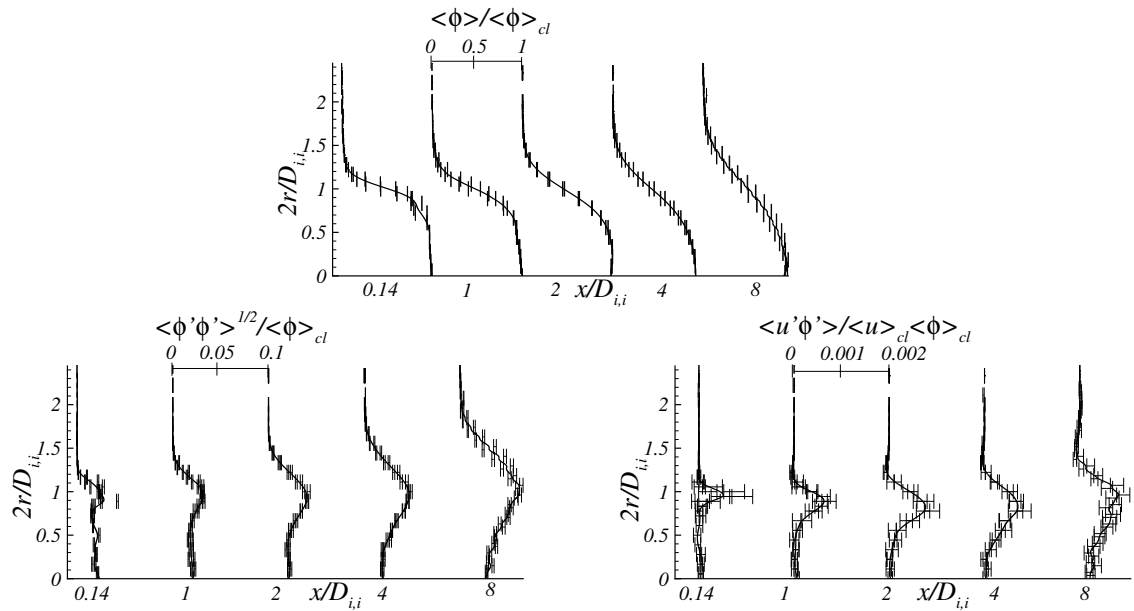


Figure 2.6: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_{i,i} = 0.14, 1, 2, 4$ and 8

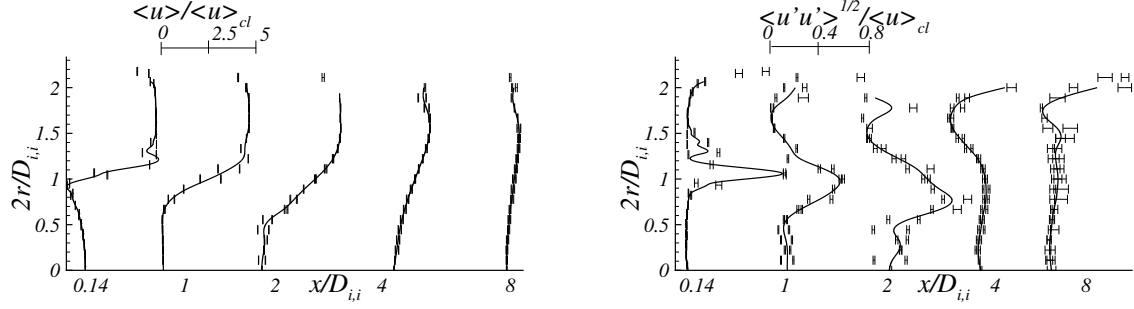


Figure 2.7: Streamwise velocity mean and fluctuation, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 6.5$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: curve fit

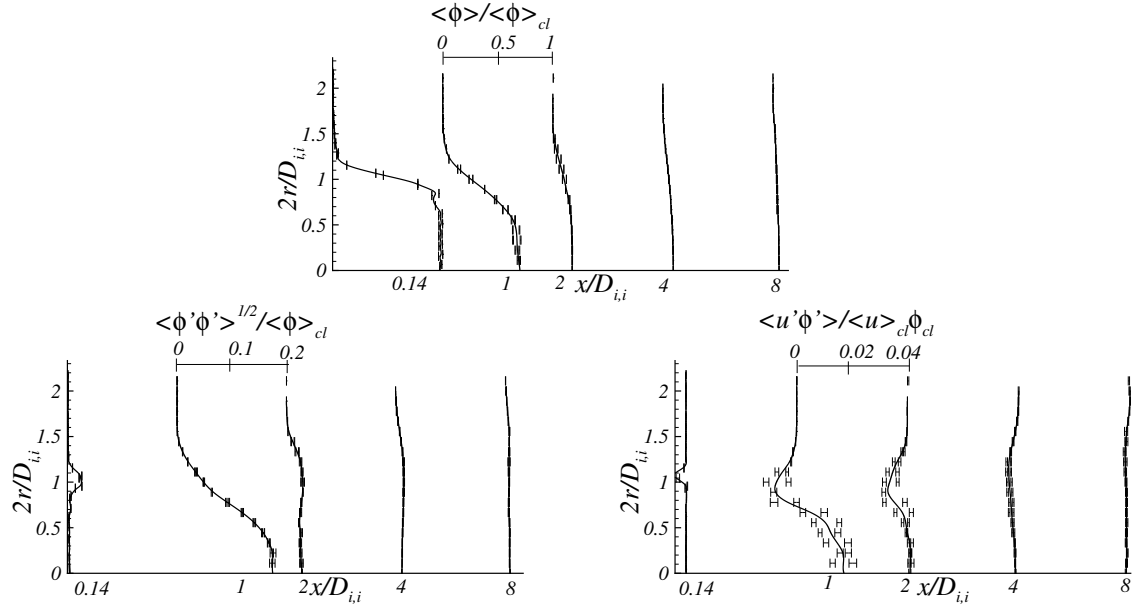


Figure 2.8: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 6.5$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: curve fit

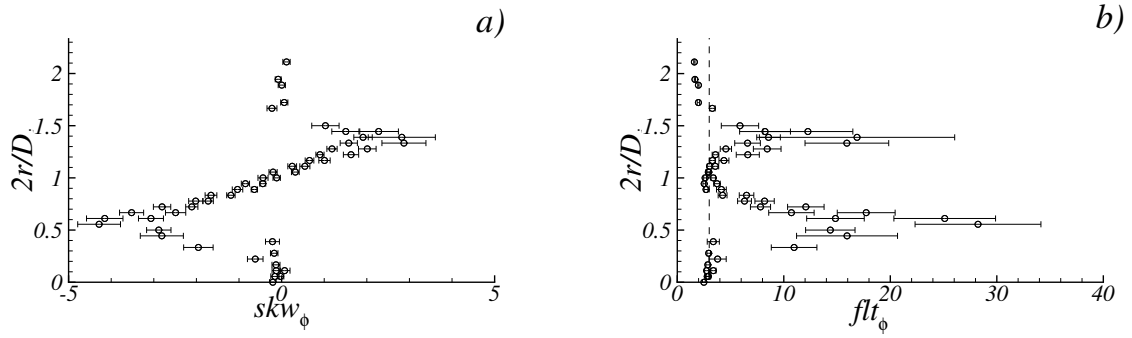


Figure 2.9: Passive scalar higher order moments of $r = 3.2$ for $x/D_{i,i} = 2$, with confidence intervals

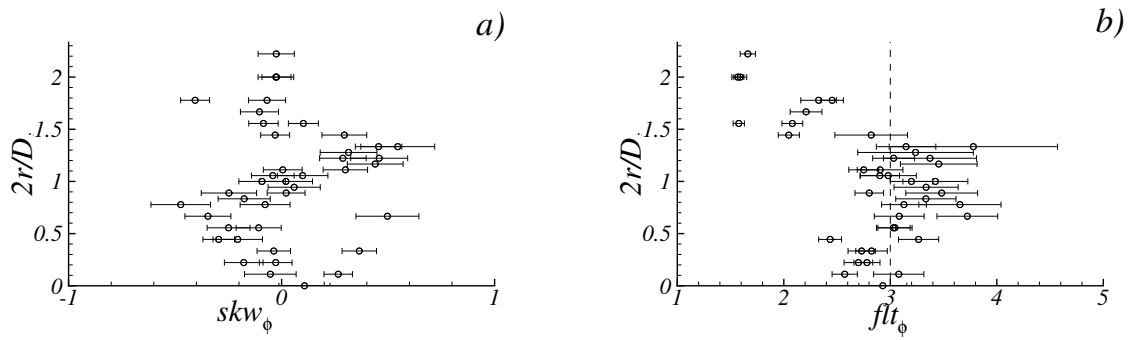


Figure 2.10: Passive scalar higher order moments of $r = 0.8$ for $x/D_{i,i} = 2$, with confidence intervals

2.4.4 Analysis of bootstrap uncertainty

The goal of this section is to determine typical values of statistical uncertainty, estimated using the bootstrap resampling method.

Uncertainty	$x/D_{i,i} = 0.14$	1	2	4	8
$(U_{\langle u \rangle} / \langle u \rangle)_{max}$	6.0	2.5	1.7	2.0	1.0
$(U_{\langle \phi \rangle} / \phi_{in})_{max}$	0.5	0.5	0.6	0.9	1.2
$(U_{\langle \phi \rangle} / \phi_{dil})_{max}$	8.2	8.2	9.9	14.9	19.9
$U_{\langle u'u' \rangle^{1/2} / \langle u'u' \rangle^{1/2}$, where $\langle u'u' \rangle^{1/2}$ is max	2.6	2.7	2.9	2.9	2.0
$U_{\langle \phi'\phi' \rangle^{1/2} / \langle \phi'\phi' \rangle^{1/2}$, where $\langle \phi'\phi' \rangle^{1/2}$ is max	4.6	3.0	3.0	4.3	5.2
$U_{\langle u'\phi' \rangle} / \langle u'\phi' \rangle$, where $\langle u'\phi' \rangle$ is max	22.7	25.0	20.3	77.5	70.3

Table 2.6: Bootstrap uncertainties for $r = 3.2$, in % (condition 1)

Uncertainty	$x/D_{i,i} = 0.14$	1	2	4	8
$(U_{\langle u \rangle} / \langle u \rangle)_{max}$	4.1	1.2	0.8	0.8	0.6
$(U_{\langle \phi \rangle} / \phi_{in})_{max}$	0.1	0.4	0.4	0.5	0.6
$(U_{\langle \phi \rangle} / \phi_{dil})_{max}$	1.0	4.0	4.0	5.0	6.0
$U_{\langle u'u' \rangle^{1/2} / \langle u'u' \rangle^{1/2}$, where $\langle u'u' \rangle^{1/2}$ is max	3.6	1.9	1.7	3.1	3.5
$U_{\langle \phi'\phi' \rangle^{1/2} / \langle \phi'\phi' \rangle^{1/2}$, where $\langle \phi'\phi' \rangle^{1/2}$ is max	4.5	3.8	1.6	2.7	3.8
$U_{\langle u'\phi' \rangle} / \langle u'\phi' \rangle$, where $\langle u'\phi' \rangle$ is max	18.6	32.6	15.1	11.8	21.8

Table 2.7: Bootstrap uncertainties for $r = 2.0$, in % (condition 2)

2.4.4.1 Mean velocity

The relative uncertainty of $\langle u \rangle$ was maximum at the shear layer region, $2r/D_i = 1$, where the lowest velocities and higher radial gradients occur, particularly for low $x/D_{i,i}$. For $r = 3.2$ it reached a maximum of 6 % for $x/D_{i,i} = 0.14$, and was below 3 % in the other sections. The trend was the same for $r = 2.0$ and $r = 1.1$ with the minimum uncertainty occurring for $r = 0.8$, with maximum uncertainty of 2.5 % at $x/D_{i,i} = 0.14$ and about 1 % for the other sections. For $r = 6.5$, the existence of recirculation originated very low velocities in $x/D_{i,i} = 0.14$ and $x/D_{i,i} = 1$, leading to large relative error of $\langle u \rangle$, of 21 % and 11 %, respectively. For $x/D_{i,i} > 2$, the typical uncertainty of 1 % was recovered. When compared with the maximum velocity, the maximum uncertainty was of about or below 1 % for all conditions.

Uncertainty	$x/D_{i,i} = 0.14$	1	2	4	8
$(U_{\langle u \rangle} / \langle u \rangle)_{max}$	4.2	0.7	0.6	0.5	1.0
$(U_{\langle \phi \rangle} / \phi_{in})_{max}$	0.1	0.3	0.3	0.3	0.4
$(U_{\langle \phi \rangle} / \phi_{dil})_{max}$	0.7	1.8	1.9	1.9	2.5
$U_{\langle u'u' \rangle^{1/2} / \langle u'u' \rangle^{1/2}$, where $\langle u'u' \rangle^{1/2}$ is max	2.6	2.8	6.0	4.6	9.4
$U_{\langle \phi'\phi' \rangle^{1/2} / \langle \phi'\phi' \rangle^{1/2}$, where $\langle \phi'\phi' \rangle^{1/2}$ is max	3.3	3.2	3.3	3.2	3.6
$U_{\langle u'\phi' \rangle} / \langle u'\phi' \rangle$, where $\langle u'\phi' \rangle$ is max	30.0	36.9	23.5	19.7	18.1

Table 2.8: Bootstrap uncertainties for $r = 1.1$, in % (condition 3)

Uncertainty	$x/D_{i,i} = 0.14$	1	2	4	8
$(U_{\langle u \rangle} / \langle u \rangle)_{max}$	2.5	0.7	0.5	0.5	0.5
$(U_{\langle \phi \rangle} / \phi_{in})_{max}$	0.2	0.1	0.2	0.2	0.3
$(U_{\langle \phi \rangle} / \phi_{dil})_{max}$	1.0	0.5	1.0	1.0	1.5
$U_{\langle u'u' \rangle^{1/2} / \langle u'u' \rangle^{1/2}$, where $\langle u'u' \rangle^{1/2}$ is max	2.7	3.0	2.8	11.8	7.4
$U_{\langle \phi'\phi' \rangle^{1/2} / \langle \phi'\phi' \rangle^{1/2}$, where $\langle \phi'\phi' \rangle^{1/2}$ is max	2.1	3.3	3.4	3.2	2.9
$U_{\langle u'\phi' \rangle} / \langle u'\phi' \rangle$, where $\langle u'\phi' \rangle$ is max	28.6	21.1	16.9	16.6	18.0

Table 2.9: Bootstrap uncertainties for $r = 0.8$, in % (condition 4)

Uncertainty	$x/D_{i,i} = 0.14$	1	2	4	8
$(U_{\langle u \rangle} / \langle u \rangle)_{max}$	21.4	10.6	6.9	1.0	1.3
$(U_{\langle \phi \rangle} / \phi_{in})_{max}$	0.1	0.5	0.5	0.5	1.1
$(U_{\langle \phi \rangle} / \phi_{dil})_{max}$	1.7	17	17	17	36
$U_{\langle u'u' \rangle^{1/2} / \langle u'u' \rangle^{1/2}$, where $\langle u'u' \rangle^{1/2}$ is max	1.3	3.9	1.3	5.8	5.5
$U_{\langle \phi'\phi' \rangle^{1/2} / \langle \phi'\phi' \rangle^{1/2}$, where $\langle \phi'\phi' \rangle^{1/2}$ is max	1.7	1.2	2.4	2.6	5.1
$U_{\langle u'\phi' \rangle} / \langle u'\phi' \rangle$, where $\langle u'\phi' \rangle$ is max	26.0	7.5	30.4	88.3	76.7

Table 2.10: Bootstrap uncertainties for $r = 6.5$, in % (condition 5)

2.4.4.2 Mean passive scalar

The passive scalar uncertainty, related to the interior jet value was of about 1 % for $r = 3.2$ and about 0.2 % for $r = 0.8$. When comparison was made to the fully mixed concentration in the test section, the uncertainty remains close to 1 % for $r = 0.8$, but for $r = 3.2$ is always higher than 10 % and reaches 20 % for $x/D_{i,i} = 8$. For $r = 2.0$, the maximum uncertainty was about 0.5 % of the interior jet concentration and about 5 % of the fully diluted concentration. For $r = 1.1$, the maximum uncertainty was about 0.3 % of the interior jet concentration and about 2 % of the fully diluted concentration.

2.4.4.3 Turbulent quantities

For $\langle u'u' \rangle^{1/2}$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, the maximum uncertainty was at about the same location of the highest values. At those locations, The relative uncertainty of $\langle u'u' \rangle^{1/2}$ was of about 3 % for $r = 3.2$ (all sections) and for $r = 0.8$, $x/D_{i,i} \leq 4$, while for $x/D_{i,i} = 4$ and $x/D_{i,i} = 8$ values near 10 % were reached. For $\langle \phi'\phi' \rangle^{1/2}$, the values were about 4 % for $r = 3.2$ and about 3 % for $r = 0.8$. For $\langle u'\phi' \rangle$ the uncertainty at the maximum value location was of about 20 % for all sections, for $r = 0.8$ and for $r = 3.2$, $x/D_{i,i} \leq 2$, whereas about 70 % was reached for $x/D_{i,i} = 4$ and $x/D_{i,i} = 8$. For $r = 2$, the uncertainty at the maximum value location was of about 4 % for $\langle u'u' \rangle^{1/2}$ and $\langle \phi'\phi' \rangle^{1/2}$ and of about 20 % for $\langle u'\phi' \rangle$. For $r = 1.1$ the uncertainty at the maximum value location was of about 5 % for $\langle u'u' \rangle^{1/2}$, 3 % for $\langle \phi'\phi' \rangle^{1/2}$ and of about 25 % for $\langle u'\phi' \rangle$. For $r = 6.5$ the uncertainty at the maximum value location was very much dependent on location. For $x/D_{i,i} = 1$, the lowest uncertainty values of all conditions for $\langle \phi'\phi' \rangle^{1/2}$ (1 %) and for $\langle u'\phi' \rangle$ (8 %) are reached. This is because $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ reach the highest values there. As the mixing is almost completed by $x/D_{i,i} = 4$, and $\langle u'\phi' \rangle$ becomes close to zero, the uncertainty of $\langle u'\phi' \rangle$ becomes high, about 80 %.

The conclusion is that the sample size is adequate for achieving reasonably small statistical uncertainty for $\langle u \rangle$, $\langle \phi \rangle$, $\langle u'u' \rangle^{1/2}$ and $\langle \phi'\phi' \rangle^{1/2}$, but in the shear layer region larger samples would be desirable. For $\langle u'\phi' \rangle$, the statistical uncertainty is higher than 20 %: the sample size was not sufficient. However, the trend of the variable is not hidden and meaningful comparison to experiment can be done.

The bootstrap method was used to determine statistical uncertainty, from which the uncertainty confidence intervals and typical relative uncertainties were computed. Dependence of the statistical uncertainty on the velocity ratio was not strong. It is found that $\langle u \rangle$ has very low uncertainty, although the shear-layer zone could be improved with larger time series. $\langle u'u' \rangle^{1/2}$ has reasonably low uncertainty. $\langle \phi \rangle$ and $\langle \phi'\phi' \rangle^{1/2}$ have low uncertainty when measuring high concentration values, but high uncertainty when measuring low values. Unlike the velocity, however, low values of passive scalar appear and are important in the outer shear layer. $\langle u'\phi' \rangle$ has a large uncertainty, but not so large as to hide the profile shape.

2.4.5 Noise in scalar measurement: amplitude, consequences and sources

Noise is defined as the passive scalar fluctuation measured when the expected value is zero. Two types of noise can be distinguished:

1. Zero level noise: the mean and fluctuation measured where the passive scalar mean and fluctuation are known to be zero.
2. Finite level noise: the fluctuation measured where the passive scalar is known to be constant and fluctuation is known to be zero, after removal of zero level noise.

The noise affects directly the instantaneous values, but these are not crucial in our investigation. The zero-level mean and fluctuation can be subtracted from the mean and fluctuation statistics, as it is uncorrelated with those. Finite-level noise cannot be removed from $\langle \phi' \phi' \rangle^{1/2}$ in the same way of the zero level $\langle \phi' \phi' \rangle_0^{1/2}$ because it varies with the concentration measured (*e.g.*, it is always smaller for $x/D_{i,i} = 100$ than for $x/D_{i,i} = 0.14$) in a way that is not known. No way to remove either noise type from $\langle u' \phi' \rangle$ or from the PDF and its third and fourth moments (skewness and kurtosis) has been found.

The finite-level noise effect on the mean after averaging has been computed by Lima (2000) using a t-Student distribution and is negligible (0.2 mV). However, it is included in the fluctuation, $\langle \phi' \phi' \rangle^{1/2}$, and again on $\langle u' \phi' \rangle$, on the PDF or in skewness and kurtosis. Finite level noise adds to $\langle \phi' \phi' \rangle^{1/2}$, causing overevaluation. Both noise types decorrelate u and ϕ and cause underevaluation of $\langle u' \phi' \rangle$. Assuming a normal distribution for the noise (reasonable, since noise comes from various sources), the effect on the PDF will be a superposition of the noise normal distribution overlapping the passive scalar real distribution and hiding the spikes on the passive scalar bounding values; Skewness and (Kurtosis-3) are also underevaluated.

In figure 2.11 the probability density functions of passive scalar in the region where ϕ is constant and equal to 1 are presented, for $r = 0.8$. This is the worst case, since this was the condition with highest values of $\langle \phi' \phi' \rangle^{1/2}$ there (9 mV) and shows the noise impact on the measurements. One major effect is that the boundedness of the passive scalar cannot be directly observed, as it is masked by the noise, leading to values of ϕ higher than one on the PDF.

Wherever unmixed fluid is not present, the passive scalar value is constant and $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ are zero. Non-zero $\langle \phi' \phi' \rangle^{1/2}$ or $\langle u' \phi' \rangle$ values in these regions are due to noise rather than turbulence. This provides a way to quantify the effect of noise. The statistical significance of this deviation from the zero expected value is established by comparing with the bootstrap uncertainty; for $\langle \phi' \phi' \rangle_{0.14}^{1/2}$ and $\langle \phi' \phi' \rangle_{100}^{1/2}$ the uncertainty averages 5 %, so the differences to zero are statistically significant. For $\langle u' \phi' \rangle_{0.14} / (\langle u \rangle_{bi} \phi_{in})$ the uncertainty

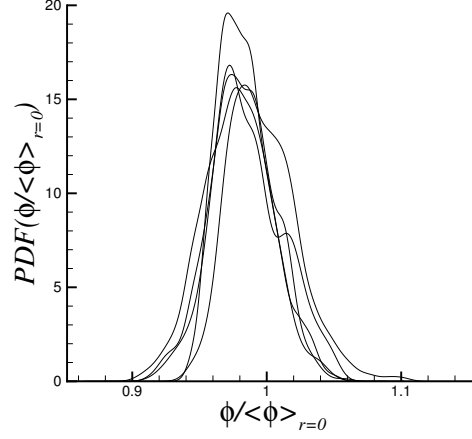


Figure 2.11: Passive scalar PDF, for $r = 0.8$ and $x/D_{i,i} = 0.14$ between $r = -2$ and $r = 2$, where ϕ is constant

averages 110 % and for $\langle u'\phi' \rangle_{100} / (\langle u \rangle_{bi} \phi_{in})$ 70 % so the differences to zero are statistically insignificant and are not presented.

r	$\langle \phi' \phi' \rangle^{1/2}$					
	$x/D_{i,i} = 0.14$		1		100	
	mV	%	mV	%	mV	%
3.2	2.2	19.1	2.2	4.0	0.6	90
2.0	2.3	20.0	2.2	6.6	0.3	98
1.1	4.4	29.0	4.1	19.6	—	—
0.8	9.0	47.6	9.2	60.6	—	—
6.5	1.2	13.1	—	—	0.2	90

Table 2.11: Noise related $\langle \phi' \phi' \rangle^{1/2}$ in fully mixed spots: centreline, close to test section inlet and exit (in mV and in % of section maxima).

The passive scalar fluctuation $\langle \phi' \phi' \rangle^{1/2}$ in fully mixed spots is consistently above zero. Table 2.11 presents values of finite level noise in fully mixed spots (outlet and centreline close to inlet). The impact on the uncertainty is assessed by comparing the noise value with the maximum value being measured at the section in the columns headed by a % sign. A clear pattern emerges: the impact on uncertainty of $\langle \phi' \phi' \rangle^{1/2}$ of the noise is much lower for large velocity ratio, therefore large velocity ratio flow is a better candidate for validation of $\langle \phi' \phi' \rangle^{1/2}$ profiles.

For each condition, the values are very similar in $x/D_{i,i} = 0.14$ and $x/D_{i,i} = 1$, but the value seems to depend on the condition, increasing with decrease in the velocity ratio

(this decrease is based on increasing Re_{in}). For $r = 0.8$, 9 mV are reached, doubling the 4 mV reported in Lima (2000) for the standard deviation of a measurement of constant concentration equal to ϕ_{in} . The relative impact on $x/D_{i,i} = 100$ is of the order of 90 %, showing that measurements there are unreliable.

As an explanation, we propose that even though the mean passive scalar is constant, small amounts of scalar fluctuation may still be present in the test section inlet. In this case, a part of the finite level noise would be this residual inlet fluctuation. An investigation on criteria for fully developed mixing Guilkey et al. (1997a,b) reports that $\langle\phi'\phi'\rangle^{1/2}$ is up to 10^{-4} (corresponding to about 4 mV) for $x/D_{i,i} = 200$, close to the developing pipe normalised length for $r = 0.8$. Noise figures higher than the values obtained in Lima (2000) calibration tests (4 mV, about 3 times the digital board 1.22 mV resolution) are probably not caused by the measurement system itself. The connection of these higher values with high Reynolds number in the interior pipe flow suggests that residual fluctuation may be occurring.

Sources and effects of scalar measurement noise were reviewed, and a way to quantify the effect on $\langle\phi'\phi'\rangle^{1/2}$ was found. The effect of the noise on the uncertainty is asymmetrical: it leads to overevaluation of $\langle\phi'\phi'\rangle^{1/2}$ and to underevaluation of $\langle u'\phi'\rangle$ and of differences to the normal distribution. Higher values of noise occurred for the conditions with lower r (higher Re_{in}), indicating that residual fluctuations are present at the test section inlet. The relative weight of noise on the measurement of $\langle\phi'\phi'\rangle^{1/2}$ is up to twenty times smaller for $r = 3.2$ compared to $r = 0.8$, indicating that $r = 3.2$ is a better candidate for comparison of $\langle\phi'\phi'\rangle^{1/2}$ with numerical simulation.

2.4.6 The evolution of probability density functions in the shear layer

The goal of this section is to study the evolution of the velocity and concentration by observing their probability density functions (PDF's). Study of the evolution of PDF's on shear layers in previous works (*e.g.*, Cortesi et al., 2001; Balarac et al., 2007b), lead to the identification of two distinct behaviours:

- PDF evolution is called *marching* when the PDF peaks (most probable values) are close to the mean and depend on the location (in our case, of r). This is typical of slow mixing, either molecular or with small structures, and of mixing reaching an homogeneous state.
- PDF evolution is called *non-marching* when the PDF peaks remain close to the free stream values, for large variations in location. This is the case for fast mixing, governed by large-scale structures.

In the figures and on the following analysis we distinguish between the *outer layer*, from $2r/D_i = 1.55$ to $2r/D_i = 1$ and the *inner layer*, from $2r/D_i = 1$ to $2r/D_i = 0.1$

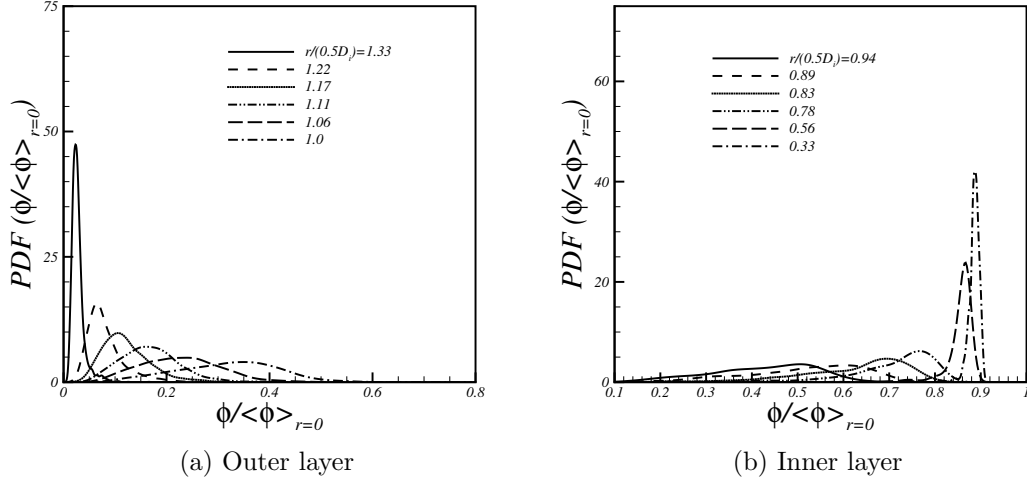


Figure 2.12: Evolution of the passive scalar PDF, for $r = 3.2$ and $x/D_{i,i} = 1.0$ in the inner and outer mixing layers

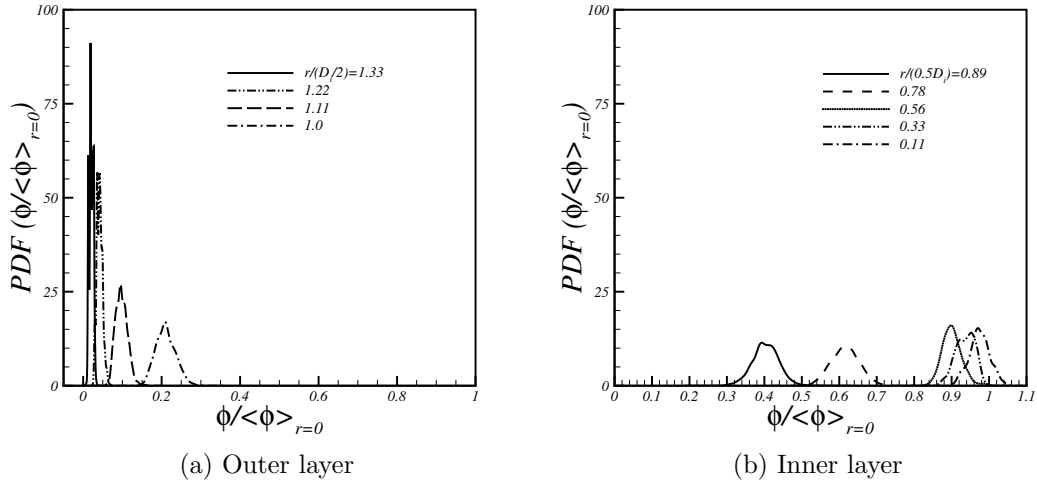


Figure 2.13: Evolution of the passive scalar PDF, for $r = 0.8$ and $x/D_{i,i} = 1.0$ in the inner and outer mixing layers

When analysing the various statistics, large gradients appeared close to the shear layer but the PDF evolution was smooth. An example of marching behaviour can be seen on figure 2.13 and non-marching on figure 2.12. The following brief analysis is based on the full set of PDF figures, not shown.

We start our analysis by the flow condition with $r = 3.2$. At $x/D_{i,i} = 0.14$ both behaviours can be observed. The velocity PDF shows a non-marching behaviour, particularly in the inner layer. In contrast, the passive scalar PDF evolution is marching. This may indicate that the large scales that are mixing the streamwise momentum still carry little passive scalar, whose mixing is governed by small structures. For $x/D_{i,i} = 1$ a general smoothing of the axial velocity PDF's is observed with the peaks less pronounced; the non-marching behaviour still predominates. In the passive scalar, however, a significant difference is observed: the shear layer PDF's now spread over large ranges and show large tails, with the a non-marching similar to the velocity PDF's. The PDF smoothing continues for $x/D_{i,i} = 2$. At $x/D_{i,i} = 4$, the interior jet peak has disappeared, which is consistent with the end of the potential core. High values of concentration no longer exist, the largest one being of about 0.5. The flow is now a single shear layer, with the PDF's presenting a marching behaviour, that indicates homogeneous mixing. By $x/D_i = 8$ most of the mixing has taken place and the most probable value is now almost independent of r , indicating that mixing is almost completed. Further downstream, narrower and narrower passive scalar PDF's are observed.

For $r = 0.8$, the velocity PDF evolution at $x/D_i = 0.14$ has the non-marching behaviour indicating the large-scale structure impact also seen for $r = 3.2$. However, the downstream evolution is much slower and the PDF's dependence on r for each section is similar, with the internal jet PDF's gradually approaching the annular jet ones. The process is far from completed at $x/D_{i,i} = 8$. The passive scalar PDF's show a marching behaviour throughout all the shear layer, indicating that the passive scalar mixing does not involve structures capable of transporting unmixed fluid to the inner jet or vice versa. By $x/D_{i,i} = 8$ both $\phi = 0$ and $\phi = 1$ can still be found, demonstrating the slow mixing characteristic of this velocity ratio.

In general, for $r = 3.2$, the passive scalar and velocity PDF evolution is of the same type. This does not occur for $r = 0.8$.

2.5 Conclusions

In this section, the main conclusions of the chapter are summarised.

A systematic description of the geometry is made, to ensure an accurate representation in numerical simulations. The Schmidt number is between 500 and 2500. We recommend to use $Sc = 1000$ in simulations, with two additional simulations with different Sc (say 500 and 2500) to assess the effect of this uncertainty in Sc .

A review of scientific database software was made to conclude on use of ASCII text files was decided, since the large storage requirements were not an issue: after adequate post-processing the whole database was stored on one data CD.

The quality of Lima (2000) measurements was confirmed by doing and improving the data post-processing. The symmetry of the measurements was verified and is proof that attenuation effects are of small importance. On the whole, results similar to Lima (2000) were achieved.

The evolution of probability density functions was analysed in terms of marching behaviour. Non-marching evolution dominates for $r = 3.2$, compatible with mixing by large scale structures. Conversely, marching evolution occurs for $r = 0.8$, indicating mixing by small structures.

In the remaining of this section the various uncertainty studies are reviewed, to fulfil the goal of choosing the best conditions for numerical experiment. An overview of the uncertainty analysis is made with the help of table 2.12, where minimum and maximum values of uncertainty with the various approaches are summarised.

There cannot be a correct passive scalar field if the velocity field was incorrect. We will thus review the velocity first and passive scalar next and the mean first and turbulent quantities next.

$\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$ profiles Visual inspection of the $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$ profiles shows good symmetry for all conditions. The mean velocity uncertainty analysis by classical uncertainty estimation lead to 1.5 % uncertainty for all conditions. The bootstrap was in general below this value, but an important exception was the shear layer region close to the inlet, where low velocity values occur. The condition with lowest uncertainty in this region was $r = 0.8$ (2.5 %) whereas $r = 6.5$ reached 21 %. Another way of assessing the $\langle u \rangle$ measurements quality is to analyse the mass flux uncertainty. The mass flux was set with rotameters and the lowest rotameter uncertainty appears for $r = 0.8$, with an interior mass flux uncertainty of 4 % and a velocity ratio uncertainty of 6 %. Higher velocity ratios have higher uncertainty, with $r = 6.5$ showing an uncertainty of 29 % in the velocity ratio and interior mass flux. The mass flux computed from profile integration varied less than the rotameter uncertainty would suggest: below 1 % for $r = 0.8$ and *circa* 5 % for $r = 6.5$.

The fluctuation $\langle u'u' \rangle^{1/2}$ bootstrap uncertainty is below 12 % for all conditions and below 3 % for the best condition, $r = 3.2$. In what concerns the velocity field, the most accurate measurements are for $r = 0.8$, with $r = 3.2$ a good compromise between $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$ uncertainty.

$\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ profiles Visual inspection shows good $\langle \phi \rangle$ and $\langle \phi'\phi' \rangle^{1/2}$, whereas $\langle u'\phi' \rangle$ show larger confidence intervals and less symmetry. The uncertainty in the interior

mass flux governs the $\langle\phi\rangle$ uncertainty, leading to a minimum uncertainty of 4 % for $r = 0.8$ and to higher uncertainty with larger r , with 14 % for $r = 3.2$ and 28 % for $r = 6.5$. This was the uncertainty when measuring the largest concentration; if the fully diluted value is used as the reference, uncertainty is doubled. The passive scalar mass flux obtained by integration shows minimal variation for $r = 1.1$ and $r = 0.8$ (about 10 % was the maximum variation), but $r = 6.5$ shows higher than 100 % variation: the condition was useless for comparison with numerical simulation. The bootstrap uncertainty was smallest for $r = 0.8$ (about 1 %) and still reasonable for $r = 3.2$ (even for the diluted concentration, it was about 20 %).

The $\langle\phi'\phi'\rangle^{1/2}$ bootstrap uncertainty was similar for all conditions. In what concerns $\langle\phi'\phi'\rangle^{1/2}$, the effect of noise was more crucial than the bootstrap uncertainty. This effect can be evaluated in the centre of the first section, where the whole of $\langle\phi'\phi'\rangle^{1/2}$ is noise. This constitutes 60 % of the maximum values for $r = 0.8$ but much less for $r = 3.2$: 20 %. For $\langle u'\phi'\rangle$, the bootstrap uncertainty was again similar to all conditions, but higher, with 30 % being typical and 80 % occurring occasionally. The effect of noise on $\langle u'\phi'\rangle$ could not be quantified, but is expected to be similar to $\langle\phi'\phi'\rangle^{1/2}$, thus making $r = 3.2$ the better condition. The 0-level fluorescence noise could not be removed from $\langle u'\phi'\rangle$ and in combination with the optical and electronic noise quantified for $\langle\phi'\phi'\rangle^{1/2}$ is likely to make the measured $\langle u'\phi'\rangle$, proportional to the correlation between u and ϕ fluctuations, much smaller than the real value.

For $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$, the noise was more important than the experimental uncertainty computed with the bootstrap method and therefore the experiment $\langle\phi'\phi'\rangle^{1/2}$ is likely overevaluated and $\langle u'\phi'\rangle$ is likely underevaluated. This finding is important for comparison with numerical simulations: overevaluation of $\langle\phi'\phi'\rangle^{1/2}$ and underevaluation of $\langle u'\phi'\rangle$ cannot be blamed on the experiments.

Global conclusion: Velocity ratio $r = 0.8$ was the condition with lower $\langle u\rangle$ and $\langle\phi\rangle$ uncertainty and provides a case with passive scalar mixing governed by small scale structures. The condition with $r = 3.2$ was a good compromise between uncertainty on the mean values and on the turbulent passive scalar quantities and provides a case with passive scalar mixing governed by large scale structures.

Uncertainty	$r = 3.2$	$r = 2.0$	$r = 1.1$	$r = 0.8$	$r = 6.5$
$\langle u \rangle$					
Local – Classic	1.5	1.5	1.5	1.5	1.5
Local – Bootstrap	1.0–6.0	0.6–4.1	0.5–4.2	0.5–2.5	1.0–21.4
Bulk – Rotameter	4.2–13.9	4.3–8.7	4.1–5.3	3.5–3.3	4.3–28.6
Bulk – Integration	1.0–8.0	1.0–3.0	0.0–3.0	1.0–2.0	0.0–5.0
Visual Inspection	4	4	3	4	3
$\langle \phi \rangle$					
Local – Classic	13.9–26.0	9.0–17.2	5.8–10.9	4.1–8.0	28.0–51.5
Local – Boot in	0.5–1.2	0.1–0.6	0.1–0.4	0.1–0.3	0.1–1.1
Local – Boot dil	8.2–19.9	1.0–6.0	0.7–2.5	1.0–1.5	1.7–36.0
Bulk – Rotameter	4.2–13.9	4.3–8.7	4.1–5.3	3.5–3.3	4.3–28.6
Bulk – Integration	11.0–34.0	9.0–22.0	1.0–6.0	5.0–11.0	1.0–127.0
Visual Inspection	4	3	4	3	4
$\langle u'u' \rangle^{1/2}$					
Local – Bootstrap	2.0–2.6	1.7–3.6	2.6–9.4	2.7–11.8	1.7–3.6
Visual Inspection	3	3	3	3	2
$\langle \phi'\phi' \rangle^{1/2}$					
Local – Bootstrap	3.0–5.2	1.6–4.5	3.2–3.6	2.1–3.4	1.2–5.1
Local – Noise	4.0–19.1	6.6–20.0	19.6–29.0	47.6–60.6	1.2–13.0
Visual Inspection	3	3	3	3	4
$\langle u'\phi' \rangle$					
Local – Bootstrap	20.3–77.5	11.8–32.6	18.1–36.9	16.6–28.6	7.5–88.3
Visual Inspection	3	3	2	2	2

Table 2.12: Uncertainty analysis summary

Chapter 3

Mathematical Model and Numerical Techniques

Abstract

The techniques used in the computer simulation of confined coaxial jets are presented in this chapter. The simulation was based on a non-orthogonal second order code, that required modifications, described here. This chapter is the basis for the LES simulations presented later.

3.1 Introduction

The great majority of the present study was based on the second order non-orthogonal computer code (VISCT), previously developed by Silva Lopes (2000), briefly described in 3.3.1. The use of this code in the simulation of confined coaxial jets required several modifications, which included the subgrid-scale modelling of passive scalar transport. These additions to the VISCT code are the main focus of the chapter.

3.2 Governing equations

3.2.1 The filtered Navier-Stokes equations

The continuity and Navier-Stokes equations in Cartesian coordinates are spatially filtered, yielding (3.1) and (3.2) (*cf.* Pope, 2000).

$$\frac{\partial}{\partial x_i}(\rho \bar{u}_i) = 0, \quad (3.1)$$

$$\frac{\partial}{\partial t}(\rho \bar{u}_i) + \frac{\partial}{\partial x_j}(\rho \bar{u}_j \bar{u}_i) = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_i}, \quad (3.2)$$

where the overline indicates a spatially filtered quantity.

Following the LES methodology, the shear stress tensor has two components,

$$\tau_{ij} = \bar{\tau}_{ij} + \tau_{ij}^{\text{sgs}},$$

a resolved component,

$$\bar{\tau}_{ij} = 2\mu \bar{S}_{ij}$$

where $\bar{S}_{ij} = 1/2(\partial \bar{u}_i/\partial x_j + \partial \bar{u}_j/\partial x_i)$ is the resolved strain rate tensor for a Newtonian fluid, and a subgrid component,

$$\tau_{ij}^{\text{sgs}} = -\rho(\overline{u_i u_j} - \bar{u}_i \bar{u}_j)$$

that represents the effects of the small subgrid scales, unresolved, on the large, resolved, ones and must be modelled, subsection 3.2.3.

3.2.2 The filtered passive scalar transport equation

The filtered passive scalar transport equation in Cartesian coordinates is

$$\frac{\partial(\rho \bar{\phi})}{\partial t} + \frac{\partial(\rho \bar{\phi} \bar{u}_j)}{\partial x_j} = \frac{\partial q_j}{\partial x_j} \quad (3.3)$$

The passive scalar flux has two components,

$$q_j = \bar{q}_j + q_j^{\text{sgs}},$$

a resolved component $\bar{q}_j = \alpha \partial \bar{\phi} / \partial x_j$ and a subgrid-scale component, $q_j^{\text{sgs}} = \rho(\overline{\phi u_j} - \bar{\phi} \bar{u}_j)$ that accounts for the effects of the subgrid scales on the resolved ones. It is usual to relate

the mass diffusivity α with the viscosity, through a (molecular) Schmidt number, $Sc = \nu/\alpha$; a dimensionless number that represents the ratio of momentum and mass diffusivity, similar to the Prandtl number in heat transfer problems.

In the remaining of the thesis, the spatial filter sign is only shown when filtered and unfiltered quantities appear in the same discussion, to improve readability.

3.2.3 Subgrid-scale models

In this section, the subgrid-scale models used are presented, namely the adaptation of the dynamic model to the passive scalar transport equation. Effective viscosity/diffusivity models were used; the models are based on the assumption that the effect of the small scales on the large ones is an increase in the effective diffusion of momentum and mass; the models use an eddy viscosity/diffusivity to model the effects of the subgrid scales on the large scales. The coefficients were computed using the dynamic procedure.

3.2.3.1 Momentum equations

The subgrid component τ_{ij}^{sgs} was modelled by

$$\tau_{ij}^{\text{sgs}} - \frac{\delta_{ij}}{3}\tau_{kk} = 2\nu^{\text{sgs}}\bar{S}_{ij}, \quad (3.4)$$

where ν^{sgs} is the subgrid-scale eddy viscosity and $\bar{S}_{ij}$ is the resolved shear-stress tensor. All that remains is to find a suitable value for ν^{sgs} .

The most common alternative is the well known Smagorinsky model (Smagorinsky, 1963),

$$\nu^{\text{sgs}} = C_{ev}\bar{\Delta}^2|\bar{S}|, \quad (3.5)$$

where C_{ev} is the Smagorinsky constant, $\bar{\Delta}$ is a grid-related length scale (the filter width) and the product $\bar{\Delta}|\bar{S}|$ is a velocity difference scale.

Whereas the Smagorinsky constant value can be determined from turbulence theory for simple flows (*e.g.*, isotropic turbulence), it is flow dependent and variable in space for complex industrial flows, such as confined coaxial jets. To determine C_{ev} , we use the dynamic procedure. It involves calculating a number of tensors in a coarser grid (the test filter, $2\times$ coarser in each grid direction), which is represented by $\hat{\cdot}$, the test-filter width being $\hat{\Delta}$. The test filter for the dynamic model uses the trapezoidal rule (*cf.* Sagaut, 2004),

$$\hat{\phi} = \frac{1}{2} \left[\left(\frac{\bar{\phi}_{i-1} + \bar{\phi}_i}{2} + \frac{\bar{\phi}_i + \bar{\phi}_{i+1}}{2} \right) \right] = \frac{1}{4}\bar{\phi}_{i-1} + \frac{1}{2}\bar{\phi}_i + \frac{1}{4}\bar{\phi}_{i+1}, \quad (3.6)$$

defined here for a single computational direction.

The Smagorinsky constant is obtained from the tensors,

$$C_{ev} = -\frac{1}{2} \frac{\langle \mathcal{L}_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}, \quad (3.7)$$

where $\langle . \rangle$ is a suitable average. To perform the average we used the Lagrangian averaging procedure of Meneveau (1996).

The model is based on the Germano identity: $\mathcal{L}_{ij} = T_{ij} - \widehat{\tau_{ij}}$, where the resolved turbulent stress tensor, $\mathcal{L}_{ij}$ is computed according to

$$\mathcal{L}_{ij} = \widehat{\overline{u_i u_j}} - \widehat{\overline{u_i}} \widehat{\overline{u_j}} \quad (3.8)$$

and applying Germano identity another tensor is computed

$$M_{ij} = -a^2 \overline{\Delta}^2 |\widehat{S}| \widehat{S}_{ij} + \overline{\Delta}^2 |\widehat{S}| \widehat{S}_{ij}, \quad a = \frac{\widehat{\Delta}}{\overline{\Delta}}. \quad (3.9)$$

3.2.3.2 Passive scalar transport

By analogy with (3.4), a subgrid-scale diffusivity model is used for the modelling of q_j^{sgs} ,

$$q_j^{\text{sgs}} = -\alpha^{\text{sgs}} \frac{\partial \overline{\phi}}{\partial x_j}. \quad (3.10)$$

To complete the closure, the subgrid-scale diffusivity α^{sgs} is obtained from

$$\alpha^{\text{sgs}} = C_{ed} \overline{\Delta}^2 |\widehat{S}|, \quad (3.11)$$

where the simplest way to determine the constant C_{ed} , based on a subgrid-scale Schmidt number, yields

$$C_{ed} = \frac{C_{ev}}{Sc^{\text{sgs}}}. \quad (3.12)$$

The modelled passive scalar transport equation is now

$$\frac{\partial(\rho \overline{\phi})}{\partial t} + \frac{\partial(\rho \overline{\phi} \overline{u_j})}{\partial x_j} = -\frac{\partial}{\partial x_j} \left((\mu/Sc + \mu^{\text{sgs}}/Sc^{\text{sgs}}) \frac{\partial \overline{\phi}}{\partial x_j} \right). \quad (3.13)$$

If $Sc^{\text{sgs}} = 1$ this is equivalent to $\alpha^{\text{sgs}} = \nu^{\text{sgs}}$, the so-called Reynolds analogy, where the assumption is that the effect of the subgrid scales on the large ones is identical on both the velocity and passive scalar fields. Following Keating (2004), the dynamic procedure was applied to get a C_{ed} based on filtering the passive scalar and velocity field, which can be seen as a dynamic procedure to calculate a spatially varying Sc^{sgs} number. Tensors $\mathcal{F}_j$

Term	Momentum	Passive-scalar
Diffusive	$\frac{\partial \tau_{ij}}{\partial x_j} = \frac{\partial(\bar{\tau}_{ij} + \tau_{ij}^{\text{sgs}})}{\partial x_j}$	$\frac{\partial q_j}{\partial x_j} = \alpha \frac{\partial(\bar{q}_j + q_j^{\text{sgs}})}{\partial x_j}$
Resolved stress/flux	$\bar{\tau}_{ij} = 2\nu \bar{S}_{ij}$	$\bar{q}_j = \alpha \frac{\partial \bar{\phi}}{\partial x_j}$
SGS stress/flux	$\tau_{ij}^{\text{sgs}} - \frac{\delta_{ij}}{3} \tau_{kk} = -2\nu_t^{\text{sgs}} \bar{S}_{ij}$	$q_j^{\text{sgs}} = -\alpha_t^{\text{sgs}} \frac{\partial \bar{\phi}}{\partial x_j}$
Eddy viscosity/diffusivity	$\nu_t^{\text{sgs}} = C_{ev} \bar{\Delta}^2 \bar{S} $	$\alpha_t^{\text{sgs}} = C_{ed} \bar{\Delta}^2 \bar{S} $
Dynamic model tensors	$\mathcal{L}_{ij} = \widehat{\bar{u}_i \bar{u}_j} - \widehat{\bar{u}_i} \widehat{\bar{u}_j}$	$\mathcal{F}_j = \widehat{\bar{\phi} \bar{u}_j} - \widehat{\bar{\phi}} \widehat{\bar{u}_j}$
Dynamic model tensors	$M_{ij} = -a^2 \bar{\Delta}^2 \widehat{\bar{S}} \widehat{\bar{S}}_{ij} + \widehat{\bar{\Delta}^2 \bar{S} \bar{S}_{ij}}$	$N_j = a^2 \bar{\Delta}^2 \widehat{\bar{S}} \frac{\partial \widehat{\bar{\phi}}}{\partial x_j} - \widehat{\bar{\Delta}^2 \bar{S} \frac{\partial \bar{\phi}}{\partial x_j}}$
Smagorinsky constant	$C_{ev} = -\frac{1}{2} \frac{\langle \mathcal{L}_{ij} M_{ij} \rangle}{\langle M_{ij} M_{ij} \rangle}$	$C_{ed} = -\frac{\langle \mathcal{F}_j N_j \rangle}{\langle N_j N_j \rangle}$

Table 3.1: Analogy between momentum and passive scalar transport dynamic model

(3.14) and N_j (3.15) are computed and C_{ed} is calculated from (3.16). Again, $\langle . \rangle$ indicates an averaging procedure, and in this work we used the Lagrangian averaging procedure.

$$\mathcal{F}_j = \widehat{\bar{\phi} \bar{u}_j} - \widehat{\bar{\phi}} \widehat{\bar{u}_j} \quad (3.14)$$

$$N_j = a^2 \bar{\Delta}^2 |\widehat{\bar{S}}| \frac{\partial \widehat{\bar{\phi}}}{\partial x_j} - \widehat{\bar{\Delta}^2 |\bar{S}| \frac{\partial \bar{\phi}}{\partial x_j}} \quad (3.15)$$

$$C_{ed} = -\frac{\langle \mathcal{F}_j N_j \rangle}{\langle N_j N_j \rangle} \quad (3.16)$$

Table 3.1 shows the analogy between the dynamic model for the momentum and passive scalar dynamic models.

3.2.4 The inlet boundary condition

The inlet of a coaxial confined flow is a two-dimensional unsteady, turbulent field, with memory of all the flow details prior to it. However, numerical cost considerations make inlet modelling, as opposed to simulation of all the prior details, desirable.

The experiment time series cannot be used as an inlet condition: they have no spatial structure, being point by point measurements. This means one is forced to reconstruct the inlet conditions from the statistical description available.

Statistical reconstruction from mean and variance is easy to implement and numerically inexpensive. However, it is a poor representation of reality and the best possible inlet

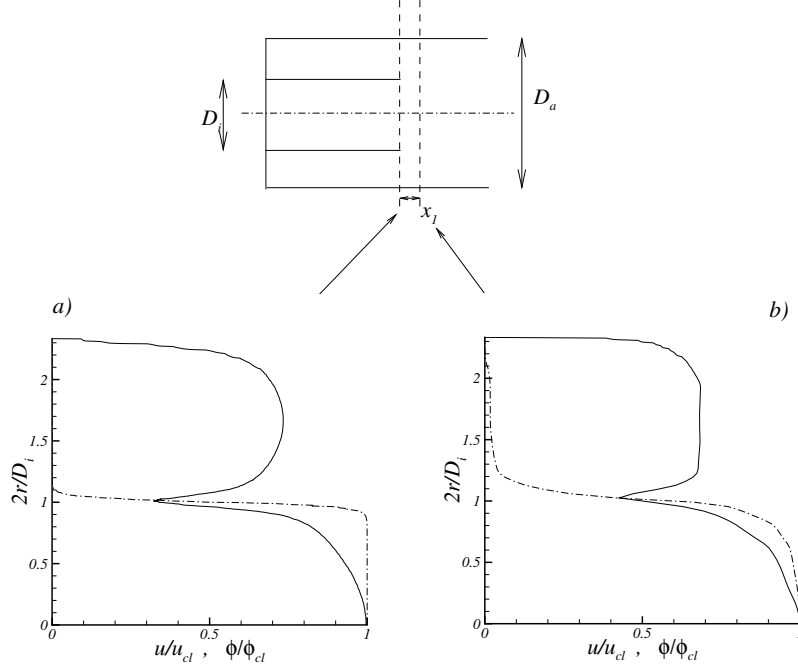


Figure 3.1: Inlet average profile, for fully developed and rescaled simulations

condition was needed to compensate for the resolution drawbacks caused by the use of non-orthogonal grids. It has been shown in Chung and Sung (1997), cited in Sagaut (2004), that this approach creates a region of the computational domain (can be more than 50 % of the total simulation points) in which the solution regenerates the space time consistency specific to the Navier-Stokes equations and that is not usable. This would be the whole near-field, the target of our study.

When the inlet consists of fully, or at least reasonably, developed flows, the use of precursor simulations works well. So as a first approach, the inlet velocity field was obtained using two fully developed precursor simulations, one for the interior tube and the other for the annulus, that were then blended and interpolated to the final grid. When compared with the experiment in $x/D_i = 0.14$, the inner pipe flow is closely matched, but the outer annular pipe was designed to be undeveloped and shows a flatter mean velocity profile and decreased, but not negligible, fluctuation.

By using precursor simulation and rescaling, we try to include as much information from the measurements as possible in an "equilibrium turbulent field", with spatial structure. Slices are collected in the fully developed precursor simulations and are rescaled to fit the experiments at $x/D_i = 0.14$, using the method suggested in Pierce (2001). This, outlined in figure 3.1, is based on shifting the inlet fields so that they matched the measurements for the mean velocity $\langle u \rangle(r)$, velocity fluctuation $\langle u'u' \rangle^{1/2}(r)$, mean scalar $\langle \phi \rangle(r)$ and scalar

fluctuation $\langle \phi' \phi' \rangle^{1/2}(\mathbf{r})$. For the velocity component u , this procedure was carried out by obtaining an azimuthally averaged profile $\langle u(\mathbf{r}, t) \rangle$ and shifting the slices $u(y, z, t)$ to match the target profile $\langle u \rangle(\mathbf{r})$. This is implemented as

$$u(y, z, t) \rightarrow \frac{\langle u' u'(\mathbf{r}) \rangle^{1/2}}{\langle u' u'(y, z, t) \rangle^{1/2}} [u(y, z, t) - \langle u(\mathbf{r}, t) \rangle] + \langle u(\mathbf{r}) \rangle. \quad (3.17)$$

The technique was extended to the scalar field by doing a first simulation using a flat scalar profile, with no fluctuation, and then collecting slices of velocity and scalar that were rescaled to the correct values of both velocity and scalar mean and turbulent fluctuation. Two points of slice collection in the fully developed simulation were tried: $x/D_i = 0.14$ and x/D_i chosen so that the centreline profile matched the experiments *e.g.*, $x/D_i = 3$ for $r = 3.2$.

3.2.5 The outlet boundary condition

A convective condition (Orlansky, 1976, (3.18)) was applied at the outlet.

$$\frac{\partial \bar{u}_i}{\partial t} + \langle u \rangle_b \frac{\partial \bar{u}_i}{\partial x} = 0 \quad (3.18)$$

Discretization was explicit Euler and a buffer region with expanding grid was used to smooth the wiggles. Note that a first order boundary condition does not degrade the whole simulation, as demonstrated by Wesseling (2001). In this condition, about 30 % of the domain is to be discarded.

3.3 Numerical techniques

3.3.1 Fractional-step Navier-Stokes solver

The computer code development was part of the doctoral thesis of Silva Lopes (2000) followed by studies of isotropic turbulence in a distorted box (Silva Lopes and Palma, 2002) and of wall-bounded flow in an S-duct (Silva Lopes and Piomelli, 2006). Here, the level of detail was the strictly necessary for understanding of the present work, and the reader is referred to the studies above if further information is needed.

According with the fractional-step algorithm, on which the code is based, the Navier-Stokes equations are split into three uncoupled equations (for u , v and w) that are advanced explicitly in time using a second order Adams-Bashfort method. At the end of the time step the pressure is solved (Poisson equation), to ensure mass conservation (more exactly,

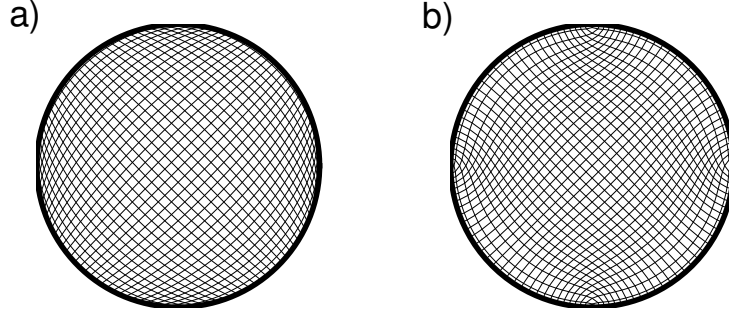


Figure 3.2: Grids for pipe flow simulation. (a) Grid generated by transfinite interpolation (b) Grid generated with elliptic methods (for clarity, only one every four points is shown)

an explicit pressure gradient term has been included in the momentum equations and a pressure correction is obtained). Pressure-velocity coupling is ensured by the pressure-weighted interpolation procedure (Rhie and Chow, 1983).

The Cartesian velocity components are stored along with the pressure at the centres of the control volumes (collocated arrangement). The midpoint rule is used for the surface integrals and the gradients are obtained at the cell centres using Gauss theorem (Ferziger and Peric, 2002). Both values and gradients are interpolated to the cell faces using linear interpolation. This is a non dissipative discretization (*i.e.*, it is identical to central differencing, for uniform grids) with no coordinate transformations, and is a procedure typical of unstructured codes, although the code only allows single block structured grids. The main advantage of using the approach above in a structured code is the lower amount of geometric information, which translates into memory savings *circa* 30 %. Use of linear interpolation is 2nd order accurate in orthogonal grids, but loses accuracy with increasing non-orthogonality.

3.3.2 Grid generation

Two grid generation methods were used in this work: The first, in fig. 3.2 (a), was obtained by transfinite interpolation (*cf.* Thompson et al., 1985) ; the second, in fig. 3.2 (b), was an elliptic Poisson grid generator, based on control maps, as described in Spekreijse (1999). It is important to control the distance to the wall. The grid generated using Spekreijse method had control over the wall distance in the first grid point, which varied between 0.5 and 2 wall units, and was adequate to turbulent flow. The transfinite interpolation grid was good enough to laminar flow but unconvincing in turbulent flow, due to a large variation in the distance to the wall of the first grid point, between 0.1 and 10.0 wall units. One wall unit corresponds to $r = \lambda_\nu = \nu/u_\tau$, where λ_ν is the viscous length, $u_\tau = \sqrt{\tau_w}$ and $\tau_w = \mu \partial u / \partial r \mid (r = D_o/2)$.

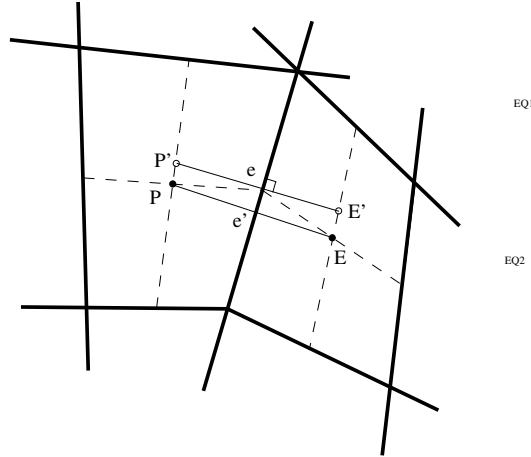


Figure 3.3: A numerical cell, focusing on the east face

The finer grids required for the grid refinement study were obtained by division of the base 66^3 grid, leaving the wall cells untouched.

3.3.3 Dealing with high non-orthogonality

This section describes how an LES code was used to perform simulations in complex grids without losing accuracy near singular points arising in the grid generation process. To assess the validity of this approach, both laminar and turbulent pipe flows are presented in appendix B. The pipe flow was simulated using non-orthogonal structured grids, figure 3.2, where a circle was mapped into a square. Close to the map corners, regions of high non-orthogonality appear, providing a test of the code in a complex grid in simple and well documented flows. The cell distortion at the artificial corners is much larger than the values used in previous tests (Armenio and Piomelli, 2000; Silva Lopes and Palma, 2002). A deferred correction approach to continuity enforcement and a 2nd-order accurate gradient reconstruction procedure were used in these highly non-orthogonal grids. In the following, the discretizations used in the various terms are presented, with emphasis in the modifications introduced in the original code of Silva Lopes (2000).

3.3.3.1 Spatial discretization

For the sake of presentation, the spatial discretization, valid for 2D and 3D grids, structured or unstructured, will be based on the East face of a control volume, figure 3.3, with the extension to the other faces being straightforward. In our notation, borrowed from Ferziger and Peric (2002), upper and lower cases refer to quantities defined at the cell centre and face.

Convective fluxes The discretization of the convective fluxes is given by (3.19), where $\dot{m}_e$ is the mass flux obtained in the previous time step that satisfies the continuity equation.

$$F_{i,e}^c = \int_{S_e} \rho u_i \mathbf{v} \cdot \mathbf{n} dS \approx \dot{m}_e u_{i,e}. \quad (3.19)$$

In the original version of the code, the u velocity at the east face, $u_{i,e}$, was obtained by linear interpolation, which for a generic variable ϕ is given by

$$\begin{aligned} \phi_{e'} &= \lambda_e \phi_P + (1 - \lambda_e) \phi_E \\ \lambda_e &= \frac{\|\mathbf{r}_E - \mathbf{r}_{e'}\|}{\|\mathbf{r}_E - \mathbf{r}_P\|} \end{aligned} \quad (3.20)$$

This is recommended by Ferziger and Peric (2002) as the best compromise for industrial codes. Only in an orthogonal grid e' coincides with the cell face centre e and $\phi_e = \phi_{e'}$ is a 2nd order approximation; in case of a non-orthogonal grid, $\phi_e = \phi_{e'}$ becomes a 1st order accurate approximation if e' is far from the face centre. In this work, a 2nd order accurate estimate of ϕ_e was obtained using the gradient correction,

$$\phi_e = \phi_{e'} + (\text{grad } \phi)_{e'} \cdot (\mathbf{r}_{e'} - \mathbf{r}_e) \quad (3.21)$$

where $\mathbf{r}_{e'}$ and $\mathbf{r}_e$ are the position vectors of e' and e (the actual face centre, as shown in fig. 3.3).

Gradient calculation The gradients at the cell centres are calculated using Gauss theorem.

$$\left(\frac{\partial \phi}{\partial x_i} \right)_P \approx \frac{\int_{\Omega} \frac{\partial \phi}{\partial x_i} d\Omega}{\Delta \Omega} = \frac{\int_S \phi \mathbf{i}_i \cdot \mathbf{n} dS}{\Delta \Omega} \approx \frac{\sum_c \phi_c S_c^i}{\Delta \Omega} \quad (3.22)$$

The cell face values ϕ_c (c is successively replaced by all six faces of the control volume) are required. Extension of the methodology in (3.21) to the gradient evaluation requires an iterative procedure. The face values are first calculated using linear interpolation only and the gradients thus calculated are used in a next step to correct the face values in (3.22). The procedure can be repeated as many times as required. It should be noted, however that one iteration in the gradient calculation increases the overall computing time by 30%.

Diffusive fluxes The diffusive flux for the x direction was found after all gradients were interpolated to the faces from cell centre values.

$$F_{i,e}^d = \int_{S_e} \tau_{ij} \mathbf{i}_j \cdot \mathbf{n} dS \approx (\tau_{xj})_e S_e^j \quad (3.23)$$

To avoid the instabilities due to the odd-even decoupling problem a stabilising term, the second term on the right hand side of (3.24), was added,

$$F_{i,e}^d = (\tau_{xj})_e S_e^j + \frac{\nu_e S_e}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}} (u_E - u_P - (\text{grad } u)_e \cdot (\mathbf{r}_E - \mathbf{r}_P)). \quad (3.24)$$

The diffusive term can be rearranged, yielding

$$\int_{S_e} \nu \frac{\partial u}{\partial n} dS + \int_{S_e} \nu \frac{\partial u_j}{\partial x_i} \mathbf{i}_j \cdot \mathbf{n} dS, \quad (3.25)$$

$$\left(\frac{\partial \phi}{\partial n} \right)_e \approx \frac{\phi_{E'} - \phi_{P'}}{\|\mathbf{r}_{E'} - \mathbf{r}_{P'}\|} = \frac{\phi_{E'} - \phi_{P'}}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}}, \quad (3.26)$$

$$\mathbf{r}_{P'} \approx \mathbf{r}_e - [(\mathbf{r}_e - \mathbf{r}_P) \cdot \mathbf{n}] \mathbf{n}, \quad \mathbf{r}_{E'} \approx \mathbf{r}_e - [(\mathbf{r}_e - \mathbf{r}_E) \cdot \mathbf{n}] \mathbf{n} \quad (3.27)$$

$$\phi_{P'} = \phi_P + (\text{grad } \phi)_P \cdot (\mathbf{r}_{P'} - \mathbf{r}_P), \quad \phi_{E'} = \phi_E + (\text{grad } \phi)_E \cdot (\mathbf{r}_{E'} - \mathbf{r}_E). \quad (3.28)$$

where the first term is a normal derivative, that can be obtained to 2nd order accuracy using a reconstruction procedure based on the gradient correction (3.21). To understand it, refer to figure 3.3: ϕ_P and ϕ_E are the known values, at the cell centre. Using E and P instead of E' and P' in (3.26) leads to a loss of order of accuracy. To recover second order accuracy, The positions of E' and P' are obtained using (3.27) and the values $\phi_{P'}$ and $\phi_{E'}$ using (3.28). Now, (3.26) is second order accurate.

3.3.3.2 Pressure-velocity coupling and continuity

Pressure weighted interpolation Pressure-velocity coupling was achieved using the pressure weighted interpolation method of Rhie and Chow (1983). After advancing the momentum equations in time (with or without a pressure gradient term), the mass flux at the faces was calculated by

$$\begin{aligned} \dot{m}_e^* &= \rho_e v_{n,e}^* S_e, \\ v_{n,e}^* &= \overline{(v_{n,e}^*)} - \Delta t \left[\left(\frac{\partial p}{\partial n} \right)_e - \overline{\left(\frac{\partial p}{\partial n} \right)_e} \right]. \end{aligned} \quad (3.29)$$

The formulation used in Silva Lopes (2000) was maintained. The velocity at the cell face $\overline{(v_{n,e}^*)}$ was found by projecting linearly interpolated Cartesian components into the

face normal vector, $\mathbf{S}_e$. Gradient reconstruction of this velocity using (3.21) was tested but required an expensive recalculation of the velocity gradients and was abandoned, also because observed differences were small.

The pressure gradients in (3.29) were approximated by

$$\left(\frac{\partial p}{\partial n}\right)_e \approx \frac{p_E - p_P}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}} + \frac{(\text{grad } p)_E \cdot (\mathbf{r}_{E'} - \mathbf{r}_E) - (\text{grad } p)_P \cdot (\mathbf{r}_{P'} - \mathbf{r}_P)}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}} \quad (3.30)$$

$$\approx \frac{p_E - p_P}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}}, \quad (3.31)$$

$$\overline{\left(\frac{\partial p}{\partial n}\right)_e} \approx \frac{\overline{(\text{grad } p)_e} \cdot (\mathbf{r}_E - \mathbf{r}_P)}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}}. \quad (3.32)$$

This was enough to prevent pressure oscillations with no need for the second additive term due to non-orthogonality in (3.30).

Continuity in orthogonal grids The mass fluxes obtained in (3.29) do not satisfy continuity (3.33) nor the Poisson equation for pressure, *cf.* Pope (2000), *i.e.*, res_0 in (3.33) is not zero.

$$\sum_c \dot{m}_c^* = res_0(i, j, k) \quad (3.33)$$

To correct this, a mass correction (3.36) was defined in terms of the pressure correction (p') gradient normal to cell face, $\dot{m}'_e = \rho_e \delta t S_e \left(\frac{\partial p'}{\partial n}\right)_e$. In orthogonal grids $\partial p' / \partial n$ is approximated to 2nd order accuracy by

$$\left(\frac{\partial p'}{\partial n}\right)_e \approx \frac{p'_E - p'_P}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}}. \quad (3.34)$$

Substitution into the continuity equation (3.35) for every control volume yields a system of equations for the pressure correction (3.37).

$$\sum_c (\dot{m}_c^* + \dot{m}'_c) = 0. \quad (3.35)$$

$$\dot{m}'_e = a_E (p'_E - p'_P) \quad (3.36)$$

$$a_E = - \frac{\rho_e \delta t S_e}{(\mathbf{r}_e - \mathbf{r}_P) \cdot \mathbf{n}}$$

$$a_E(i, \dots)(p'_E - p'_P) + a_E(i-1, \dots)(p'_W - p'_P) + \dots = -res_0 \quad (3.37)$$

The system has a seven diagonal coefficient matrix and can be solved efficiently using iterative methods. Once solved, the mass correction can be obtained from (3.36). The corrected mass fluxes satisfy continuity up to the iterative solver residual and the corrected pressures satisfy the Poisson equation to 2nd order accuracy.

Continuity in non-orthogonal grids The application of the above procedure in complex grids is not trivial. If a good approximation of the normal pressure gradient is used *e.g.*, equation (3.26), a large computational stencil is obtained yielding an expensive system of equations. If the terms associated to non-orthogonality are neglected (*i.e.*, if the procedure for orthogonal grids is applied without changes) instability can occur. This can be dealt with using a deferred correction approach. Ferziger and Peric (2002) suggest a second order approximation to the pressure gradient in non-orthogonal grids,

$$\left(\frac{\partial p'}{\partial n}\right)_e \approx \frac{p'_E - p'_P}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}} + \frac{(\text{grad} p')_E \cdot (\mathbf{r}_{E'} - \mathbf{r}_E) - (\text{grad} p')_P \cdot (\mathbf{r}_{P'} - \mathbf{r}_P)}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}}. \quad (3.38)$$

A first estimate of the pressure correction is obtained using the method described for orthogonal grids. At the end of this step, the mass residual is equal (to machine precision) to the iterative solver residual and is defined by

$$res_1 = a_E(i, \dots)(p'_E - p'_P) + a_W(i, \dots)(p'_W - p'_P) + \dots + res_0 \approx \sum_c (\dot{m}_c^* + \dot{m}'_c). \quad (3.39)$$

A new pressure correction p'' is then defined by,

$$\left(\frac{\partial p''}{\partial n}\right)_e \approx p''_E - p''_P + srce_1, \quad (3.40)$$

including estimates of the non-orthogonal terms based on p' .

$$srce_1 = \frac{(\text{grad} p')_E \cdot (\mathbf{r}_{E'} - \mathbf{r}_E) - (\text{grad} p')_P \cdot (\mathbf{r}_{P'} - \mathbf{r}_P)}{(\mathbf{r}_E - \mathbf{r}_P) \cdot \mathbf{n}} \quad (3.41)$$

We substitute in the continuity equation to obtain a new system of equations,

$$\begin{aligned} a_E(i, \dots)(p''_E - p''_P) + a_W(i, \dots)(p''_W - p''_P) + \dots = \\ res_1 - a_E(i, \dots)srce_1(i, \dots) + a_E(i-1, \dots)srce_1(i-1, \dots), \end{aligned} \quad (3.42)$$

with the same coefficients matrix and with the non-orthogonal terms appearing in the right hand side. The inclusion of res_1 in (3.42) ensures consistency between the solver and the mass flux residual and is an improvement over section 8.8 of Ferziger and Peric (2002), where it was neglected.

The extension of the above procedure to an arbitrary number of corrections is straightforward and was implemented. In the grids used in this study, three to five corrections were usually required.

3.3.4 Bounded convection term discretization schemes

The passive scalar field, unlike the velocity one, has a boundedness property *i.e.*, given initial and boundary values between two extremes, $\phi(\mathbf{r}, t)$ must remain between those values for all $(\mathbf{r}, t)$. This is demonstrated in Pope (2000), as a property of the transport equation for any conserved passive scalar.

When discretizing the passive scalar transport equation, the convection term needs special treatment. Simply using the second-order scheme presented in subsection 3.3.3, and used in the Navier-Stokes equations, leads to unboundedness when applied to the passive scalar transport. Part of the problem had to do with mass conservation in the velocity field: it was found that it was beneficial to solve the scalar transport equation using an incompressible velocity field - *i.e.*, using Adams-Bashfort instead of Runge-Kutta for integration in time. This was enough in plane channel simulations, but the problem remained in the coaxial jets simulations.

We used two boundedness preserving schemes: a fairly standard TVD scheme (TVD, from Wesseling, 2001, section 3.3.4.2) adapted to the convection term of collocated finite volume second order codes, and a scheme by Herrmann et al. (2004) (BLINT, section 3.3.4.3) that directly enforces the boundedness property.

3.3.4.1 Introduction: upwind and hybrid schemes

Upwind scheme The well known upwind discretization scheme

$$\begin{cases} \phi_e^u = \phi_i, & \text{if } \dot{m}_e > 0, \\ \phi_e^u = \phi_{i+1}, & \text{if } \dot{m}_e < 0, \end{cases} \quad (3.43)$$

is, by construction, monotone and wiggle-free. This, however, comes at the cost of accuracy and the scheme is only first order accurate. In fact, numerical analysts have proved the *order barrier theorem*: only first order schemes are absolutely monotonous (*cf.* Toro, 1999).

Hybrid scheme To combine the stability of the upwind scheme with the accuracy of higher (than one) order schemes has been a long time quest of the numerical analysis community. This is only possible using nonlinear methods, and many such schemes appear in the literature (Toro, 1999).

The hybrid scheme was recommended in Patankar (1980) for the first industrial type RANS. This scheme is governed by the Peclet number, $Pe = u(x_e - x_w)/D$, an important non-dimensional parameter because if $|Pe| < 2$, the central scheme (linear interpolation, in the context of finite volume codes) is monotonous. The hybrid scheme uses linear interpolation if $|Pe| < 2$ and reverts to upwind for $|Pe| > 2$, as formalised in

$$\phi_e^h = \phi_e^c s(Pe) + \phi_e^u (1 - s(Pe)), s = \begin{cases} 1. & |Pe| \leq 2, \\ 0. & |Pe| > 2. \end{cases} \quad (3.44)$$

The scheme is monotonous and reverts to second order linear interpolation when $Pe > 2$. However, high Pe does not always lead to oscillations. The criterion is too loose and effectively becomes first order in underresolved convection dominated flows (Ferziger and Peric, 2002).

3.3.4.2 TVD: A second order TVD scheme

Flux limited schemes To avoid oscillations in second order (or higher) schemes, a flux limiter must be introduced. In the context of a finite volume method, the goal of the limiter is to reduce the slopes used to interpolate variables to the control volume face. Where there are discontinuities, or very large gradients, the limiter must reduce the slope to zero, *i.e.*, the upwind scheme is recovered.

The ratio of consecutive gradients r is the parameter that detects unsmoothness (large gradients and/or discontinuities) and governs the flux limiting function Ψ , that switches between upwind, linear interpolation or some weighted average of the two. It is defined in terms of upstream, central and downstream nodes,

$$r = \frac{\phi_C - \phi_U}{\phi_D - \phi_C} \quad (3.45)$$

A general TVD scheme (*cf.* Wesseling, 2001) is presented below,

$$\begin{cases} \phi_e = \phi_i + \frac{1}{2}\Psi(r_i)(\phi_{i+1} - \phi_i), & \text{if } \dot{m}_e > 0. \\ \phi_e = \phi_{i+1} + \frac{1}{2}\Psi(1/r_{i+1})(\phi_i - \phi_{i+1}), & \text{if } \dot{m}_e < 0. \\ r_i = \frac{\phi_i - \phi_{i-1}}{\phi_{i+1} - \phi_i} \end{cases} \quad (3.46)$$

where Ψ is the flux limiting function that distinguishes between the many TVD schemes available.

Modifying as little as possible the tried and tested second order scheme recommended in Ferziger and Peric (2002), the basis of our own Navier-Stokes solver, we modified (3.46) so that $\Psi=1$ yields linear interpolation,

$$\begin{cases} \phi_e = \phi_i + (1 - \lambda_e)\Psi(r_i)(\phi_{i+1} - \phi_i), & \text{if } \dot{m}_e > 0. \\ \phi_e = \phi_{i+1} + \lambda_e\Psi(1/r_{i+1})(\phi_i - \phi_{i+1}), & \text{if } \dot{m}_e < 0. \\ r_i = \frac{\phi_i - \phi_{i-1}}{\phi_{i+1} - \phi_i} \end{cases} \quad (3.47)$$

The scheme is identical to the central differences limiter from Wesseling (2001) in regular grids, and is therefore of second order in regular grids wherever $\Psi=1$. In irregular grids, it is nevertheless asymptotically second order in smoothly varying grids (*cf.* Ferziger and Peric, 2002).

A second order flux limiting function The flux limiting function adds an anti-diffusive term, when flow is smooth. In this way a scheme of positive type is obtained, while retaining as much as possible second order accuracy. We apply the second order flux limiting offered in Wesseling (2001), equation (3.48).

$$\begin{cases} \Psi(r) = 0., & r < 0. \\ \Psi(r) = \frac{2r}{(1+r)^2}(1 + 2r - r^2), & 0. < r < 1. \\ \Psi(r) = 1., & r > 1. \end{cases} \quad (3.48)$$

In our work, we focused in second order limiting functions, since high-order schemes are hard to apply in non-orthogonal grids and much or all of the accuracy would be only nominal, due to the non-orthogonality itself. However, an improvement would be to add the gradient correction described in (3.21) to the second term in (3.47).

3.3.4.3 BLINT: Bounded linear interpolation

Herrmann et al. (2004) presented a bounded QUICK scheme (BQUICK) that ensured boundedness by switching between two interpolating functions. We adapted the method to the second order finite volume scheme (identical to the one used in the Navier-Stokes equations) based on linear interpolation.

In this method, two right-hand sides (RHSs) are computed for the Adams-Bashfort explicit time-advancement scheme: one using the second order finite volume with linear

interpolation (eq. 3.49 LINT RHS) and another using upwind interpolation (eq. 3.3.4.3 - Upwind RHS). The solution was then advanced in two substeps:

- Prediction step, where $\phi^p(t + \Delta t)$ is obtained from $\phi^0(t)$ using the LINT RHS
- Correction step, where **if** $\phi^p > \phi_{max}$ **or** $\phi^p < \phi_{min}$, $\phi^p(t + \Delta t)$ is obtained from $\phi^0(t)$ using the Upwind RHS

$$\phi_e = \phi_i + (1 - \lambda_e)(\phi_{i+1} - \phi_i) \quad (3.49)$$

$$\begin{cases} \phi_e = \phi_i, & \text{if } \dot{m}_e > 0. \\ \phi_e = \phi_{i+1}, & \text{if } \dot{m}_e < 0. \end{cases}$$

We call this method the BLINT scheme. The method was tested in plane channel flow and good agreement with Keating (2004) is shown in appendix B.

If one wishes to see both schemes in the same light one can picture BLINT as a TVD method (3.47) where the limiter Ψ is no longer governed by r but is instead 1 when global boundedness is preserved or 0 (upwind scheme) when it isn't.

$$\text{if } \phi < 0 \text{ or } \phi > 1, \Psi = 0 \text{ else } (0 < \phi < 1), \Psi = 1$$

This has the added advantage of clearly showing the global boundedness nature of BLINT, and makes it comparable to schemes of the TVD family by plotting $\langle \Psi \rangle$. Plots of $\langle \Psi \rangle$ allow a quantitative assessment of the accuracy of each method by comparison of the ensemble average of $\langle \Psi \rangle$ over the whole domain.

Chapter 4

Large-Eddy Simulations of Confined Coaxial Jets

Abstract

Large-eddy simulations of confined coaxial jets are presented and analysed in this chapter. Two ratios of annulus to pipe bulk velocity were studied, 3.2 and 0.8, for an outer to inner diameter ratio of 2.33, a Reynolds number of about 30000 and a Schmidt number of 1000. The goal was to determine the prediction capability of an industrial type flow, based on non-orthogonal grids, by comparison with experiment. Accurate reproduction of $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$ was achieved, and fair agreement with $\langle \phi \rangle$. Turbulent fluxes $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ were also compared with the experiments and discrepancies analysed, by computing the transport equation budget of the statistics. A connection to the Taylor diffusivity independence hypothesis, by use of a hyperbolic passive scalar transport equation, is proposed.

4.1 Introduction

The objective of the work in the present chapter was to develop and test tools for the LES of passive scalar mixing, using confined coaxial jets as the testing ground. The main focus was on the tool developed: a passive scalar transport LES code, using a dynamic procedure and a non-orthogonal grid. Comparison with experiments allowed examination of numerical and modelling choices and pointed out limitations of the tool. The chapter includes analysis of the effects of the discretization of the convective terms and of transport equation budgets.

Two flow conditions, selected from Lima (2000) were used: $r = 0.8$, with the lowest

experimental uncertainty for $\langle u \rangle$ and $\langle \phi \rangle$ and with mixing mainly governed by small scales, and $r = 3.2$, with larger experimental $\langle \phi \rangle$ uncertainty but lower $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ relative uncertainty and with mixing governed by large scale structures. This matches the conclusions from chapter 2 (section 2.5).

For high Peclet number, $Pe = Re \times Sc$, it is necessary to validate LES by comparison with experimental results, as DNS results are impossible to obtain. There are important applications in which $\langle \phi \rangle$ is not enough and a large part of our work was devoted to comparison of $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ of LES against experiment. In pollutant dispersion and chemical reaction, including combustion, the instantaneous value of ϕ is crucial, so an estimate of the fluctuation, obtained with a simple model, is added to the $\bar{\phi}$ produced by the LES simulation. However, the accuracy of the extreme values of ϕ is connected with the accuracy of $\langle \phi' \phi' \rangle^{1/2}$: the way to access the accuracy of $\bar{\phi}$ for high Pe is to compare $\langle \phi' \phi' \rangle^{1/2}$ with $\langle \phi' \phi' \rangle^{1/2}$ from the experiment. The turbulent scalar flux, $\langle u' \phi' \rangle$, appears in the evolution equation for $\langle \phi \rangle$ (equation A.21) and represents the effect of the fluctuation on the mean field. It is the term modelled in RANS type closures and use of LES to improve RANS closures is dependent on an accurate reproduction of this quantity in the LES simulation.

In this work $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ were computed and many tests performed (section 4.3) to either improve agreement or understand its absence, including a study of the transport equation budgets (section 4.4). A connection with Taylor diffusivity independence hypothesis and the relevance to SGS modelling are presented in the final part of the chapter (section 4.5).

4.2 Mathematical model and numerical techniques

In this section, a brief review of chapter 3 is made, and details of the simulations are presented.

4.2.1 Mathematical and numerical models

As detailed in chapter 3, section 3.3.1, the Navier-Stokes equations were discretized using a second-order finite volume method and the temporal advancement was ensured by a second-order Adams-Bashfort.

Solution of the passive scalar transport equation required a special treatment of the convective terms, to preserve boundedness. Two schemes were used: a second order TVD scheme (section 3.3.4.2, henceforth called TVD), and a bounded second order scheme (section 3.3.4.3, henceforth called BLINT).

To account for the effects of the filtered small scales on the large resolved ones, a

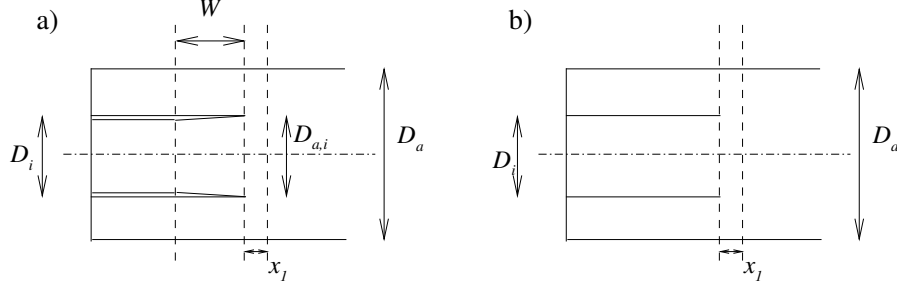


Figure 4.1: Geometry: a) experiment, b) computer simulations

Lagrangian dynamic subgrid model was used for the velocity and passive scalar fields (section 3.2.3).

The inlet boundary condition was obtained from a precursor simulation and submitted to a rescaling procedure to match the measurements at $x/D_i = 0.14$ (section 3.2.4). The walls were resolved, using no slip conditions for the velocity and zero-gradient conditions for the passive scalar. A convective condition (equation (3.18)) was applied at the outlet.

4.2.2 Geometry details

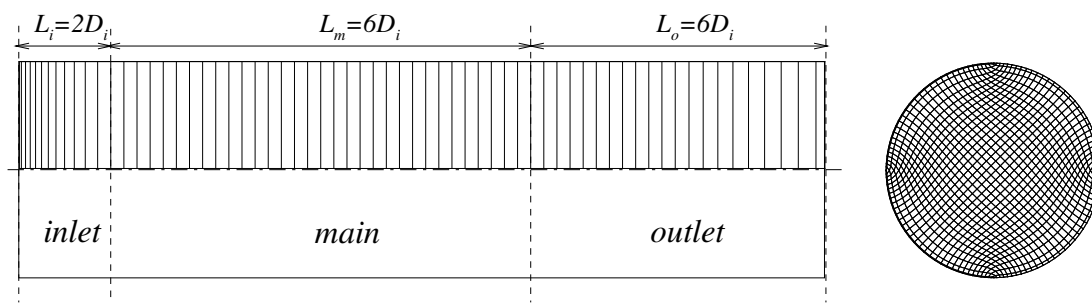
Both the integration domain and the experimental arrangement by Lima (2000) are shown in figure 4.1. The $2/18 D_i$ internal pipe wall is replaced by a zero thickness wall, leading to a diameter ratio, $\beta = 42/18 = 2.33$. The effect of including this wall is not investigated because the numerical resolution for accurately representing such a wall was insufficient, an option also followed in previous works (Akselvoll and Moin, 1996; Dianat et al., 2006).

Two velocity ratios $r = u_o/u_i$ were studied, $r = 3.2$ and $r = 0.8$. The bulk Reynolds number, $Re = \langle u \rangle_b D_o / \nu$ is 29400 for $r = 3.2$ and 35000 for $r = 0.8$. The Sc number is high and we used $Sc = 1000$ as a reasonable estimate, see section 2.2.2 for a discussion.

The grid generation procedure (Spekreijse, 1999) described in subsection 3.3.2 was used. In the streamwise direction (x) the domain length was $L = 14D_i$, enough to prevent unphysical effects of the outlet condition in the region of interest: $x/D_i < 8$. For $x < D_i$, an expansion factor ($f = 1.13$ for 66^3) was used. An expanding grid was also used in the outlet region ($x > 8D_i$), ($f = 1.03$ for 66^3). A plot of the grids used is presented in figure 4.2; the grid dimensions tested are summarised in table 4.1.

Table 4.1: Grids used in the simulations

Grid	NI	×	NJ	×	NK
1	66	×	66	×	66
2	98	×	98	×	98
3	128	×	128	×	128

Figure 4.2: The 66^3 grid used in most simulations

4.2.3 Computer resources

Most of the work was performed in a Dell machine, Dell₂₀₀₄, equipped with two Intel Pentium 4, 3.2 GHz and 512 Kbyte cache, 2 Gbytes RAM memory and 400 Gbytes storage, running linux kernel 2.4.18. The grid refinement tests were performed on another machine, Dell₂₀₀₉, with two Intel Xeon, 4 cores each, at 3.2 GHz and 8 Mbytes cache, 25 Gbytes RAM memory and 2 Tbytes hard drive storage, running linux kernel 2.6.22.

A test with 20 time steps was made, and the corresponding time, for a complete simulation, including precursor simulations and two runs, one to collect slices and another with rescaled slices, is presented in Table 4.2. A segmentation fault occurred for the larger grids in Dell₂₀₀₄, most likely due to memory issues (128^3 requires 4.5 GBytes of memory and 192^3 requires 14.8 GBytes).

The finer grids were used for grid refinement studies. Numerical and modelling tests required a large number of simulations and were performed in the 66^3 grid.

4.2.3.1 Cost and effect of gradient correction

For the quantities under study (mean, fluctuation, turbulent scalar flux), the contours were quite insensitive to the singular points; for the 66^3 grid, no corner effects were present when plotting mean and instantaneous fields and no changes were observed in the statistics when

Table 4.2: Time for a complete simulation, in days

	66^3	98^3	128^3	192^3
Dell ₂₀₀₄ ^a	4.4	7.1	—	—
Dell ₂₀₀₉ ^b	1.	1.8	4.7	47

^a Intel Pentium 4 (2×), 3.2 GHz, 2 Gbytes RAM^b Intel Xeon (2×4 cores), 3.2.GHz, 25 Gbytes RAM

gradient correction was turned on.

The computation of two gradient corrections plus the computation of deferred correction terms yields an increase of 70% in the computing time. Since the cost is significant, the corrections were not used in the simulations.

4.2.4 Averaging procedure

The averages were obtained by interpolating the mean 2D slices at a given x to a circular grid and than averaging over azimuthal. Finer and coarser circular grids were compared and showed little difference to the grid used. The averaging time was two cross-over times; the averaging starts after two cross-over times, to clean up transients. Doubling or halving the clean-up and averaging times had no effect. Even though half cross over time was enough in the case tested (66^3 grid, $r = 3.2$), two cross-over times seemed more reasonable and were the time used.

4.3 Effects of numerical and modelling parameters

A large set of calculations summarised in table 4.3 were performed, before reaching a working understanding of the most appropriate modelling and numerical tools. These included:

- Grid refinement (section 4.3.2.1): the 66^3 grid used as a reference, runs 3 and 4, was compared against results on grid 98^3 , runs 7 and 8, and 128^3 , runs 9 and 10.
- ϕ convection term discretization (section 4.3.2.2): the TVD discretization, runs 3 and 4, was compared against BLINT, runs 1 and 2, and upwind (UPW), runs 5 and 6, discretizations.
- Inlet (section 4.3.3.1): The fully developed inlet was compared against a rescaled one, for runs 3 and 4.

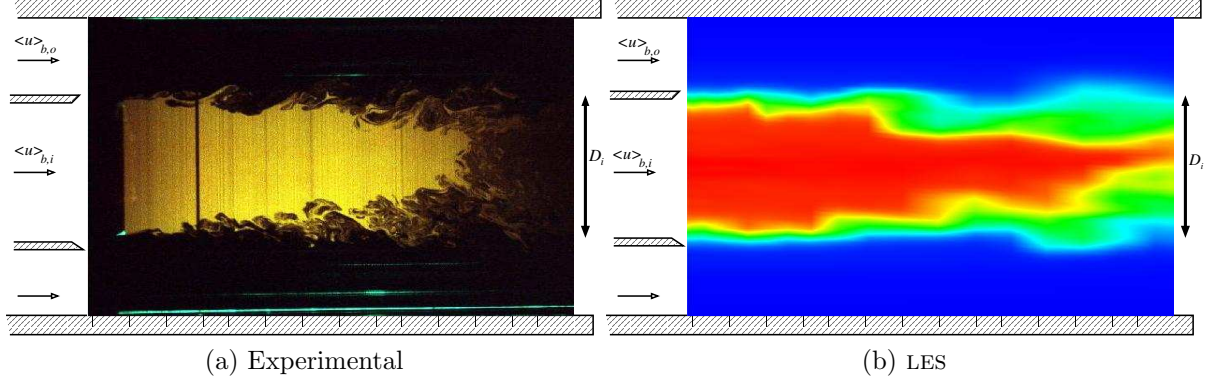


Figure 4.3: Visualisation of the entry region ($x/D_{i,i} \lesssim 3.5$) for $r = 3.2$

- The physical Sc number (section 4.3.3.2): $Sc = 1000$, runs 3 and 4, was compared against $Sc = 1$, runs 17 and 18.
- The passive scalar SGS model (section 4.3.3.3): various constant Sc^{sgs} (0.25, 0.5 and ∞ , runs 10 to 18) were compared against dynamic Sc^{sgs} , runs 3 and 4, where the spatial variation of Sc^{sgs} is shown. The goal of the parametric tests with Sc^{sgs} was not to fit Sc^{sgs} , but rather to gain insight on the link between Sc^{sgs} and the statistics.
- No diffusive terms (section 4.3.3.4): $Sc = Sc^{sgs} = \infty$, runs 19 and 20.

The main criteria used for selection was the comparison with experiment, namely the agreement in $\langle u \rangle$, $\langle u'u' \rangle^{1/2}$, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$. Other aspects, such as formal order of accuracy, were also considered. The reasons behind the numerical (section 4.3.2) and modelling (section 4.3.3) options used in the reference simulations are thus presented. Achievements and limitations of the reference simulations are presented next (section 4.3.4), followed by a summary of conclusions from modelling and numerical tests (section 4.3.5). Then the budgets of transported variables are shown (section 4.4) and the connection to the diffusivity independence hypothesis is proposed (section 4.5.1).

4.3.1 Instantaneous fields

Flow visualisation is available (Lima, 2000), in figure 4.3a for $r = 3.2$ and in 4.4a for $r = 0.8$ and can be compared with instantaneous fields from the LES simulation. Figure 4.3b is an instantaneous ϕ field for velocity ratio $r = 3.2$. The development of the mixing layer between the annular and the inner jet can be seen, via large turbulent structures developed and increased in size with the downstream distance. Comparing with the experimental visualisation of figure 4.3a, the effect of the coarser resolution of LES simulation was seen, since the smaller structures are not present and the central region behaviour seems indeed

Table 4.3: Details of simulation setups

RUN	$r = u_o/u_i$				Grids			Conv. Disc.			SGS Sc^{sgs}				Sc			Figure ¹
	0.8	3.2	1	2	3	TVD	BLT	UPW	Dyn	0.25	0.50	∞	1	10^3	∞			
01	●	—	●	—	—	—	●	—	●	—	—	—	—	●	—	—	4.13	
02	—	●	●	—	—	—	●	—	●	—	—	—	—	●	—	—	4.9	
03	●	—	●	—	—	●	—	—	●	—	—	—	—	●	—	—	4.30	
04	—	●	●	—	—	●	—	—	●	—	—	—	—	●	—	—	4.28	
05	●	—	●	—	—	—	—	●	●	—	—	—	—	●	—	—	4.14	
06	—	●	●	—	—	—	—	●	●	—	—	—	—	●	—	—	4.10	
07	●	—	—	●	—	●	—	—	●	—	—	—	—	●	—	—	4.8	
08	—	●	—	●	—	●	—	—	●	—	—	—	—	●	—	—	4.6	
09	●	—	—	—	●	●	—	—	●	—	—	—	—	●	—	—	4.8	
10	—	●	—	—	●	●	—	—	●	—	—	—	—	●	—	—	4.6	
11	●	—	●	—	—	●	—	—	—	●	—	—	—	●	—	—	4.23	
12	—	●	●	—	—	●	—	—	—	●	—	—	—	●	—	—	4.21	
13	●	—	●	—	—	●	—	—	—	—	●	—	—	●	—	—	—	
14	—	●	●	—	—	●	—	—	—	—	●	—	—	●	—	—	—	
15	●	—	●	—	—	●	—	—	—	—	—	●	—	●	—	—	4.24	
16	—	●	●	—	—	●	—	—	—	—	—	●	—	●	—	—	4.22	
17	●	—	●	—	—	●	—	—	●	—	—	—	●	—	—	—	—	
18	—	●	●	—	—	●	—	—	●	—	—	—	●	—	—	—	—	
19	●	—	●	—	—	●	—	—	—	—	—	●	—	—	●	—	—	
20	—	●	●	—	—	●	—	—	—	—	—	●	—	—	●	●	4.25	

^aPlots that add no information were not included: RUNs 13, 14 and 19 are similar to RUN 3, RUNs 17 and 18 are similar to RUN 4.

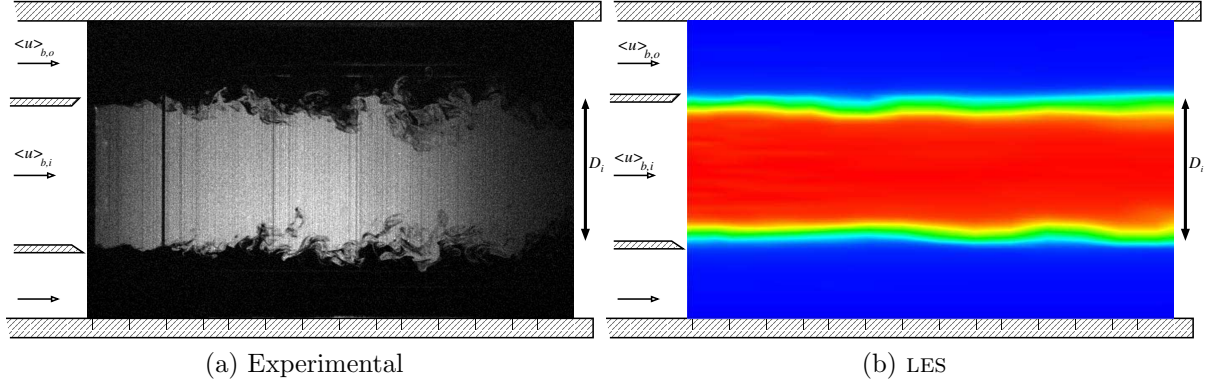


Figure 4.4: Visualisation of the entry region ($x/D_{i,i} \lesssim 3.5$) for $r = 0.8$

a filtered version of the experiment. For velocity ratio $r = 0.8$ (figure 4.4b) mixing was much slower (compare with figure 4.4a) and again the LES plot did look like a filtered version of the experiment. The plots are from the 66^3 grids and plots from the finer grids (see table 4.1) were similar.

4.3.2 Numerical tests

This subsection deals with grid refinement and passive scalar discretization tests, both tightly connected with the grid resolution.

4.3.2.1 The effect of grid refinement

The grid refinement test covered both cases $r = 3.2$ and $r = 0.8$. The base 66^3 grid was refined twice, with a factor of $\sqrt{2}$, to 98^3 and 128^3 . For $r = 3.2$, run 4 is compared with run 8 and 10 (figures 4.5 and 4.6), whereas, for $r = 0.8$, run 3 is compared with runs 7 and 9 (figures 4.7 and 4.8).

For $r = 3.2$, the mean velocity and velocity fluctuation agreed with the experiment even in the coarsest 66^3 grid and the agreement improved slightly with refinement. The major improvement occurred in the mean passive scalar, that was much closer to experiment in the 98^3 grid and even closer in the 128^3 one. However, the passive scalar turbulent quantities, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ remained significantly higher in the simulations, regardless of the grids used.

For $r = 0.8$ the mean and fluctuating velocity and the mean passive scalar improve slightly with the first refinement, from 66^3 to 98^3 , but the second one, to 128^3 , had no impact on $\langle u \rangle$ and $\langle u' u' \rangle^{1/2}$ whereas $\langle \phi \rangle$ became slightly worse near inlet and slightly better away. The passive scalar turbulent quantities, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, are much higher

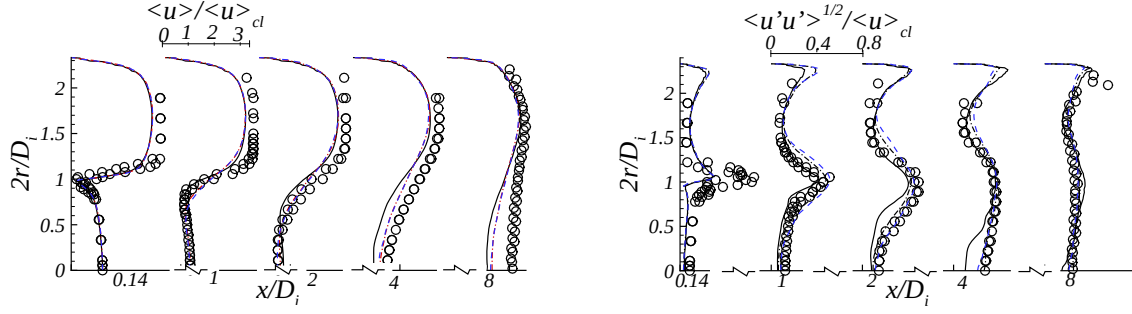


Figure 4.5: Streamwise velocity mean and fluctuation, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run4: $66 \times 66 \times 66$ - solid line; run8: $98 \times 98 \times 98$ - dash dot line; run10: $128 \times 128 \times 128$ - dashed line)

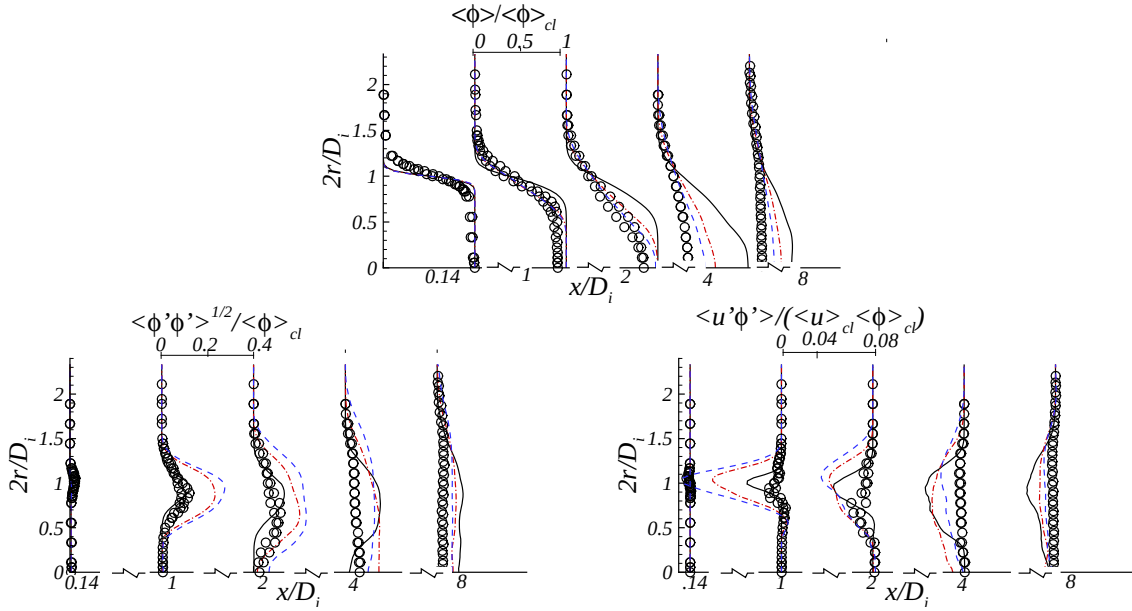


Figure 4.6: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run4: $66 \times 66 \times 66$ - solid line; run8: $98 \times 98 \times 98$ - dash dot line; run10: $128 \times 128 \times 128$ - dashed line)

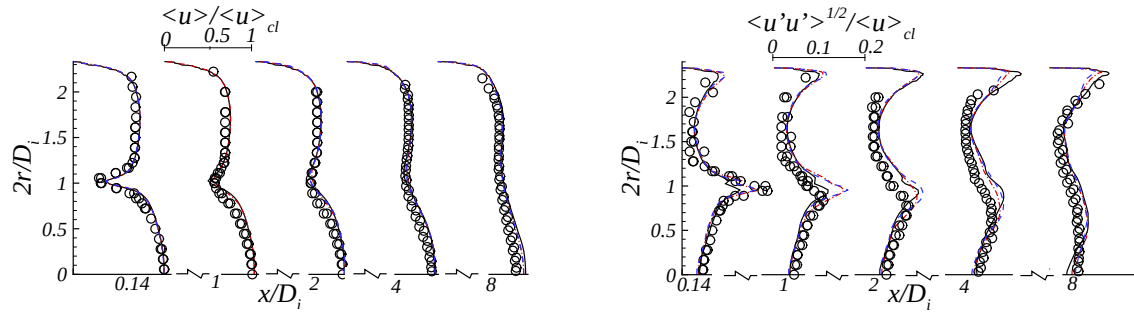


Figure 4.7: Streamwise velocity mean and fluctuation, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run3: $66 \times 66 \times 66$ - solid line; run7: $98 \times 98 \times 98$ - dash dot line; run9: $128 \times 128 \times 128$ - dashed line)

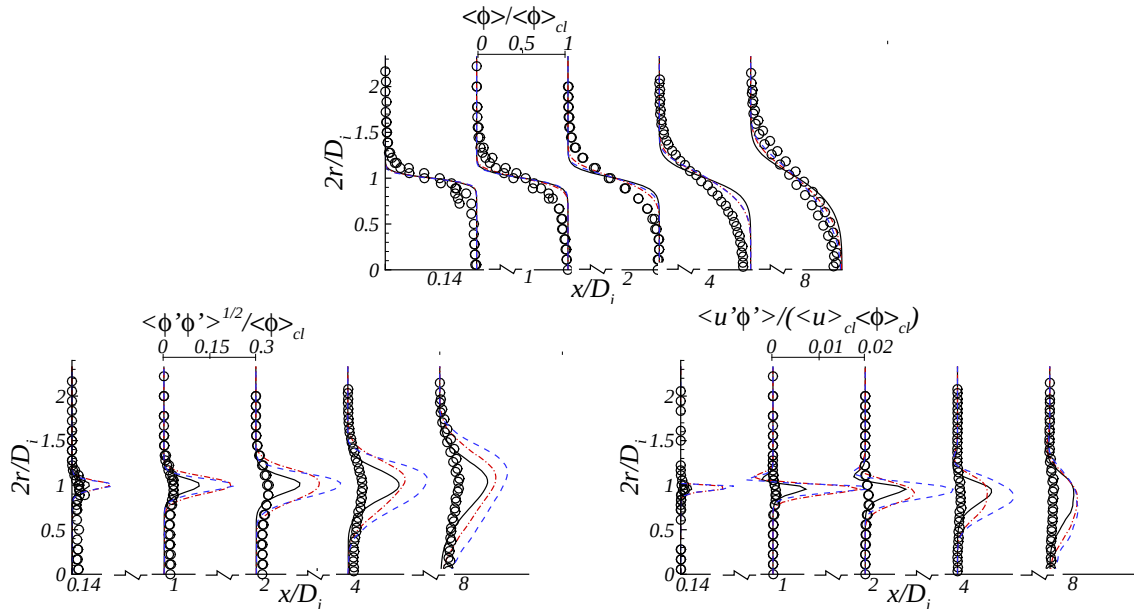


Figure 4.8: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run3: $66 \times 66 \times 66$ - solid line; run7: $98 \times 98 \times 98$ - dash dot line; run9: $128 \times 128 \times 128$ - dashed line)

than the experimental measurements and increase with grid refinement.

We conclude that fine grids are required for accurate reproduction of $\langle\phi\rangle$ for $r = 3.2$ and that passive scalar turbulent quantities are significantly higher than experimental values for all grid resolutions tested.

4.3.2.2 The effect of passive scalar convective term discretization

Figures 4.9 and 4.10 show the effect of BLINT (run 2) and upwind (run 6) over TVD discretization (run 4), for $r = 3.2$. TVD was a major improvement over BLINT for $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$, but was noticeably worse in the reproduction of $\langle\phi\rangle$ for $x/D_i > 4$. (figure 4.9). Upwind (figure 4.10) was similar to TVD in reproduction of $\langle\phi\rangle$ and even better in $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$.

As detailed in section 3.3.4.2, Ψ is the parameter that controls the average weight of the central scheme on the discretization ($\Psi = 0$ upwind, $\Psi = 1$, central scheme). In the TVD, the Ψ parameter was computed by the flux limiter used. In BLINT, $\Psi = 1$ is used first, and where boundedness is violated, Ψ is set to zero. The ensemble average $\langle\Psi\rangle_b$ over the whole domain was 0.55 for the TVD scheme and 0.85 for the BLINT scheme. This meant that the weight of the upwind scheme was $3\times$ higher in the TVD scheme (45 %) than on the BLINT scheme (15 %). The local variation is shown in figures 4.11 and 4.12. The pattern was similar for TVD and BLINT, with the lowest values appearing close to the inlet in the unmixed fluid region. This is fortunate, since this region is not critical. However, the BLINT scheme was almost a pure central scheme (Ψ higher than 99 %) in a large part of the domain, a rare occurrence in TVD; the BLINT scheme has a higher formal order of accuracy.

For $r = 0.8$, figure 4.13 shows the effect of BLINT discretization, whereas in figure 4.14 a test using upwind discretization is presented. The general appraisal is similar to the one made for $r = 3.2$. TVD reproduced $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$ much better, but BLINT was better for $\langle\phi\rangle$, even though agreement is satisfactory even for TVD. Again, use of the upwind scheme (figure 4.14) led to an improvement in $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$ and had no effect on $\langle\phi\rangle$ (not shown).

To conclude this section, we state that the discretization of the passive scalar convective terms was the parameter that influenced the results most. Use of the upwind scheme proved necessary. Average upwind weight ($1-\langle\Psi\rangle$) was 15 % on BLINT and 45 % on TVD, meaning that BLINT had higher formal accuracy. $\langle\phi\rangle$ was indeed better with BLINT, whereas $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$ were incorrect with both schemes but significantly better with TVD. Upwind was the best method in the case of $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$. It was not chosen, since it is a first order method and can become inaccurate, but the result is important and an explanation for it will be proposed later in the chapter (section 4.5.2). Formal order of accuracy was higher in BLINT, whereas TVD respected the boundedness property not only in a global

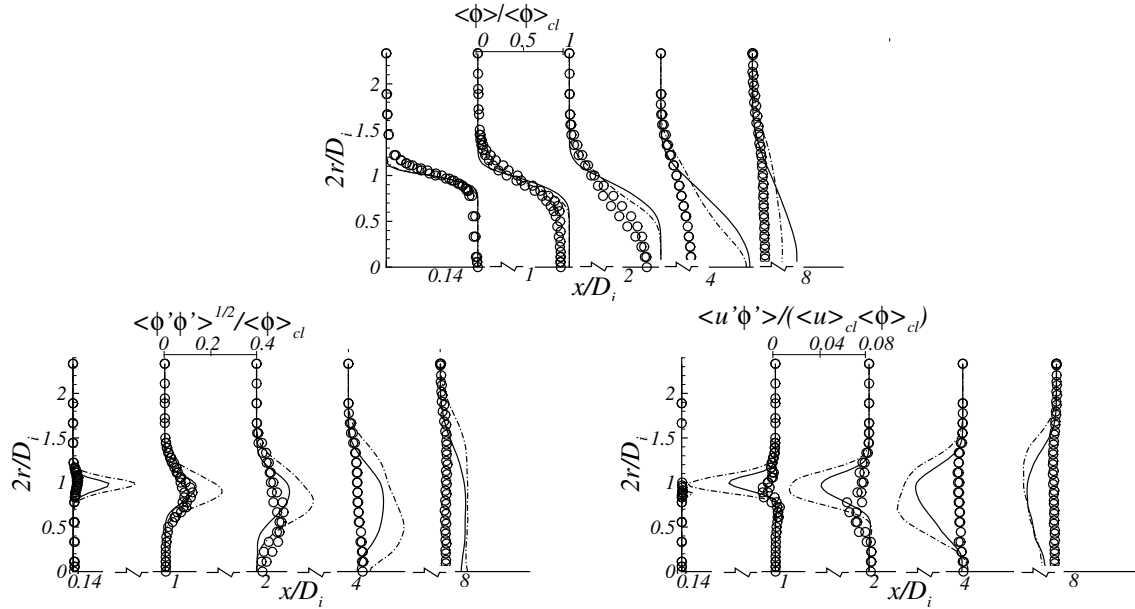


Figure 4.9: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: TVD- solid line; run 2: BLINT- dash dot line)

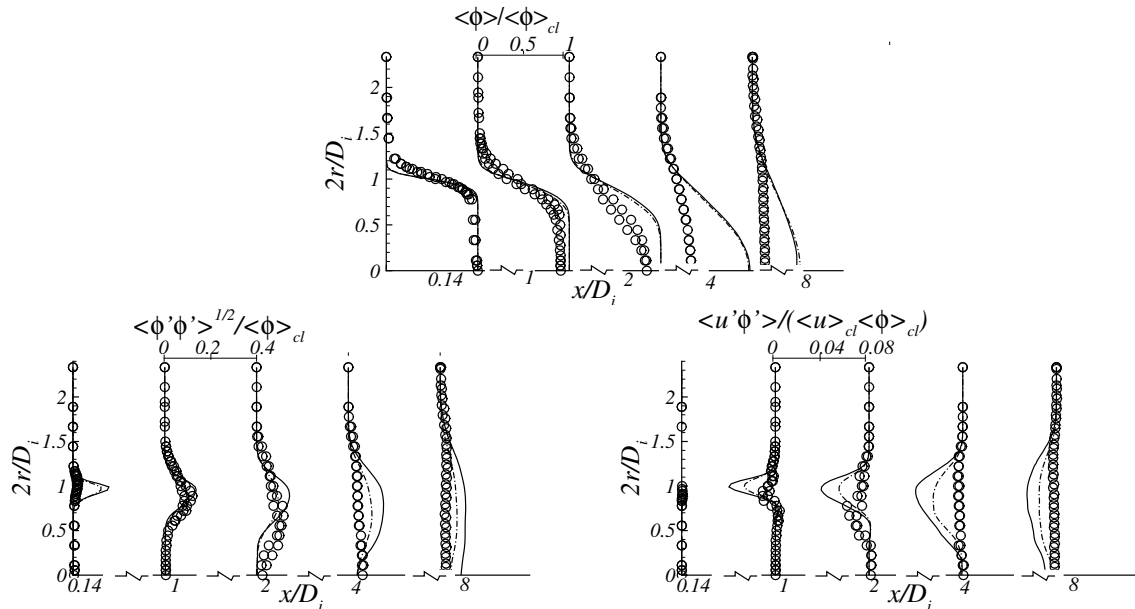
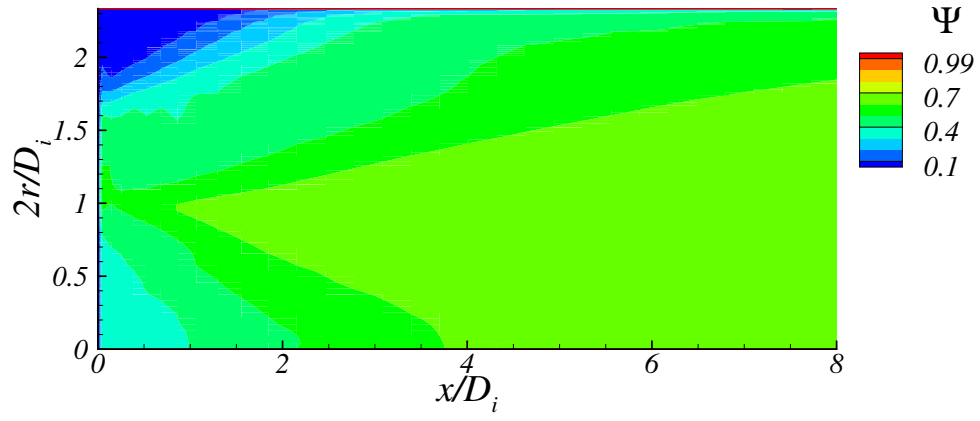
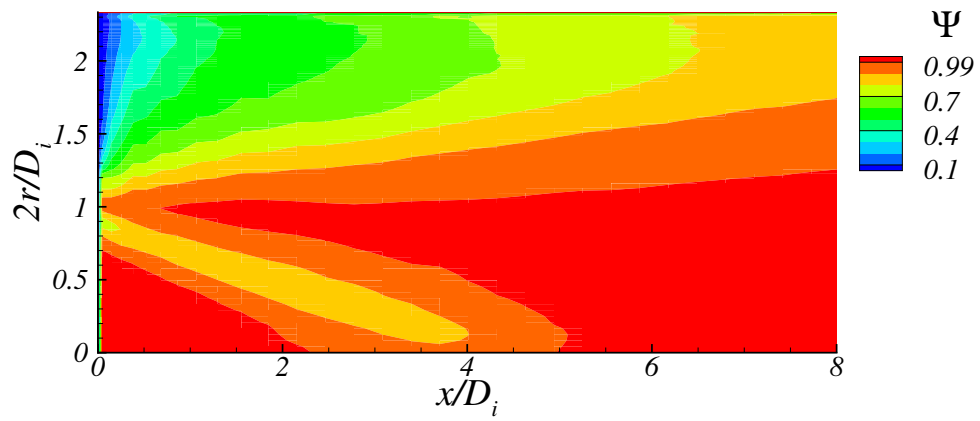


Figure 4.10: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: TVD- solid line; run 6: UPW- dash dot line)

Figure 4.11: $\langle \Psi \rangle$ for the TVD scheme for velocity ratio $r = 3.2$ (run 4)Figure 4.12: $\langle \Psi \rangle$ for the BLINT scheme for velocity ratio $r = 3.2$ (run 2)

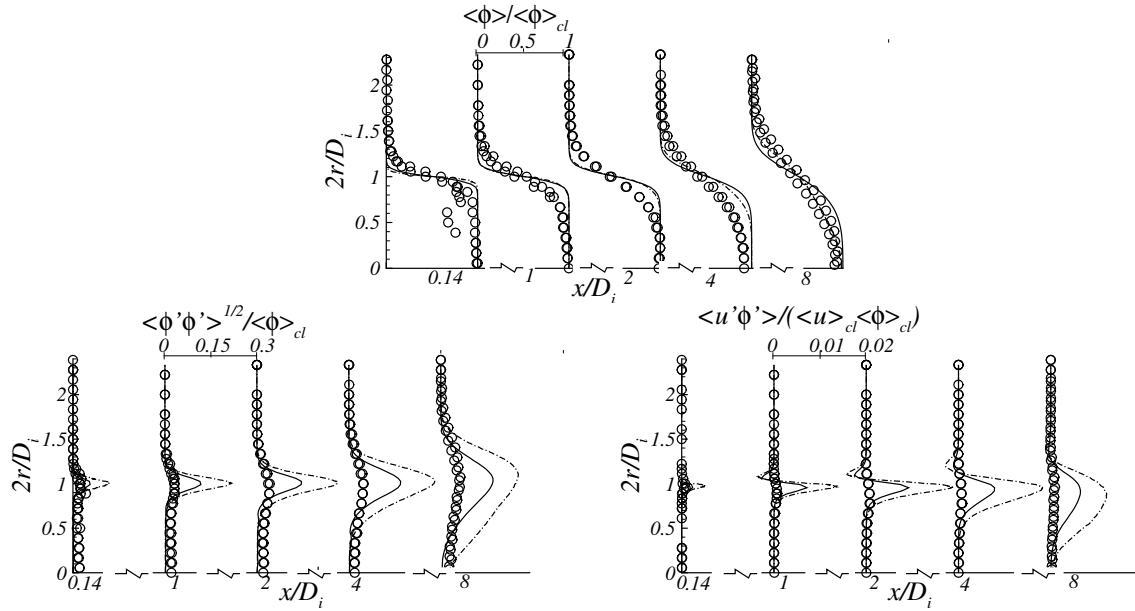


Figure 4.13: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: TVD- solid line; run 1: BLINT- dash dot line)

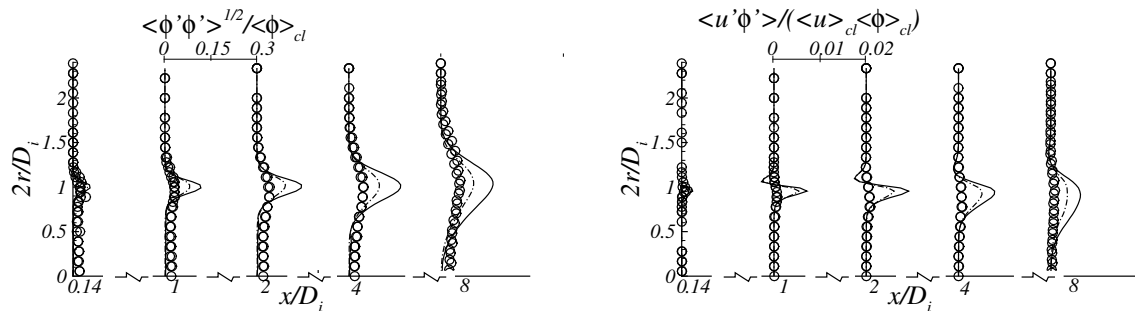


Figure 4.14: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: TVD- solid line; run 5: UPW- dash dot line)

sense, as BLINT, but also locally. The TVD method was chosen to be used as a reference, as it showed better overall agreement with the available data and is a reliable method.

4.3.2.3 Spatial resolution

The results in the previous subsections required the assessment of the resolution requirements based on physical principles.

Velocity We start by examining the resolution requirements for the velocity field. The length scale used to evaluate the resolution in wall bounded flows is the viscous length scale:

$$\lambda_\nu = \nu / u_\tau, u_\tau = \sqrt{\tau_w}, \tau_w = \mu \frac{\partial u}{\partial r}(x, y, z = D_o/2). \quad (4.1)$$

The cell size is expressed in λ_ν units, henceforth called wall units. We obtained an estimate for λ_ν using the relation from Kays and Crawford (1980), $C_f/2 = 0.039 Re^{-0.25}$ where $Re = \langle u \rangle_b D_i / \nu$ and $u_\tau = \langle u \rangle_b \sqrt{C_f/2}$.

Applying these length scales to the wall region (annulus outer wall), in the $r = 3.2$ condition, the most demanding in resolution requirements, due to higher Re , the distance of the first control volume centre to the wall varied between 0.5 and 3 wall units. The distance in the directions tangent to the wall reached a maximum of 25 wall units. All these values are within standard for resolved LES wall simulations (*cf.* Sagaut, 2004, chapter 9, Boundary Conditions).

In the shear-layer region, if one demands the same resolution as close to a wall, this zone is under-resolved, with the cell size averaging $20 \times \lambda_\nu$ in the radial direction, for the 66^3 grid and $10 \times \lambda_\nu$ for the finest 128^3 grid. If $r^+ = r/\lambda_\nu$, to solve the internal wall a point of about $r^+ = 1$ would be needed, plus a few points between $r^+ = 1$ and $r^+ = 20$ to represent the near wall gradient. If one considers the effects of non-orthogonality, the resolution in the shear layer region is in fact 41 % worse than it seems, according to Piomelli (private communication), quoting analysis made in the immersed boundary context. Therefore, resolution for the velocity is coarse, according to established criteria (*cf.* Sagaut, 2004), if trying to start the simulation from $x/D_i = 0$ and represent the wall. However, the profile by $x/D_i = 0.14$ was more like a free-shear layer than wall bounded and the appropriate length scale is 25 wall units, according to Miller and Dimotakis (1991).

We conclude that the velocity shear-layer was resolved, since the rescaling procedure lessens the need to resolve the internal wall boundary layers, and makes the available grid satisfactory.

Passive scalar To evaluate the resolution of the passive scalar transport equations based on the "smallest strain limited diffusion length scale",

$$\lambda_D = \lambda_\nu Sc^{-1/2}, Sc = \nu/\alpha. \quad (4.2)$$

With this scale, the passive scalar length scale should be $Sc^{1/2}$ times smaller than the viscous length scale (equation 4.1). For $Sc = 1000$ of Rhodamine-B in water, this means resolution is $33\times$ worse in the passive scalar field than in the velocity field.

Unlike in the velocity, there is no consensus as to the length scale to use (Mi and Nathan, 2003). Our choice is recommended in Miller and Dimotakis (1991). We conclude that the passive scalar shear layer was under-resolved, due to the high Sc number.

Another view of the resolution is given by the connection with the discretization scheme. Upwinding proved necessary and using central scheme more often, as in BLINT, by relaxing the boundedness property at local level, yielded poorer results. The better results of the first order scheme are in this context an indication of under-resolution.

We conclude the analysis of resolution by stating that the grid used in the shear-layer region was coarser than is recommended in the literature, and coarser than that used by Akselvoll and Moin (1996) and Dianat et al. (2006). Nonetheless, it was sufficient to reproduce $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$. For the passive scalar, there are no clear guidelines in the literature, but the relation between the length scales indicates a resolution about $30\times$ finer would be required to the passive scalar with $Sc = 1000$.

In the revision stage of the thesis refinement by a factor of 2 in each direction was achieved. The mean passive scalar $\langle \phi \rangle$ improved for $r = 3.2$, where it had some room for improvement. However, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ remained much higher than the experimental measurements.

4.3.3 Modelling tests

This subsection deals with the effect of the inlet boundary condition and of the molecular (Sc) and subgrid scale (Sc^{sgs}) Schmidt numbers, including the spatially variable Sc^{sgs} computed in the dynamic model and the neglecting of diffusive terms, corresponding to $Sc = Sc^{sgs} = \infty$.

4.3.3.1 The effect of the inlet boundary condition

Here results using fully developed inlet conditions and rescaled inlet conditions are compared. Figures 4.15 and 4.16 show the effect of inlet rescaling in the $r = 3.2$ condition (run 4). Rescaling allowed almost perfect agreement for $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, figure 4.15. Rescaling was also beneficial to the passive scalar statistics. $\langle \phi \rangle$ improved significantly, but remained poor for $x/D_i = 4$, whereas a minor improvement was observed in $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$.

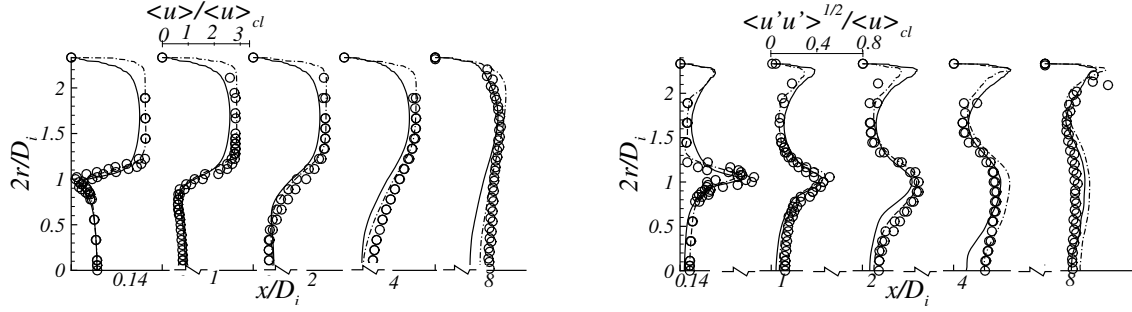


Figure 4.15: Streamwise velocity, mean and turbulent values, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$ for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: fully developed - solid line; rescaled - dash dot line)

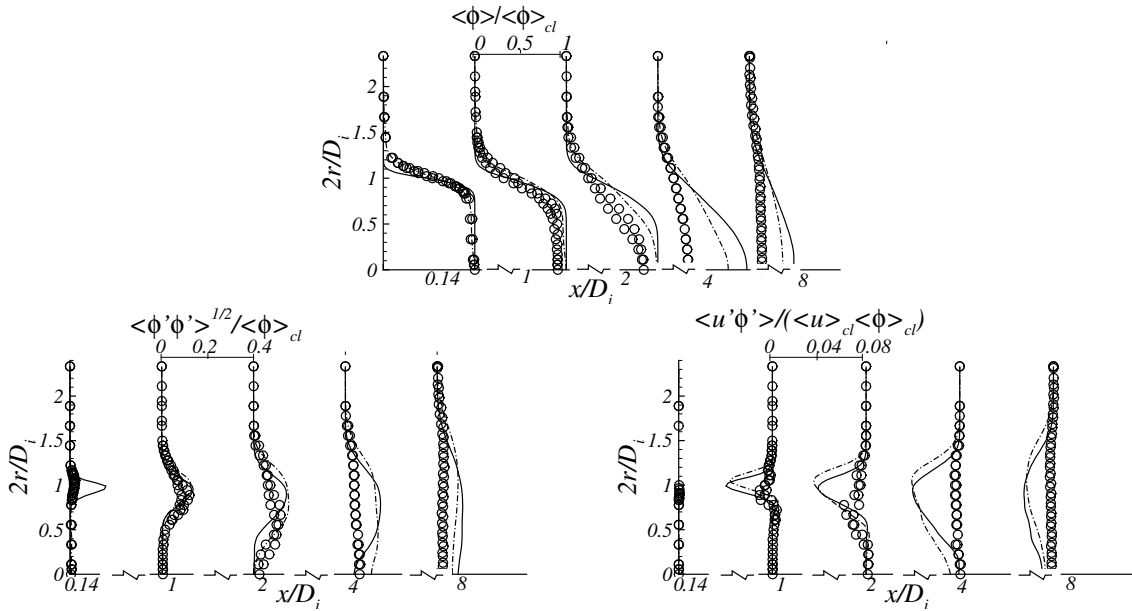


Figure 4.16: Passive scalar, mean and turbulent values $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: fully developed - solid line; rescaled - dash dot line)

Figures 4.17 and 4.18 show the effect of inlet rescaling in the $r = 0.8$ condition (run 3). The velocity profiles have reasonable agreement in both simulations, figure 4.17. Rescaling improved $\langle u \rangle$ in the annulus region for $x/D_i < 2$ and $\langle u'u' \rangle^{1/2}$ everywhere. With an inlet based on a sharp hyperbolic tangent profile, $\langle \phi \rangle$ was inaccurate for $x/D_i \leq 2$ but reasonable for $x/D_i = 4$ and $x/D_i = 8$. Rescaling improved $x/D_i < 2$ profiles, leading to good overall agreement. $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, figure 4.18, were highly inaccurate already at $x/D_i = 0.14$ and got worse with the increase in downstream distance. Rescaling improved the agreement, that nevertheless remained poor.

The passive scalar ϕ is fully mixed in the interior pipe and zero in the annulus. Therefore, at the inlet a flat profile occurs. Two effects occurred in the measured flow: molecular diffusion to the interior of the pipe and annulus and, most importantly, incipient recirculation to the interior of the pipe and annulus. Negative velocities were in fact present in the experiment time series. Apart from including part of the tube and annulus in the simulation (Akselvoll and Moin, 1996; Dianat et al., 2006), an option not available when using non-orthogonal grids, there is no implementation of an inlet boundary condition that could allow such effects, to the best of the author's knowledge.

The superiority of the rescaled inlet condition was not surprising, as it matches the annulus profile and, by starting at $x/D_i = 0.14$, avoids the need to represent numerically the flat scalar profile and the fast mixing that takes place between $x/D_i = 0$ and $x/D_i = 0.14$. Also, the mean profiles are smoother at $x/D_i = 0.14$, reducing the resolution requirements.

In most simulations, the fully developed velocity profiles are blended (averaged over 4 cells) in the shear layer region, and a smoothly varying hyperbolic tangent profile is set for the passive scalar. This improved the simulation stability, but had no impact on the results and plots are not shown. Two points of slice collection in the fully developed simulation were tried: $x/D_i = 0.14$ and x/D_i chosen so that the centreline profile matched the experiments, typical value was $x/D_i = 3$ for $r = 3.2$. No significant differences were found in the results after rescaling, and the simpler collection at $x/D_i = 0.14$ is the option followed in the remaining tests.

We conclude by stating that, for both velocity ratios, rescaling had a significant impact on the velocity profiles, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, and on the passive scalar mean $\langle \phi \rangle$ but had a minor impact on $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$.

4.3.3.2 The effect of the molecular Schmidt number

The effect of varying the Sc number was tested for both velocity ratios, by applying $Sc = 1$ and $Sc = \infty$ instead of the correct $Sc = 1000$:

- For $r = 0.8$: run 3 *versus* run 17,
- For $r = 3.2$: run 4 *versus* run 18.

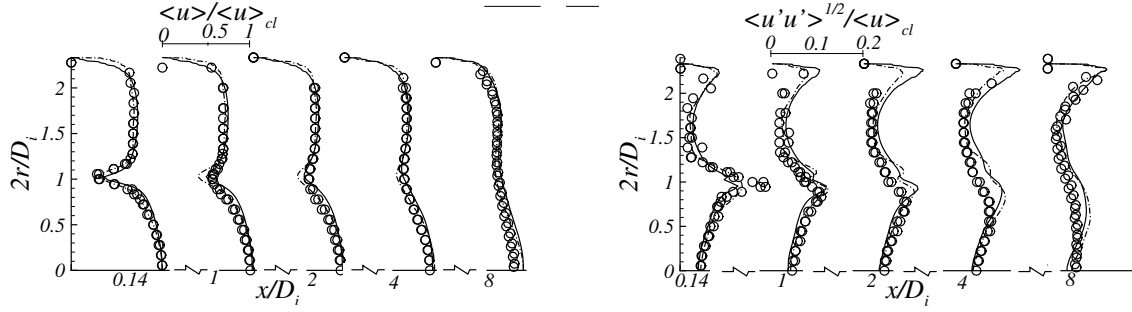


Figure 4.17: Longitudinal velocity, mean and turbulent values, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: fully developed - solid line; rescaled - dash dot line)

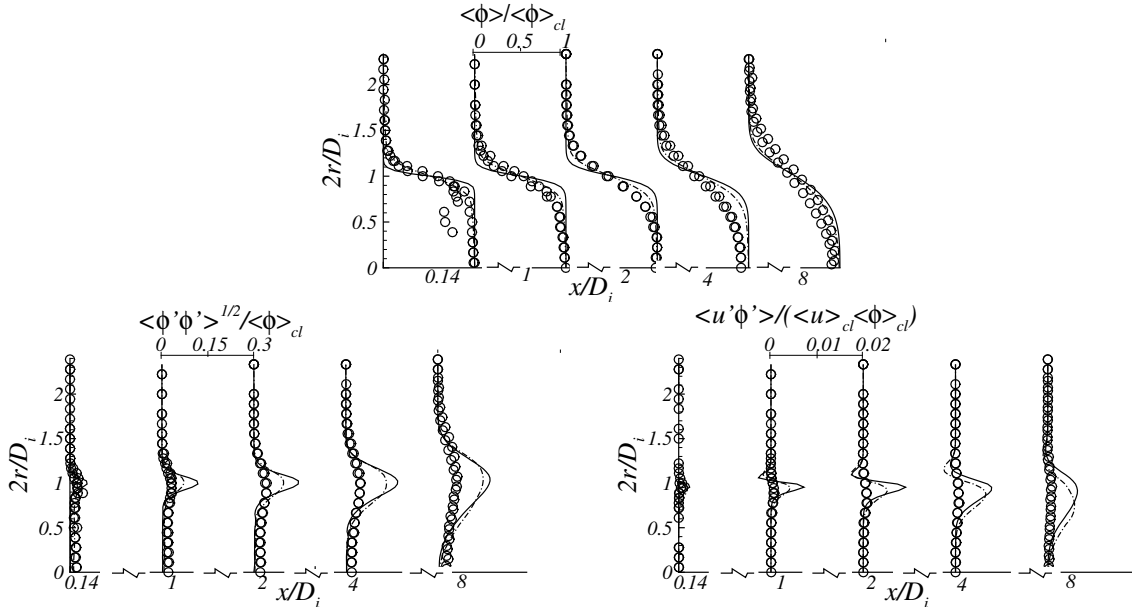


Figure 4.18: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: fully developed - solid line; rescaled - dash dot line)

For all Sc tested, including $Sc = \infty$, there was no observable impact on $\langle \phi \rangle$, and effects on $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ were very small.

In our model the Sc number affects only the molecular diffusivity terms that, away from walls, are small due to the high Re number. Similar results have been reported in Jahnke et al. (2004). To quantify this effect was one of the reasons for computing the passive scalar transport equation budgets (section 4.4).

4.3.3.3 The effect of the passive scalar subgrid-scale model

Here, the use of a dynamic SGS model for the passive scalar is compared to using a uniform Sc^{sgs}

- $Sc^{sgs} = 0.25$, runs 11 and 12,
- $Sc^{sgs} = 0.5$, runs 13 and 14,
- $Sc^{sgs} = \infty$, runs 15 and 16.

The dynamic model computes a spatially varying Sc^{sgs} number, figs. 4.19 and 4.20. A Sc^{sgs} close to 0.5 appeared in a large part of the domain, indicating that there was little impact on using a dynamic model as opposed to a constant Sc^{sgs} close to 0.5. A test was made setting $Sc^{sgs} = 0.5$ and results were very close to the ones obtained using the dynamic model, and are not shown.

The increase in Sc^{sgs} close to the shear layer in figs. 4.19 and 4.20 was similar to the limiting behaviour of Sc^{sgs} close to a wall in Keating (2004), where a higher Sc yields a higher Sc^{sgs} near the wall whereas away from the wall 0.5 is a typical value. The behaviour of Sc^{sgs} in our work was similar.

A numerical problem occurred in the shear layer region and, more rarely, near the walls. The tensor norm $\langle \mathcal{N}_j \mathcal{N}_j \rangle_{\mathcal{L}}$ became zero, yielding infinity values of C_ϕ . The problem was dealt with by imposing a lower bound on $\langle \mathcal{N}_j \mathcal{N}_j \rangle$ of 3×10^{-8} .

$$\frac{\partial(\rho\bar{\phi})}{\partial t} + \frac{\partial(\rho\bar{\phi}\bar{u}_j)}{\partial x_j} = -\frac{\partial}{\partial x_j} \left(\mu/Sc \frac{\partial\bar{\phi}}{\partial x_j} \right). \quad (4.3)$$

A test was made where no passive scalar model was used, leading to equation 4.3, a modification of eq. 3.13 with $Sc^{sgs} = \infty$. The results are shown on figures 4.22 ($r = 3.2$) and 4.24 ($r = 0.8$). The subgrid model had little ($r = 3.2$) or no ($r = 0.8$) effect on $\langle \phi \rangle$ and led to a minor improvement in $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for both conditions.

The use of artificially lower, increased turbulent diffusion, values of Sc^{sgs} was tested. For $r = 0.8$, figure 4.23 shows that decreasing the Sc^{sgs} number improves all statistics,

particularly $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$. This behaviour was identical, but more pronounced for $r = 3.2$ (figure 4.21). Lower Sc^{sgs} values were tested: for $Sc^{\text{sgs}} = 0.1$, $r = 0.8$ improved slightly, but NAN values appeared in the $r = 3.2$ calculation. Similar behaviour (NANs) occurred for $r = 0.8$ when $Sc^{\text{sgs}} = 0.01$ was used.

We conclude by highlighting the surprising behaviour found: the details of the eddy diffusivity subgrid-scale model had little impact on the results. The dynamic Sc^{sgs} was typically 0.5, with higher values in limited regions. In fact, use of a constant $Sc^{\text{sgs}} = 0.5$ was identical to use of the dynamic model. A general improvement on the results was observed when lower values of Sc were used.

The typical $Sc^{\text{sgs}} = 0.5$ found is also quoted in Keating (2004) away from the walls. Using scaling arguments, Flohr and Vassilicos (2000) quotes 0.6 as a theoretical value, but values between 0.1 and 1 are quoted in the literature (Sagaut, 2004). The subject is revisited later in the chapter, section 4.4.

4.3.3.4 Neglecting diffusive terms: $Sc = Sc^{\text{sgs}} = \infty$

$$\frac{\partial(\rho\bar{\phi})}{\partial t} + \frac{\partial(\rho\bar{\phi}\bar{u}_j)}{\partial x_j} = 0. \quad (4.4)$$

Here, not only the diffusivity is neglected but also no subgrid-scale model is used. Therefore, the passive scalar transport is modelled by a hyperbolic equation (eq. 4.4), with convective terms only. The profiles for $\langle \phi \rangle$ were identical (not shown), and $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ profiles varied slightly, as shown in figure 4.25 for $r = 0.8$ and in figure 4.26 for $r = 3.2$.

A hyperbolic equation ($Sc = Sc^{\text{sgs}} = \infty$) was enough to reproduce $\langle \phi \rangle$ and produced $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ similar to the ones obtained using a standard dynamic model. The conclusion was that $\langle \phi \rangle$ can be well reproduced with a hyperbolic equation, and so can the resolved parts of $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$.

4.3.4 The reference simulations

In accordance with the results of the numerical (section 4.3.2) and modelling tests (section 4.3.3) a good choice of parameters is TVD discretization, inlet rescaling, to fit measurements at $x/D_i = 0.14$, $Sc = 1000$, dynamic passive scalar SGS model and a 66^3 grid.

Figures 4.27 and 4.28 present the reference simulation for the $r = 3.2$ velocity ratio (run 4). The velocity statistics were well reproduced (figure 4.27); $\langle u \rangle$ showed almost perfect agreement, whereas $\langle u' u' \rangle^{1/2}$ was slightly over-predicted for $x/D_i \geq 4$. The fast mixing of $\langle \phi \rangle$ was not fully captured, and significant differences in magnitude for $x/D_i > 4$ can be seen in figure 4.28. The same figure showed a good reproduction of $\langle \phi' \phi' \rangle^{1/2}$ and of

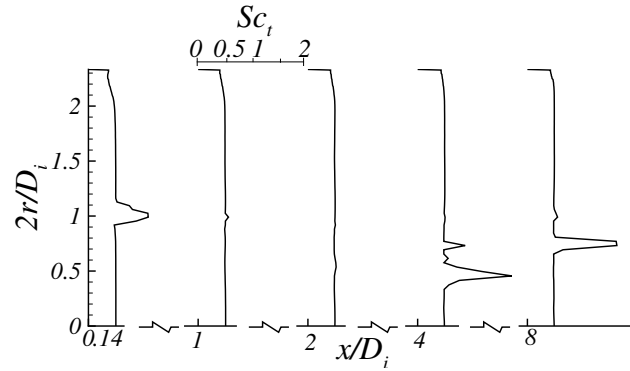


Figure 4.19: Sc^{sgs} spatial variation for $r = 3.2$ (run 4) at $x/D_i = 0.14, 1, 2, 4$ and 8

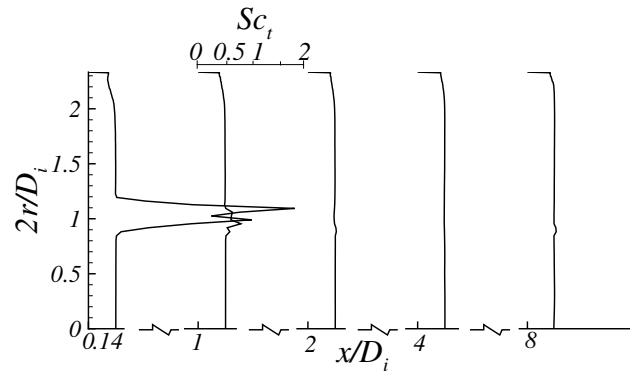


Figure 4.20: Sc^{sgs} spatial variation for $r = 0.8$ (run 3) at $x/D_i = 0.14, 1, 2, 4$ and 8

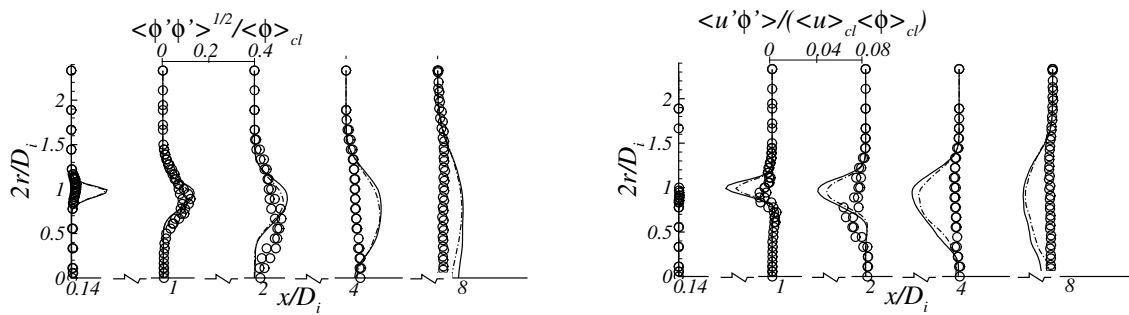


Figure 4.21: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: Sc^{sgs} dyn - solid line ; run 12: $Sc^{sgs} = 0.25$ - dash dot line)

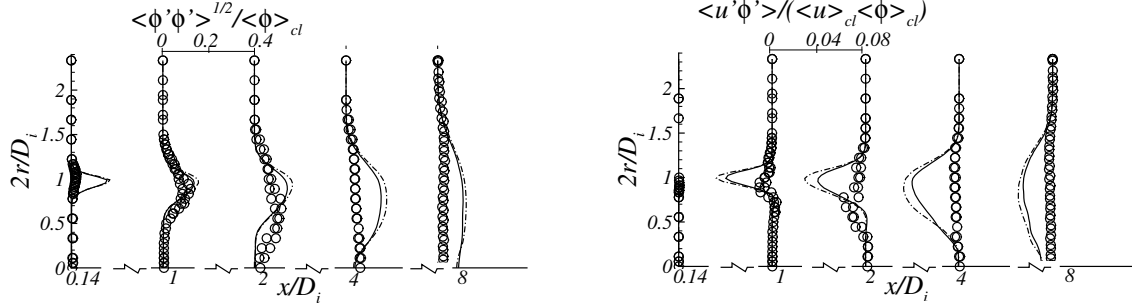


Figure 4.22: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: $Sc^{sgs} \text{ dyn}$ - solid line ; run 16: $Sc^{sgs} = \infty$ (*i.e.*, no model) - dash dot line)

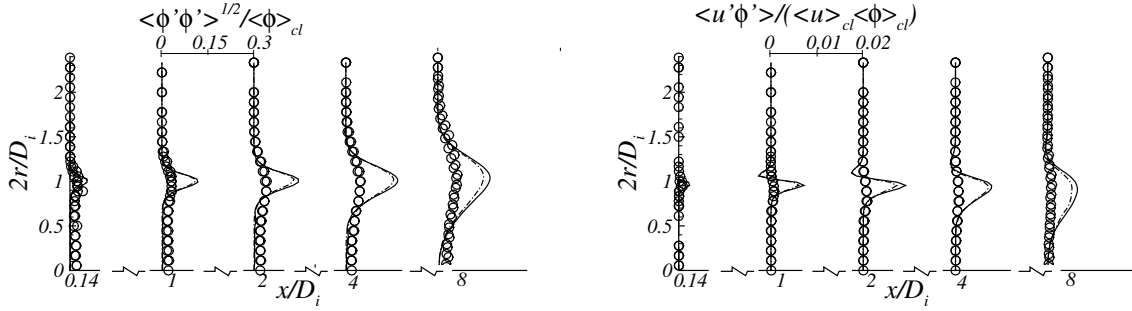


Figure 4.23: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: $Sc^{sgs} \text{ dyn}$ - solid line ; run 11: $Sc^{sgs} = 0.25$ - dash dot line)

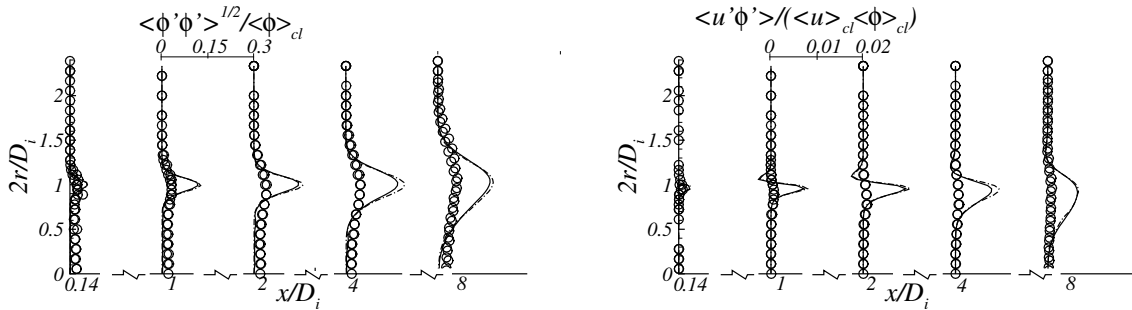


Figure 4.24: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: $Sc^{sgs} \text{ dyn}$ - solid line ; run 15: $Sc^{sgs} = \infty$ (*i.e.*, no model) - dash dot line)

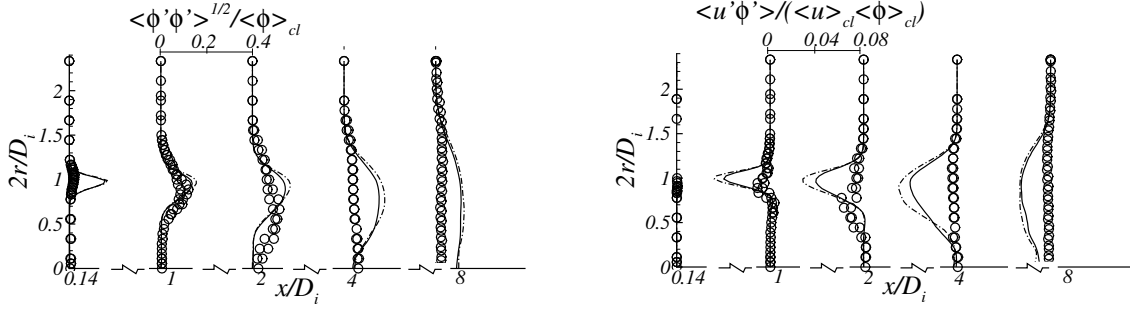


Figure 4.25: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 4: $Sc = 1000$, Sc^{sgs} dyn - solid line; run 20: $Sc = Sc^{sgs} = \infty$ - dash-dot line)

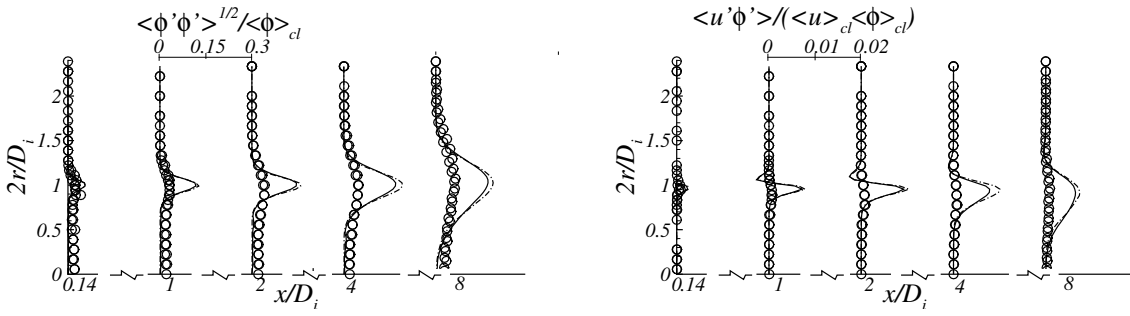


Figure 4.26: Passive scalar, turbulent values, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (run 3: $Sc = 1000$, Sc^{sgs} dyn - solid line; run 19: $Sc = Sc^{sgs} = \infty$ - dash-dot line)

$\langle u'\phi' \rangle$ for $x/D_i = 1$ and $x/D_i = 4$ and an over-prediction of around $2\times$ for $x/D_i = 4$ and $x/D_i = 8$. Although with a poor agreement with experimental results, the $\langle u'\phi' \rangle$ shape was captured with negative turbulent scalar flux in the shear layer region.

Figures 4.29 and 4.30 present the reference simulation for velocity ratio $r = 0.8$ (run 3). In figure 4.29 it can be seen that $\langle u \rangle$ was well reproduced up to $x/D_i = 8$. The agreement between LES results and experiment was almost perfect, apart from a small discrepancy at $x/D_i = 1$ and $x/D_i = 2$, still evidencing the shear layer. The fluctuation magnitude $\langle u'u' \rangle^{1/2}$ showed good agreement, with a small discrepancy close to the shear layer. The passive scalar mean $\langle \phi \rangle$ agreement was also good, with a slight difference for $x/D_i = 2$ and 4 (figure 4.30). In spite of the good agreement in $\langle \phi \rangle$, a very significant ($\approx 10\times$) over-prediction of $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ was observed, figure 4.30.

4.3.5 Conclusions

We start by summing up the behaviour of the reference simulations, runs 3 and 4. For both velocity ratios, velocity statistics, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, were well reproduced. This is a necessary condition for reproduction of the passive scalar statistics. The passive scalar mean was reproduced for $r = 0.8$, but not for $r = 3.2$ when $x/D_i \geq 4$. The passive scalar turbulent statistics $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ were not accurately reproduced. They were wrong for an order of magnitude for $r = 0.8$, whereas for $r = 3.2$ the order of magnitude was predicted close to the inlet, but not for $x/D_i > 4$. The reproduction of $\langle \phi \rangle$ was easier where there were less gradients *i.e.*, $r = 0.8$, whereas $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ magnitude was reproduced where large-scale dominated *i.e.*, $r = 3.2$.

Overestimation of $\langle u'u' \rangle^{1/2}$ in under-resolved LES has been reported on Lund et al. (1998) and further explored on Gullbrand and Chow (2003), but no satisfactory explanation of this behaviour has been found, according to Piomelli (private communication) (quoted in Keating, 2004).

The main result of the numerical test is that the use of inlet rescaling had a significant impact on the velocity statistics and on $\langle \phi \rangle$, but improvement on $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ was small.

Grid refinement, from 66^3 up to 128^3 improved the mean passive scalar $\langle \phi \rangle$ but fluctuation $\langle \phi'\phi' \rangle^{1/2}$ and turbulent scalar flux $\langle u'\phi' \rangle$ remained far from experimental measurements.

The main result of the modelling tests was the impact on statistics of the convective term discretization of the passive scalar transport equation. BLINT led to better $\langle \phi \rangle$ agreement (significant in $r = 3.2$), whereas TVD over-predicted $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ much less. Varying Sc and Sc^{sgs} , including use of a SGS dynamic model, had no impact on $\langle \phi \rangle$ and a modest effect on $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$. The details of the eddy diffusivity model had little impact. Use of constant $Sc^{sgs} = 0.5$, gave identical results to the dynamic model, that has a

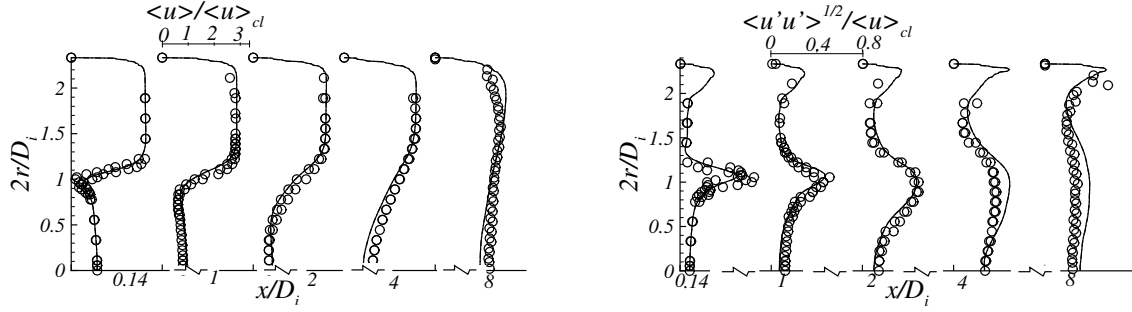


Figure 4.27: Streamwise velocity, mean and turbulent values, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$ for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (experiment - circles ; LES run 4 - solid line)

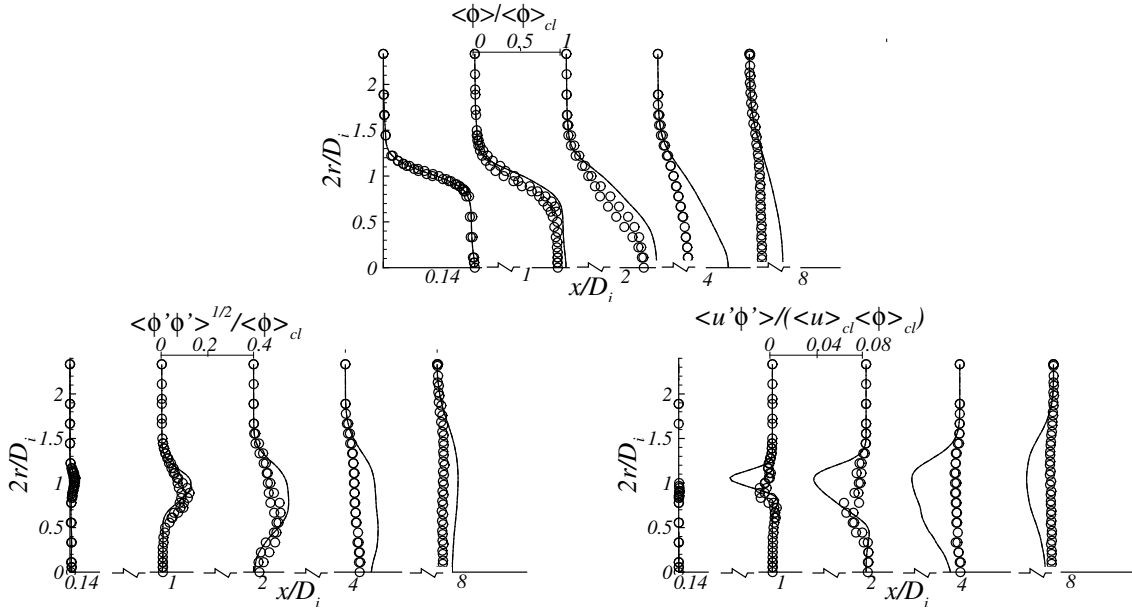


Figure 4.28: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ for velocity ratio $r = 3.2$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (experiment - circles ; LES run 4 - solid line)

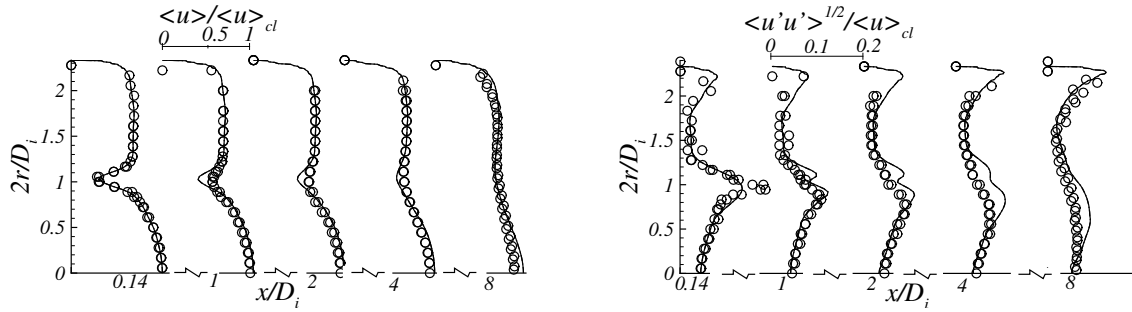


Figure 4.29: Streamwise velocity, mean and turbulent values, $\langle u \rangle$ and $\langle u'u' \rangle^{1/2}$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (experiment - circles ; LES run 3- solid line)

spatially variable Sc^{sgs} but on average led to $Sc^{\text{sgs}} = 0.5$ except in the mixing region. Ad-hoc adjustment of the Sc^{sgs} number to lower values improved the results, which may be a clue for the construction of SGS in high- Sc flow.

Suppressing the diffusive terms ($Sc = Sc^{\text{sgs}} = \infty$) had small impact on $\langle \phi \rangle$, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$. This was a surprising result, and prompted the research into the passive scalar transport equation budgets.

4.4 Momentum and passive scalar budgets

In this section, budgets for $\langle u \rangle$, $\langle u' u' \rangle^{1/2}$, $\langle \phi \rangle$, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ in confined coaxial jets are analysed, with the goal of improving the understanding of the numerical behaviour of the passive scalar transport equation, by finding out which terms, *i.e.*, parts of the numerical code, dominate the calculation. In particular, our goal was to improve understanding of why change in diffusive terms had such a small impact on results.

4.4.1 Budget plots and analysis

Budgets were computed as detailed in appendix A. Terms in the transport equations were grouped in accordance with the physical meaning of the terms that originate them: $\mathcal{C}$ originate in the convective terms, $\mathcal{D}$ in the molecular viscosity or diffusion, $\mathcal{D}^{\text{sgs}}$ in the eddy viscosity or diffusion and Π on the pressure gradient terms; $\mathcal{B}$ is the balance of the previous terms. The plots presented here are for the reference simulations, run 4, for $r = 3.2$, and run 3, for $r = 0.8$.

4.4.1.1 Reference simulations

In the $\langle u \rangle$ momentum budget, figure 4.31 convection and pressure gradient terms were the dominant ones. The molecular diffusion term was important close to the walls and inlet section, in the shear layer region. The subgrid-scale term was significant in all sections and in some parts of the shear layer became higher than the convection term. The balance was close to zero everywhere. Similar shapes were observed in the $\langle u' u' \rangle^{1/2}$ Reynolds-stress budget plots, figure 4.32.

In the $\langle \phi \rangle$ transport budget plots, figure 4.33, both the molecular diffusion term $\mathcal{D}_\phi$ and the budget sum $\mathcal{B}_\phi$ were close to zero; the transport equation was governed by the convection and subgrid scale terms. The sign change at the shear layer region is connected to the type of mixing: packets of mixed fluid reaching unmixed one for $2r/D_i > 1$ and packets of unmixed fluid reaching mixed one for $2r/D_i < 1$. When compared to the $\langle u \rangle$

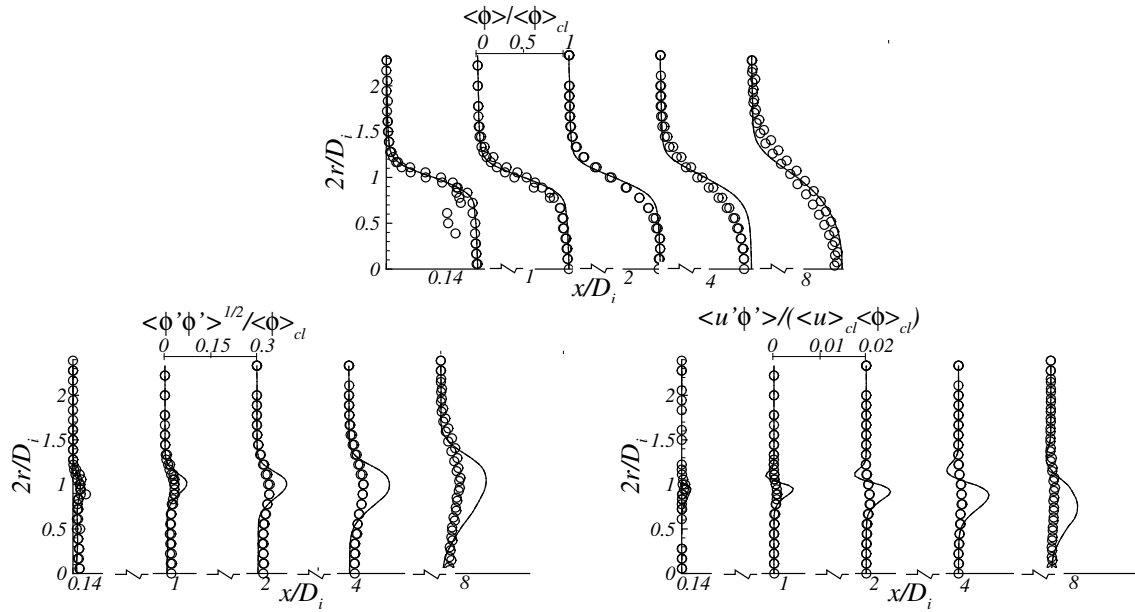


Figure 4.30: Passive scalar, mean and turbulent values, $\langle \phi \rangle$, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, for velocity ratio $r = 0.8$ at $x/D_i = 0.14, 1, 2, 4$ and 8 (experiment - circles ; LES run 3- solid line)

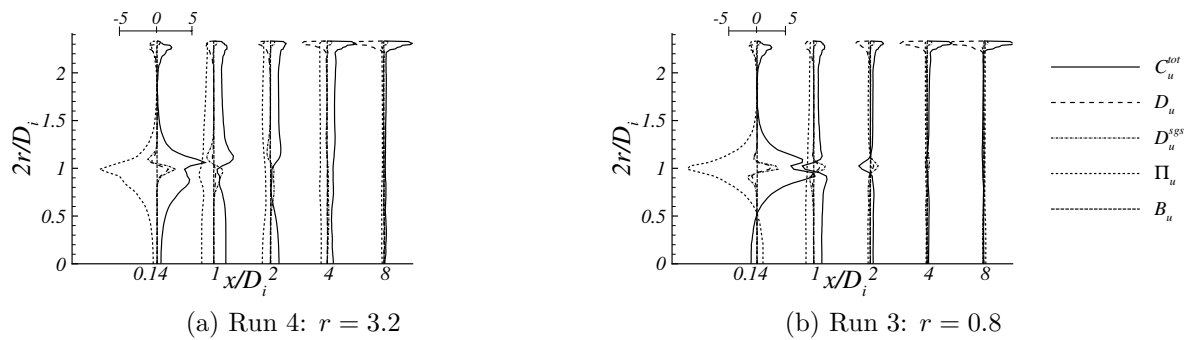
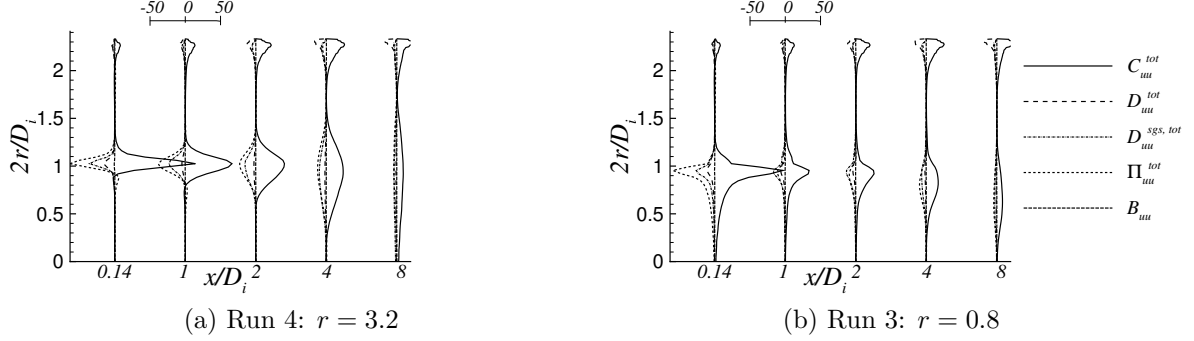
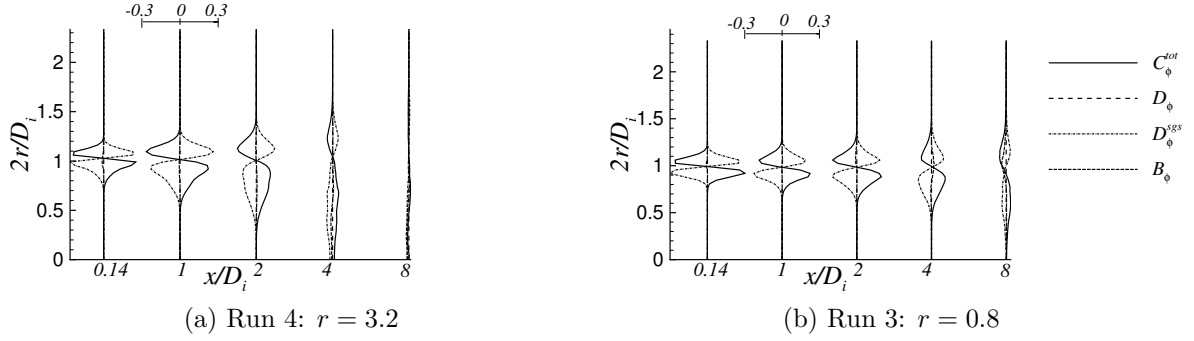


Figure 4.31: Momentum $\langle u \rangle$ budget at $x/D_i = 0.14, 1, 2, 4$ and 8

Figure 4.32: Reynolds stress $\langle u'u' \rangle^{1/2}$ budget at $x/D_i = 0.14, 1, 2, 4$ and 8 Figure 4.33: Passive scalar transport $\langle \phi \rangle$ budget at $x/D_i = 0.14, 1, 2, 4$ and 8

momentum budget, the absence of the pressure gradient term means that the behaviour of the SGS model was more crucial here than in the momentum equation.

The $\langle \phi' \phi' \rangle^{1/2}$ turbulent scalar flux budget, figure 4.34, is similar to the $\langle \phi \rangle$ one, with the caveat that the magnitude of the terms for $r = 0.8$ was lower than for $r = 3.2$. This is caused by increased mixing for $r = 3.2$. The $\langle u' \phi' \rangle$ turbulent scalar flux budget is presented in figure 4.35. Pressure gradient was important, particularly for $r = 3.2$. There were opposite signs for the convective and subgrid scale terms, which is explained by the different mixing mechanisms of each condition: large scale for $r = 3.2$ and small scale for $r = 0.8$.

4.4.1.2 No diffusion terms: $Sc = Sc^{sgs} = \infty$

In this test case, the diffusive terms are eliminated and there are only convective terms. The average value of the convective terms must be zero on average. This was confirmed in our tests (trivial plots of zero not shown).

This is in contrast with the budgets for the reference simulations, where the SGS model

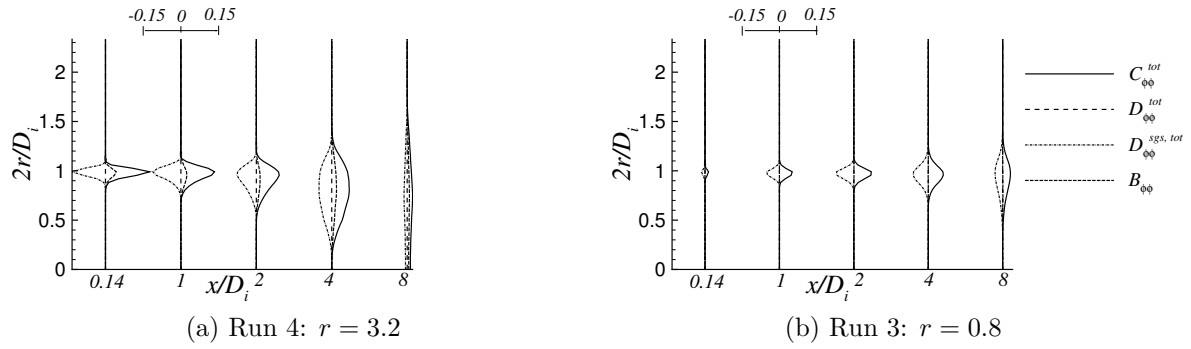


Figure 4.34: Scalar variance $\langle \phi' \phi' \rangle^{1/2}$ budget at $x/D_i = 0.14, 1, 2, 4$ and 8

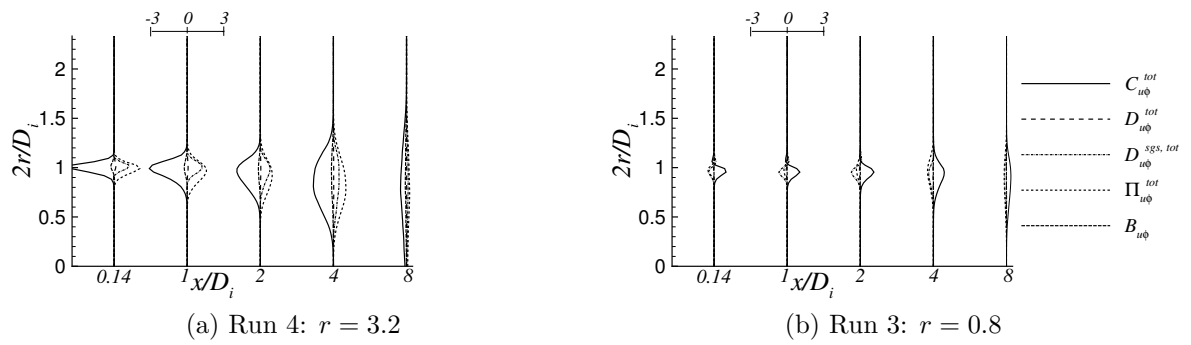


Figure 4.35: Turbulent scalar flux $\langle u' \phi' \rangle$ budget at $x/D_i = 0.14, 1, 2, 4$ and 8

balances the convection. The budgets were then significantly different, but nevertheless the $\langle\phi\rangle$ profiles remained identical, and only small changes appeared in the $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$ profiles. We propose this is connected with the diffusivity independence hypothesis, described in section 4.5.1.

4.4.2 Conclusions

Passive scalar transport, variance and turbulent scalar flux budget analysis of LES were used to analyse the results, focusing on the full numerical terms instead of on the decomposed ones. This is a novelty of the current work.

Convective terms were dominant for $\langle\phi\rangle$, $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$. In the $\langle u'\phi'\rangle$ budget, the pressure gradient also plays a major role. In all statistics, $\langle\phi\rangle$, $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$, molecular diffusivity played no role, as it was negligibly small, several orders of magnitude, when compared to SGS and convective terms. This explains why changes of the Sc number (to either 1 or ∞) had little impact on the results.

The relative weight of molecular and SGS terms can be seen as a resolution criteria. From that view point the coaxial jet simulation was under-resolved, both in velocity (where terms were of the same order of magnitude) and on the passive scalar (where the molecular part was negligibly small, due to the high Sc number).

The budgets for $r = 0.8$ and $r = 3.2$ were remarkably similar for $\langle\phi\rangle$ and $\langle\phi'\phi'\rangle^{1/2}$. Only for $\langle u'\phi'\rangle$ were significant differences observed.

When $Sc^{sgs} \approx 0.5$, as happened also when dynamic SGS is used, the turbulent diffusivity seems to be crucial in the $\langle\phi\rangle$ and $\langle\phi'\phi'\rangle^{1/2}$ budgets, as it is the term that balances the convection but is absent in the test with $Sc^{sgs} = \infty$. It seems that the subgrid scale diffusion term has no dynamical effect on $\langle\phi\rangle$.

4.5 A unified view of the results

In this section we review the results previously presented in light of a possible connection to an hypothesis not frequently mentioned in the LES context, the Taylor diffusivity independence hypothesis and the related notion of a passive scalar dominated by the velocity field.

4.5.1 The Taylor diffusivity independence hypothesis

In an effort to understand the lack of response of the simulations to changes concerning the passive scalar transport equation, we found the following idea in the literature (Pope,

1998):

For high $Pe = Re \times Sc$ flows, $\langle \phi \rangle$ is determined by the velocity field, *i.e.*, it is independent of diffusivity.

This is an interpretation of Taylor (1921) hypothesis made by Pope (1998) and can be called the diffusivity independence hypothesis. Since $\alpha = \mu/Sc$, independent of diffusivity is identical to independent of Sc . This is defended by Pope (1998) for $\langle \phi \rangle$ only and not to the probability density function of ϕ or even to second order moments like $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$. Diffusivity cannot be neglected (Pope (1998)) on $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$, which depend strongly on numerical and modelling details (*cf.* Flohr and Vassilicos (2000)).

The hypothesis is firmly established in the context of turbulent dispersion and Lagrangian methods. The consequences for LES, that is defined in Eulerian terms, particularly in LES based on eddy diffusivity models are not addressed, to the best of the author knowledge, in current published literature. Particularly, the impact on of eddy-diffusivity models, whose only effect is an increase in diffusivity, and seem to be rendered incapable to perform their task: to compensate for the subgrid scale mixing processes that are not resolved in the grid.

With this idea in mind, some other results were found that seem to support it. For high Re (and $Pe = Re \times Sc$) and away from walls, μ^{sgs} and α^{sgs} scale with velocity and length, and are independent of μ and α . Thus μ^{sgs}/μ and α^{sgs}/α increase linearly with Re (and Pe) and molecular transport becomes negligible (Pope, 2000, , pg. 95); in the centreline of a self-similar jet, $\langle \phi' \phi' \rangle^{1/2}/\langle \phi \rangle \approx 0.05$ (Pope, 2000, pg. 165, figure 5.38). This supports the hypothesis that, at high Re , the means and variances of velocities and scalar are unaffected by Re and Sc ; a recent thermal plane channel simulation, Bergant and Tiselj (2007), where a DNS is made in the velocity field, and a LES in the passive scalar claims that there is no need to resolve the scales between the Kolmogorov and Batchelor scales to reproduce the $\langle \phi \rangle$ profile, *i.e.*, even though Sc is high, there is no need to use a finer resolution than that used in the velocity. This result is an indication that diffusivity independence holds even close to the wall.

4.5.2 Relation to the current test results

In our simulations, as in others recently reported (Jahnke et al., 2005), Sc had very little effect on $\langle \phi \rangle$. If the mean field of $\langle \phi \rangle$ is determined by the velocity field, then $\langle \phi \rangle$ is dependent on accurate reproduction of the velocity field and the subgrid- scale model becomes of secondary importance.

Another way of looking at the diffusivity independence is to say that an accurate velocity field is not only a necessary but also a sufficient condition for reproduction of $\langle \phi \rangle$. This was in accordance with results in our tests: the tests that had impact on $\langle \phi \rangle$ were either

the ones that impacted on the velocity field, grid refinement or rescaling, or the ones that impacted on the way in which the velocity field entered the transport equation, *i.e.*, the convective term discretization tests.

In connection with this results, we propose that, at least away from walls, the scalar transport equation without diffusivity terms (a hyperbolic equation) is enough to compute $\langle \phi \rangle$.

$\langle u' \phi' \rangle$ appears in the mean scalar $\langle \phi \rangle$ transport equation (Pope, 2000, pg. 91–95) but in our geometry had no dynamical effect on $\langle \phi \rangle$, since simulating with a hyperbolic equation led to negligible change in $\langle \phi \rangle$.

There are reproductions of $\langle u \rangle$, $\langle u' u' \rangle^{1/2}$ and $\langle \phi \rangle$ in published literature and in the present work also good agreement was shown for these quantities. High Sc did not prevent $\langle \phi \rangle$ reproduction, which lends credit to the diffusivity independence hypothesis and explains why LES of $\langle \phi \rangle$ have been frequently reported (*e.g.*, Akselvoll and Moin (1996)) but $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ are much more difficult to obtain and have been published for geometrically and physically simple flows only. In our work, $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ remained similar when Sc and Sc^{sgs} were set to zero, indicating that their resolved part was reproduced by the hyperbolic equation. However, the unresolved part had a significant weight that explains the lack of matching with experimental measurements for $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$.

Diffusivity, or Sc , is relevant close to walls, where Pe is always low, as confirmed by the molecular diffusion term distribution in plane channel budgets, but the dynamical effect on $\langle \phi \rangle$ remains small, as indicated by Bergant and Tiselj (2007) conclusions (see section 4.5.1). In addition, particularly for $r = 3.2$, the strong mixing means that for $x/D_i = 0.14$, where our rescaled simulations start, molecular diffusion terms are already negligible. So, even with walls close to the region of interest, diffusivity independence appears to apply.

4.5.3 A note on passive scalar sgs models

For high Sc the SGS model becomes in effect irrelevant for the simulation of $\langle \phi \rangle$, as long as it does not contaminate it. However, since diffusivity is important for turbulent statistics, the SGS model is crucial if reproduction of $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ is intended and needs to be of a new kind. In the current work, the diffusive terms had impact only when they were arbitrarily increased, by use of a small Sc^{sgs} . This indicates that the computed Sc^{sgs} is too high, leading to an eddy-diffusivity that is too small.

A SGS model tailored for high- Sc number is likely to be needed, since two regions appear in the spectra of a passive scalar in high- Sc flow, the inertial convective range and the viscous convective range. Since a single grid is used, the cut-off is inevitably in the inertial convective range, therefore the whole viscous convective range must be modelled. The use of such a model was considered, but a review of the state of the art on high- Sc subgrid-scale model has found no adequate model, *e.g.*, the Sagaut (2004) textbook does

not mention any such model. It is an immature subject and even if an apparently adequate model was found, model reliability might be questionable. Diffusivity independence implies that SGS models cannot be validated by comparison with experiments $\langle\phi\rangle$, but they can be made to impact on $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$. For that to happen, it seems the SGS needs to produce a lower Sc^{sgs} , *i.e.*, a higher diffusivity. This is confirmed not only by the tests with $Sc^{sgs}=0.1$ but also by the better behaviour, in terms of $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$, of the convective discretizations with higher upwind scheme weight. The connection can be established, since use of the upwind scheme can be looked at as a numerical diffusion. Those tests had no impact on $\langle\phi\rangle$, indicating that the diffusivity independence hypothesis remains valid, in our geometry, even when diffusive terms are arbitrarily increased by a factor of $10\times$ or when a pure upwind scheme is used.

4.6 Conclusions

The LES code can predict $\langle\phi\rangle$ but not in general $\langle\phi'\phi'\rangle^{1/2}$ and $\langle u'\phi'\rangle$. This fact remained constant with the various numerical and modelling tests performed. This looks surprising at first, but in fact matches an hypothesis well known within Lagrangian methods of passive scalar dispersion, the diffusivity independence hypothesis.

Since in eddy-diffusivity type model the effect of the SGS model is to add diffusivity, it can be understood, in the context of the diffusivity independence hypothesis, that there is small impact of the SGS model on $\langle\phi\rangle$. Indeed, increase of the diffusivity by a factor of 10 still had no impact on $\langle\phi\rangle$.

If both molecular and SGS diffusion become irrelevant, convective terms are paramount. In fact, we propose that for high Pe diffusivity independent flows $\langle\phi\rangle$ can be found using a hyperbolic (no diffusion terms: $Sc = Sc^{sgs} = \infty$) transport equation. If this is correct, eddy diffusivity subgrid scale models are useless in high- Sc flow.

We present two schemes for the convection term: one that locally respects the boundedness rule (a second order TVD scheme, called TVD) and another that respects boundedness only in a global sense (the BLINT scheme) but reverts to upwind much less often. TVD is chosen as the preferred method, since it reaches better overall agreement with the experiments and retains a reasonable order of accuracy.

Chapter 5

Conclusions and Future Work

5.1 Conclusions

The post-processing of experiments confirmed, independently and with different tools, the results and analysis of Lima (2000) analysis, as it reached similar results. The way to store the experiments was investigated with ASCII text files chosen. A review of the Sc number concluded that it was between 500 and 2500, with 1000 the recommended value for numerical simulation.

The quality and uncertainty of the experimental measurements was evaluated with a variety of methods: propagation of uncertainty, bootstrap methods, mass flux uncertainty, variation of mass flux computed from the radial profiles and analysis of the effect of noise on the passive scalar measurements. We found that $r = 0.8$ had lower uncertainty on $\langle u \rangle$ and $\langle \phi \rangle$, whereas passive scalar turbulent quantities have smaller uncertainty for $r = 3.2$. The condition with $r = 3.2$ was a good compromise between uncertainty on the mean values and on turbulent passive scalar quantities and is a case with added physical and engineering interest, due to the high velocity ratio. The PDF evolution was non-marching for $r = 3.2$, indicating mixing by large-scale structures, and marching for $r = 0.8$, *i.e.*, mixing by small-scale structures. Accordingly, $r = 0.8$ and $r = 3.2$ were selected for simulation using LES.

The numerical tests in the LES simulations concluded that inlet rescaling had direct impact on the velocity profiles agreement, but was less noticeable on the passive scalar ones. Grid refinement improved the mean passive scalar for $r = 3.2$ but had little impact on velocity statistics and on the fluctuation and turbulent scalar flux. The modelling tests, focusing on the passive scalar transport solver, showed that the Sc number and subgrid-scalar Sc^{sgs} had no impact on $\langle \phi \rangle$ and only a small effect on $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$.

Analysis of the transport equation budgets showed that molecular diffusivity terms had

a negligible weight on all passive scalar statistics. The terms originating from the eddy-diffusivity were balanced by the convection terms. However, when the eddy-diffusivity was set to zero ($Sc = Sc^{\text{sgs}} = \infty$, *i.e.*, no diffusive terms) the convection terms weight became of the order of the balance error, but no effect on $\langle \phi \rangle$ was observed and $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ remained similar. The parameter that most affected the passive scalar profiles was the convection term discretization scheme. Agreement with $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$ was much better with the TVD scheme than with the bounded scheme.

For velocity ratios $r = 0.8$ and $r = 3.2$, $\langle u \rangle$ and $\langle u' u' \rangle^{1/2}$ were well reproduced. With the best available modelling and numerical choices, agreement was reached for $\langle \phi \rangle$ but not for $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$. We propose that this behaviour is connected with the diffusivity independence hypothesis, known from passive scalar studies using Lagrangian methods: behaviour of $\langle \phi \rangle$ was independent of the diffusive terms (including eddy-diffusivity) so we propose that, in LES of passive scalar, an hyperbolic equation can be used to obtain the passive scalar mean, $\langle \phi \rangle$.

5.2 Future work

The work was done taking into account time and computational resources available. In this section, the question of how to proceed is analysed. Of the many possibilities of proceeding the work, the following seem most promising:

- Improve the LES simulations. The most promising would be to use cylindrical grids, in order to have a finer control of the resolution in the shear layer region.
- Further explore the diffusivity independence hypothesis in LES and the requirements in terms of resolution and subgrid-scale model to improve the reproduction of $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$.
- The experimental measurements of Lima (2000), appropriate for numerical validation, can still be improved upon. Both jets could be as close as possible to fully developed flows and both jets could have a concentration above zero, to avoid high relative uncertainties. To avoid residual fluctuation, more effective ways of mixing the scalar could be sought. Finally, during the measurements, detection of outliers and bootstrap uncertainty should be computed, and larger timeseries used until outliers are either rejected or included and statistical uncertainty is small. The reduction of noise on the passive scalar measurement would reduce the uncertainty of $\langle \phi' \phi' \rangle^{1/2}$ and $\langle u' \phi' \rangle$.

Appendix A

Equations for Budget Analysis

To account for the behaviour of the numerical algorithm, the average weight of each term in the transport equation of $\langle u \rangle$, $\langle \phi \rangle$, $\langle u'u' \rangle^{1/2}$, $\langle \phi'\phi' \rangle^{1/2}$ and $\langle u'\phi' \rangle$ was evaluated. The equations used are presented herer; they were derived using an approach designed to ensure coherence between the solver and the budget equations.

A.1 Momentum budgets

The momentum transport equation for large-eddy simulation, repeated here,

$$\frac{\partial u_i}{\partial t} = -\frac{\partial(u_i u_k)}{\partial x_k} + \nu \frac{\partial^2 u_i}{\partial x_k \partial x_k} - \frac{\partial \tau_{ik}}{\partial x_k} - \frac{\partial P}{\partial x_k}, \quad (\text{A.1})$$

can be written as an equation for u_i ,

$$\frac{\partial u_i}{\partial t} = \mathcal{C}_i^{tot} + \mathcal{D}_i + \mathcal{D}_i^{sgs} + \Pi_i = \mathcal{B}_i. \quad (\text{A.2})$$

Applying spatial or ensemble averaging, an equation for $\langle u_i \rangle$ is obtained, and can be interpreted as a momentum budget equation,

$$\frac{\partial \langle u_i \rangle}{\partial t} = \langle \mathcal{C}_i^{tot} \rangle + \langle \mathcal{D}_i \rangle + \langle \mathcal{D}_i^{sgs} \rangle + \langle \Pi_i \rangle \quad (\text{A.3})$$

$\langle \mathcal{C}_i^{tot} \rangle = \left\langle -\frac{\partial(u_i u_k)}{\partial x_k} \right\rangle$	Total convection
$\langle \mathcal{D}_i \rangle = \left\langle \nu \frac{\partial^2 u_i}{\partial x_k \partial x_k} \right\rangle$	Molecular diffusion
$\langle \mathcal{D}_i^{sgs} \rangle = \left\langle -\frac{\partial \tau_{ik}}{\partial x_k} \right\rangle$	Subgrid scale diffusion
$\langle \Pi_i \rangle = \left\langle -\frac{\partial P}{\partial x_k} \right\rangle$	Pressure gradient
$\langle \mathcal{B}_i \rangle = \langle \mathcal{C}_i^{tot} \rangle + \langle \mathcal{D}_i \rangle + \langle \mathcal{D}_i^{sgs} \rangle + \langle \Pi_i \rangle$	(Out-of) Balance

The total convection term $\langle \mathcal{C}_i^{tot} \rangle$ includes the resolved Reynolds stresses (that would be modelled in a RANS type code):

$$\langle \mathcal{D}_{rs,i} \rangle = \frac{\partial \langle u'_i u'_k \rangle}{\partial x_k} \quad \text{Reynolds stress diffusion}$$

This is usually referred to as “convection term” and can be decomposed:

$$\langle \mathcal{C}_i \rangle = \langle \mathcal{C}_i^{tot} \rangle - \langle \mathcal{D}_{rs,i} \rangle \quad \text{Convection}$$

A.2 Reynolds-stress budgets

The Reynolds-stress budget equations can be derived following the algorithm:

- Take the difference between equations (A.1) and (A.3), to get a transport equation for u'_i .
- Replace i with j in the above equation to get a transport equation for u'_j
- Taking into account that $\frac{\partial(u'_i u'_j)}{\partial t} = u'_i \frac{\partial u'_j}{\partial t} + u'_j \frac{\partial u'_i}{\partial t}$ multiply the transport equation for u'_i with u'_j , the transport equation for u'_j with u'_i and sum the resulting equations.
- Apply an average and simplify (eliminate terms that are zero on average)
- A transport equation for $u'_i u'_j$ is now available and the budget can be computed.

We applied the algorithm keeping the terms from equations (A.1) and (A.3) in order to ensure coherence between the budget calculation and the solution of the Navier-Stokes equations, leading to:

$$\mathcal{C}_{ij}^{tot} = \langle \mathcal{C}_i^{tot} u_j \rangle + \langle \mathcal{C}_j^{tot} u_i \rangle - \langle \mathcal{C}_i^{tot} \rangle \langle u_j \rangle - \langle \mathcal{C}_j^{tot} \rangle \langle u_i \rangle \quad (\text{A.4})$$

$$\mathcal{D}_{ij}^{tot} = \langle \mathcal{D}_i u_j \rangle + \langle \mathcal{D}_j u_i \rangle - \langle \mathcal{D}_i \rangle \langle u_j \rangle - \langle \mathcal{D}_j \rangle \langle u_i \rangle \quad (\text{A.5})$$

$$\mathcal{D}_{ij}^{sgs,tot} = \langle \mathcal{D}_i^{sgs} u_j \rangle + \langle \mathcal{D}_j^{sgs} u_i \rangle - \langle \mathcal{D}_i^{sgs} \rangle \langle u_j \rangle - \langle \mathcal{D}_j^{sgs} \rangle \langle u_i \rangle \quad (\text{A.6})$$

$$\Pi_{ij}^{tot} = \langle \Pi_i u_j \rangle + \langle \Pi_j u_i \rangle - \langle \Pi_i \rangle \langle u_j \rangle - \langle \Pi_j \rangle \langle u_i \rangle \quad (\text{A.7})$$

And the budgets were then computed:

$$\frac{\partial \langle u'_i u'_j \rangle}{\partial t} = \mathcal{C}_{ij}^{tot} + \mathcal{D}_{ij}^{tot} + \mathcal{D}_{ij}^{sgs,tot} + \Pi_{ij}^{tot} = \mathcal{B}_{ij} \quad (\text{A.8})$$

$\mathcal{C}_{ij}^{tot}$	Reynolds-stress (RS) total convection
$\mathcal{D}_{ij}^{tot}$	RS total molecular (viscous) diffusion
$\mathcal{D}_{ij}^{sgs,tot}$	RS total subgrid-scale diffusion
Π_{ij}	RS total Velocity-Pressure gradient tensor
$\mathcal{B}_{ij}$	RS Balance

The coherence obtained by direct computation of the product derivation terms, using the terms from the transport equation is very important if one intends to prevent numerical errors from obfuscating the budget analysis. Numerical error is not much increased, since only a small number of products and sums of already available variables is made.

In this approach, the budget terms are organised according to their numerical origin: $\mathcal{C}_{ij}^{tot}$ originates from the convection term, $\mathcal{D}_{ij}^{tot}$, originates from the molecular diffusion, $\mathcal{D}_{ij}^{sgs,tot}$ originates from the subgrid-scale term and Π_{ij}^{tot} originates from the pressure gradient term.

Because the physical significance of these terms is obscure, being just the result of the derivation of the transport equation for the Reynolds-stresses, the terms are usually

rearranged in a more physically meaningful fashion (this rearrangement varies between studies, particularly in what respects the subgrid-scale terms):

$$\epsilon_{ij} = -2\nu \left\langle \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k} \right\rangle \quad (\text{A.9})$$

$$\mathcal{D}_{ij} = \mathcal{D}_{ij}^{tot} - \epsilon_{ij} = \nu \frac{\partial^2 \langle u'_i u'_j \rangle}{\partial x_k^2} \quad (\text{A.10})$$

$$\Pi_{ij}^{tot} = \mathcal{R}_{ij} + \Pi_{ij} \quad (\text{A.11})$$

$$\mathcal{R}_{ij} = \frac{1}{\rho} \left\langle p' \frac{\partial u'_j}{\partial x_i} + p' \frac{\partial u'_i}{\partial x_j} \right\rangle \quad (\text{A.12})$$

$$\Pi_{ij} = \frac{1}{\rho} \left\langle u'_j \frac{\partial p'}{\partial x_i} + u'_i \frac{\partial p'}{\partial x_j} \right\rangle \quad (\text{A.13})$$

$$\epsilon_{ij}^{sgs} = \left\langle \tau_{ik} \frac{\partial u'_j}{\partial x_k} + \tau_{jk} \frac{\partial u'_i}{\partial x_k} \right\rangle \quad (\text{A.14})$$

$$\mathcal{T}_{ij}^{sgs} = \mathcal{D}_{ij}^{tot,sgs} - \epsilon_{ij}^{sgs} = - \frac{\partial \langle \tau_{jk} u'_i + \tau_{ik} u'_j \rangle}{\partial x_k} \quad (\text{A.15})$$

$$\mathcal{T}_{ij} = - \frac{\partial \langle u'_i u'_j u'_k \rangle}{\partial x_k} \quad (\text{A.16})$$

$$\mathcal{P}_{ij} = - \left\langle u'_j u'_k \frac{\partial \langle u_i \rangle}{\partial x_k} + u'_i u'_k \frac{\partial \langle u_j \rangle}{\partial x_k} \right\rangle \quad (\text{A.17})$$

$$\mathcal{C}_{ij} = \mathcal{C}_{ij}^{tot} - \mathcal{P}_{ij} - \mathcal{T}_{ij} = - \langle u_k \rangle \frac{\partial \langle u'_i u'_j \rangle}{\partial x_k} \quad (\text{A.18})$$

The budget can be interpreted, with added physical meaning:

$$\frac{\partial \langle u'_i u'_j \rangle}{\partial t} = \mathcal{C}_{ij} + \mathcal{P}_{ij} + \mathcal{T}_{ij} + \mathcal{D}_{ij} + \epsilon_{ij} + \mathcal{T}_{ij}^{sgs} + \epsilon_{ij}^{sgs} + \mathcal{R}_{ij} + \Pi_{ij} \quad (\text{A.19})$$

ϵ_{ij}	Reynolds-stress (RS) viscous dissipation
ϵ_{ij}^{sgs}	RS subgrid dissipation
$\mathcal{R}_{ij}$	RS Pressure-rate of strain tensor
Π_{ij}	RS Velocity-Pressure gradient tensor
$\mathcal{D}_{ij}$	RS Molecular (viscous) diffusion
$\mathcal{T}_{ij}$	RS Turbulent diffusion (convection by the fluctuations)
$\mathcal{T}_{ij}^{sgs}$	RS Subgrid diffusion
$\mathcal{P}_{ij}$	RS production
$\mathcal{C}_{ij}$	RS convection
$\mathcal{B}_{ij}$	Balance

It is worth noting, however, that the increased physical meaning comes at the cost of increased numerical error (*i.e.*, the third order moments are harder to compute than the derivatives) and of decreased numerical meaning, *i.e.* the numerical origin of the terms is obscured. The smaller number of terms in (A.8) also simplifies the analysis, which can become cumbersome in complex geometries.

Since our work had a numerical emphasis, we chose to analyse the total numerical terms (the first set of equations) using the decomposition only on the validation of plane channel results. To the best of the author's knowledge, focus on the total numerical terms instead of the physical decomposed ones has not been done before.

A.3 Passive scalar transport budgets

The budgets are derived in the same fashion, and the equations are presented without further comments.

$$\frac{\partial \phi}{\partial t} = \mathcal{C}_{\phi}^{tot} + \mathcal{D}_{\phi} + \mathcal{D}_{\phi}^{sgs} + \mathcal{S}_{\phi} \quad (\text{A.20})$$

$$\frac{\partial \langle \phi \rangle}{\partial t} = \langle \mathcal{C}_{\phi}^{tot} \rangle + \langle \mathcal{D}_{\phi} \rangle + \langle \mathcal{D}_{\phi}^{sgs} \rangle + \langle \mathcal{S}_{\phi} \rangle = \langle \mathcal{B}_{\phi} \rangle \quad (\text{A.21})$$

$$\begin{aligned}
\langle \mathcal{C}_\phi^{tot} \rangle &= \left\langle -\frac{\partial(\phi u_k)}{\partial x_k} \right\rangle && \text{"Total" Convection} \\
\langle \mathcal{D}_\phi \rangle &= \left\langle \alpha \frac{\partial^2 \phi}{\partial x_k \partial x_k} \right\rangle && \text{Molecular diffusion} \\
\langle \mathcal{D}_\phi^{sgs} \rangle &= \left\langle -\frac{\partial q_k}{\partial x_k} \right\rangle, \quad q_k = -\alpha^{sgs} \frac{\partial \phi}{\partial x_k} && \text{Subgrid scale diffusion} \\
\langle \mathcal{S}_\phi \rangle &&& \text{Source term} \\
\langle \mathcal{D}_{tsf} \rangle &= \frac{\partial \langle \phi' u'_k \rangle}{\partial x_k} && \text{Turbulent scalar flux diffusion} \\
\langle \mathcal{C}_\phi \rangle &= \langle \mathcal{C}_\phi^{tot} \rangle - \langle \mathcal{D}_{tsf} \rangle && \text{Convection} \\
\langle \mathcal{B}_\phi \rangle &= \langle \mathcal{C}_\phi^{tot} \rangle + \langle \mathcal{D}_\phi \rangle + \langle \mathcal{D}_\phi^{sgs} \rangle + \langle \mathcal{S}_\phi \rangle && \text{Balance}
\end{aligned}$$

A.4 Turbulent scalar flux budgets

$$\frac{\partial \langle u'_i \phi' \rangle}{\partial t} = \mathcal{C}_{i\phi}^{tot} + \mathcal{D}_{i\phi}^{tot} + \mathcal{D}_{i\phi}^{sgs,tot} + \Pi_{i\phi}^{tot} + \mathcal{S}_{i\phi}^{tot} = \mathcal{B}_{i\phi} \quad (\text{A.22})$$

$$\mathcal{C}_{i\phi}^{tot} = \langle C_{m,i}^{tot} \phi \rangle + \langle C_\phi^{tot} u_i \rangle - \langle C_{m,i}^{tot} \rangle \langle \phi \rangle - \langle C_\phi^{tot} \rangle \langle u_i \rangle \quad (\text{A.23})$$

$$\mathcal{D}_{i\phi}^{tot} = \langle D_{m,i} \phi \rangle + \langle D_\phi u_i \rangle - \langle D_{m,i} \rangle \langle \phi \rangle - \langle D_\phi \rangle \langle u_i \rangle \quad (\text{A.24})$$

$$\mathcal{D}_{i\phi}^{sgs,tot} = \langle D_{m,i}^{sgs} \phi \rangle + \langle D_\phi^{sgs} u_i \rangle - \langle D_{m,i}^{sgs} \rangle \langle \phi \rangle - \langle D_\phi^{sgs} \rangle \langle u_i \rangle \quad (\text{A.25})$$

$$\Pi_{i\phi}^{tot} = \langle P_{m,i} \phi \rangle - \langle P_{m,i} \rangle \langle \phi \rangle \quad (\text{A.26})$$

$$\mathcal{S}_{i\phi}^{tot} = \langle \mathcal{S}_\phi u_i \rangle - \langle \mathcal{S}_\phi \rangle \langle u_i \rangle \quad (\text{A.27})$$

$\mathcal{C}_{i\phi}^{tot}$	TSF convection
$\mathcal{D}_{i\phi}^{tot}$	TSF total molecular (viscous) diffusion
$\mathcal{D}_{i\phi}^{sgs,tot}$	TSF total subgrid-scale diffusion
$\Pi_{i\phi}^{tot}$	TSF total scalar-Pressure gradient tensor
$\mathcal{S}_{i\phi}$	TSF from source term
$\mathcal{B}_{i\phi}$	TSF Balance

$$\epsilon_{i\phi} = -(\nu + \alpha) \left\langle \frac{\partial \phi'}{\partial x_k} \frac{\partial u'_i}{\partial x_k} \right\rangle \quad (\text{A.28})$$

$$\mathcal{D}_{i\phi} = \mathcal{D}_{i\phi}^{tot} - \epsilon_{i\phi} = \frac{\partial}{\partial x_k} \left[\left\langle \nu \phi' \frac{\partial u'_i}{\partial x_k} \right\rangle + \left\langle \alpha u'_i \frac{\partial \phi'}{\partial x_k} \right\rangle \right] \quad (\text{A.29})$$

$$\Pi_{i\phi}^{tot} = \Pi_{i\phi} = -\left\langle \phi' \frac{\partial p'}{\partial x_i} \right\rangle \quad (\text{A.30})$$

$$\epsilon_{i\phi}^{sgs} = \left\langle \tau_{ik} \frac{\partial \phi'}{\partial x_k} + q_k \frac{\partial u'_i}{\partial x_k} \right\rangle \quad (\text{A.31})$$

$$\mathcal{T}_{i\phi}^{sgs} = \mathcal{D}_{i\phi}^{tot,sgs} - \epsilon_{i\phi}^{sgs} = -\frac{\partial}{\partial x_k} \left\langle q_k u'_i + \tau_{ik} \phi' \right\rangle \quad (\text{A.32})$$

$$\mathcal{T}_{i\phi} = -\frac{\partial}{\partial x_k} \left\langle u'_i u'_k \phi' \right\rangle \quad (\text{A.33})$$

$$\mathcal{P}_{i\phi} = -\left\langle u'_k \phi' \frac{\partial \langle u_i \rangle}{\partial x_k} + u'_i u'_k \frac{\partial \langle \phi \rangle}{\partial x_k} \right\rangle \quad (\text{A.34})$$

$$\mathcal{S}_{i\phi} = \mathcal{S}_{i\phi}^{tot} \quad (\text{A.35})$$

$$\mathcal{C}_{i\phi} = \mathcal{C}_{i\phi}^{tot} - \mathcal{P}_{i\phi} - \mathcal{T}_{i\phi} = -\left\langle u_k \right\rangle \frac{\partial \langle u'_i \phi' \rangle}{\partial x_k} \quad (\text{A.36})$$

$$\frac{\partial \langle u'_i \phi' \rangle}{\partial t} = \mathcal{C}_{i\phi} + \mathcal{P}_{i\phi} + \mathcal{T}_{i\phi} + \mathcal{D}_{i\phi} + \epsilon_{i\phi} + \mathcal{T}_{i\phi}^{sgs} + \epsilon_{i\phi}^{sgs} + \Pi_{i\phi} + \mathcal{S}_{i\phi} \quad (\text{A.37})$$

$\epsilon_{i\phi}$	Turbulent scalar flux (TSF) viscous dissipation
$\epsilon_{i\phi}^{sgs}$	TSF subgrid dissipation
$\Pi_{i\phi}$	TSF Scalar-Pressure gradient tensor
$\mathcal{D}_{i\phi}$	TSF Molecular (viscous) diffusion
$\mathcal{T}_{i\phi}$	TSF Turbulent diffusion (convection by the fluctuations)
$\mathcal{T}_{i\phi}^{sgs}$	TSF Subgrid diffusion
$\mathcal{P}_{i\phi}$	TSF production
$\mathcal{S}_{i\phi}$	TSF from source term
$\mathcal{C}_{i\phi}$	TSF convection
$\mathcal{B}_{i\phi}$	TSF Balance

A.5 Scalar variance budgets

$$\frac{\partial \langle \phi' \phi' \rangle}{\partial t} = \mathcal{C}_{\phi\phi}^{tot} + \mathcal{D}_{\phi\phi}^{tot} + \mathcal{D}_{\phi\phi}^{sgs,tot} + \mathcal{S}_{\phi\phi}^{tot} = \mathcal{B}_{\phi\phi} \quad (\text{A.38})$$

$$\mathcal{C}_{\phi\phi}^{tot} = 2\langle C_{\phi}^{tot} \phi \rangle - 2\langle C_{\phi}^{tot} \rangle \langle \phi \rangle \quad (\text{A.39})$$

$$\mathcal{D}_{\phi\phi}^{tot} = 2\langle D_{\phi} \phi \rangle - 2\langle D_{\phi} \rangle \langle \phi \rangle \quad (\text{A.40})$$

$$\mathcal{D}_{\phi\phi}^{sgs,tot} = 2\langle D_{\phi}^{sgs} \phi \rangle - 2\langle D_{\phi}^{sgs} \rangle \langle \phi \rangle \quad (\text{A.41})$$

$$\mathcal{S}_{\phi\phi}^{tot} = 2\langle \mathcal{S}_{\phi} \phi \rangle - 2\langle \mathcal{S}_{\phi} \rangle \langle \phi \rangle \quad (\text{A.42})$$

$\mathcal{C}_{\phi\phi}^{tot}$	Scalar variance (SV) total convection
$\mathcal{D}_{\phi\phi}^{tot}$	SV total molecular (viscous) diffusion
$\mathcal{D}_{\phi\phi}^{sgs,tot}$	SV total subgrid-scale diffusion
$\mathcal{S}_{\phi\phi}$	SV from source term
$\mathcal{B}_{\phi\phi}$	SV Balance

$$\frac{\partial \langle \phi' \phi' \rangle}{\partial t} = \mathcal{C}_{\phi\phi} + \mathcal{P}_{\phi\phi} + \mathcal{T}_{\phi\phi} + \mathcal{D}_{\phi\phi} + \epsilon_{\phi\phi} + \mathcal{T}_{\phi\phi}^{sgs} + \epsilon_{\phi\phi}^{sgs} + \mathcal{S}_{\phi\phi} \quad (\text{A.43})$$

$$\epsilon_{\phi\phi} = 2\alpha \left\langle \frac{\partial \phi'}{\partial x_k} \frac{\partial \phi'}{\partial x_k} \right\rangle \quad (\text{A.44})$$

$$\mathcal{D}_{\phi\phi} = \mathcal{D}_{\phi\phi}^{tot} - \epsilon_{\phi\phi} = \alpha \frac{\partial^2 \langle \phi' \phi' \rangle}{\partial x_k^2} \quad (\text{A.45})$$

$$\epsilon_{\phi\phi}^{sgs} = -2 \left\langle q_k \frac{\partial \phi'}{\partial x_k} \right\rangle \quad (\text{A.46})$$

$$\mathcal{T}_{\phi\phi}^{sgs} = \mathcal{D}_{\phi\phi}^{tot,sgs} - \epsilon_{\phi\phi}^{sgs} = -\frac{\partial}{\partial x_k} \langle q_k \phi' \rangle \quad (\text{A.47})$$

$$\mathcal{T}_{\phi\phi} = -\frac{\partial}{\partial x_k} \langle u'_k \phi' \phi' \rangle \quad (\text{A.48})$$

$$\mathcal{P}_{\phi\phi} = 2 \langle u'_k \phi' \rangle \frac{\partial \langle \phi \rangle}{\partial x_k} \quad (\text{A.49})$$

$$\mathcal{S}_{\phi\phi} = S_{\phi\phi}^{tot} \quad (\text{A.50})$$

$$\mathcal{C}_{\phi\phi} = \mathcal{C}_{\phi\phi}^{tot} - \mathcal{P}_{\phi\phi} - \mathcal{T}_{\phi\phi} = -\langle u_k \rangle \frac{\partial \langle \phi' \phi' \rangle}{\partial x_k} \quad (\text{A.51})$$

$\epsilon_{\phi\phi}$	Scalar variance (SV) viscous dissipation
$\epsilon_{\phi\phi}^{sgs}$	SV subgrid dissipation
$\mathcal{D}_{\phi\phi}$	SV Molecular (viscous) diffusion
$\mathcal{T}_{\phi\phi}$	SV Turbulent diffusion (convection by the fluctuations)
$\mathcal{T}_{\phi\phi}^{sgs}$	SV Subgrid diffusion
$\mathcal{P}_{\phi\phi}$	SV production
$\mathcal{S}_{\phi\phi}$	SV from source term
$\mathcal{C}_{\phi\phi}$	SV convection
$\mathcal{B}_{\phi\phi}$	Balance

Appendix B

Validation of LES Code

The VISCT code used in the thesis has been developed by Silva Lopes (2000), and has been validated in decaying isotropic turbulence Silva Lopes and Palma (2002), and in an S-duct Silva Lopes and Piomelli (2006). In this appendix, some validation tests on the use the code are reported.

Validation of the code for the simulation of coaxial flows using structured grids, where high non-orthogonality appears in the grid corners, was made in a fully developed pipe flow. The validation of the passive scalar solver is made in a plane channel, similar to Keating (2004), including the computation of the transport equation budgets.

B.1 Turbulent plane channel flow with heat transfer

A standard grid from the reference works Armenio and Piomelli (2000); Keating (2004) was used. The Reynolds number used is $Re_\tau = 395$ to match the DNS by Moin and Mahesh (1998). Resolution is then $\Delta x = 52$, $y^+(1) = 1$ (expanding with a hyperbolic tangent) and $\Delta z = 19$. Re_τ is defined as $Re_\tau = \frac{u_\tau h/2}{\mu} = 395$ The bulk Reynolds number is $Re_b = \frac{2U_b h_i}{\mu} = 13800$. The Prandtl number is 0.71.

The velocity statistics match Armenio and Piomelli (2000) and the passive scalar ones match Keating (2004); this includes the passive scalar transport budgets, *e.g.*, in figure B.1 the $\langle u' \phi' \rangle$ budget is shown (compare to figure 3.6-48 from Keating (2004)).

B.2 Laminar pipe flow

The suitability of non-orthogonal grids for pipe flow simulation was first appraised with a laminar ($Re = \langle u \rangle_b D_o / \nu = 800$) flow, using a relatively coarse (30^3 control volumes) grid generated by transfinite interpolation. The results were fully satisfactory, since the simulated isovelocity contours and the analytical solution of the Navier-Stokes equations were identical.

$$\langle u \rangle = \langle u \rangle_{max} (1 - (\frac{2r}{D_o})^2), \text{ where } \langle u \rangle_{max} = 2\langle u \rangle_b$$

Figure B.2 shows the simulated wall shear stress for the north wall in computational coordinates. The other walls are indistinguishable. The extremes (-1 and +1) of the x axis represent the grid corners. An important part of the Navier-Stokes solver used is the gradient calculation kernel, that calculates the gradient vector at the cell centres using Gauss theorem (eq. 3.22). The four lines represent four simulations, with increasing number of iterations in the gradient calculation (see section 3.3.3). It can be seen that no iteration (*i.e.*, linear interpolation only - lint) leads to severe wiggles close to the corners. However, a single iteration (lint + 1*g.c.) reduces the error to 0,1 % while 3 iterations (lint + 3*g.c.) completely eliminate the wiggles.

B.3 Turbulent pipe flow

The turbulent pipe flow calculations were made based on the LES approach. A 66^3 grid, generated using the techniques described in Spekreijse (1999) was used (see section 3.3.2) in a test case where $Re_\tau = 180$ ($Re \approx 5000$) and domain length $L = 5D$ to match the conditions of the direct numerical simulation in Eggels et al. (1994).

The grid was such that the coarsest cells had $\Delta y^+ = \Delta z^+ < 8$ and $\Delta x^+ \approx 30$. In the y and z directions, these are DNS like resolutions, comparing with the span-wise values of $\Delta \theta^+ \approx 9$ in Eggels et al. (1994) and $\Delta z^+ = 7$ in Kim et al. (1987). The streamwise resolution is three times lower than DNS values ($\Delta x^+ = 12$ in Kim et al. (1987)). The dimensionless time step was $t^* = 0.001 u_\tau / D$, well below the Kolmogorov time scale estimate of $\tau = 0.0068 u_\tau / D$ from Eggels et al. (1994).

While the flow is symmetrical, the grid is not, so some grid effect is to be expected. The number of points in the wall region, necessary to solve the high gradient there, can be smaller than necessary far away from the corners, and accounts for part of the small grid effect detected. The distance to the wall of the first grid point varies between 0.5 and 2 wall units. While this is acceptable, it nevertheless introduces another grid effect: varying wall distance. The depart from axial symmetry is shown in fig. B.3 for the Smagorinsky model (similar plots were obtained with the other models). The comparison of isovelocity contours with concentric circles shows only a small grid effect close to the grid corners.

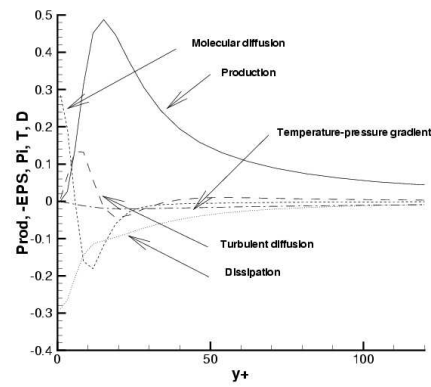


Figure B.1: Turbulent scalar flux $\langle u'\phi' \rangle$ budgets for plane channel flow

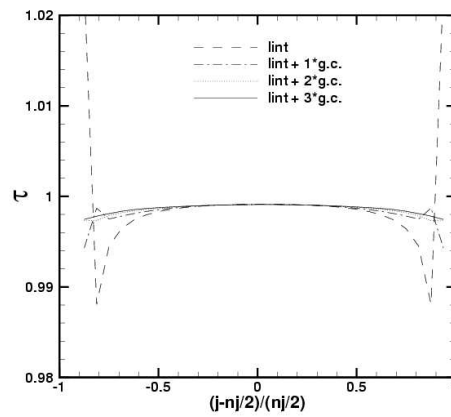


Figure B.2: Laminar pipe: wall shear stress; effect of the number of iterations in the gradient calculation; lint: linear interpolation; g.c.: gradient correction iteration

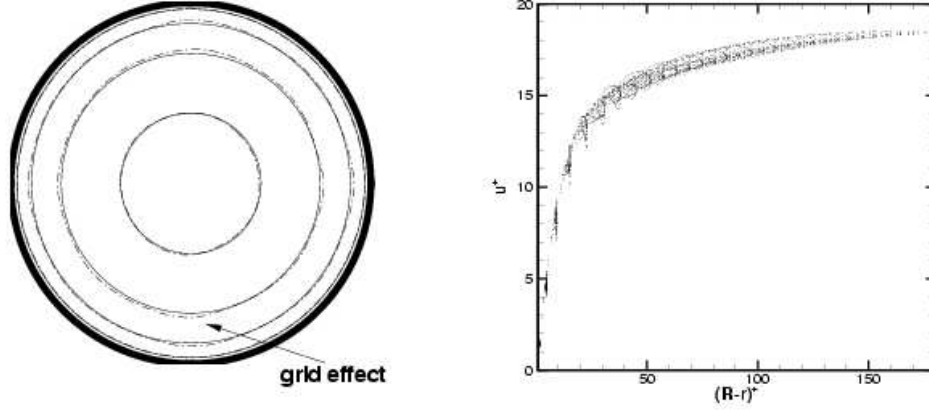


Figure B.3: Turbulent pipe. Isovelocity contours and axial velocity profile

The mean velocity profile shows good collapsing, although grid effects are present. The collapsing for the second order turbulence statistics (not shown) is also reasonable.

For comparison with the DNS results Eggels et al. (1994), the values have been interpolated to a cylindrical grid and averaged in the azimuthal direction. This operation was performed after averaging on time and on the axial direction. This is better than interpolating for each time step, which smooths the fields maxima and introduces additional filtering, even using a very fine cylindrical grid.

The comparison of the average velocity profiles for the various models (fig. B.4) with Eggels et al. (1994) shows that in all cases the log region is underpredicted (except in the Smagorinsky model, where agreement is very good) and the wake region is not captured. This underprediction is common in well resolved LES calculations, particularly when using spectral or high-order spatial discretization. The resolved axial turbulence intensity $\langle u'u' \rangle^{1/2}$ (fig. B.5) also shows the expected behaviour, being lower than the total ones, from the DNS.

In the case of the mean velocity profile, all models improved upon the no-model simulation, and seem to be working correctly. The turbulence intensities are also reasonable for all models tested.

A more comprehensive analysis of the performance of the various subgrid-scale models is beyond the scope of the current work.

The underpredictions in the velocity profile and in the $\langle u'u' \rangle^{1/2}$ turbulence intensity are atypical for 2nd order LES simulations, where overprediction has been observed (see e.g. Moin (2003)). A possible explanation for this atypical behaviour is the fine resolution in the azimuthal (or transversal, in a plane channel) direction near the wall, when compared with typical LES.

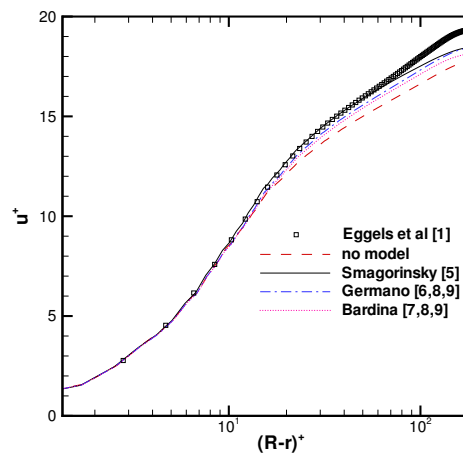
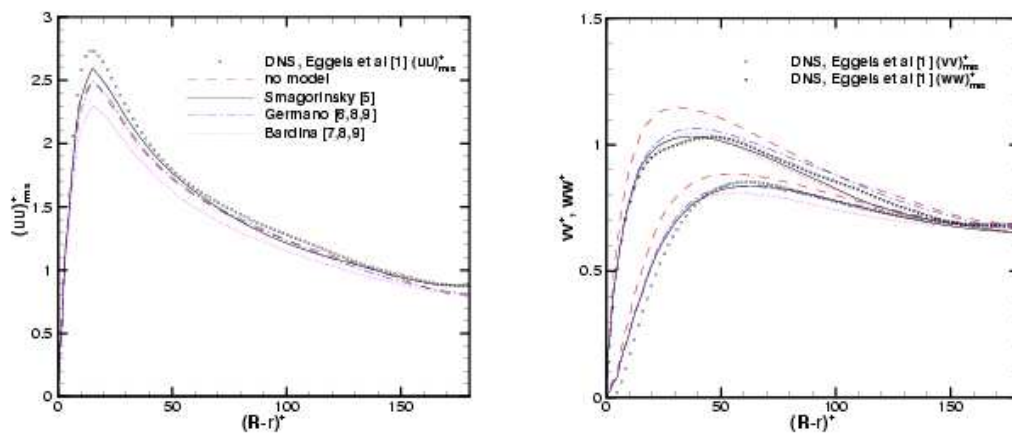
Figure B.4: Turbulent pipe: u velocity profile

Figure B.5: Turbulent pipe: turbulence intensities

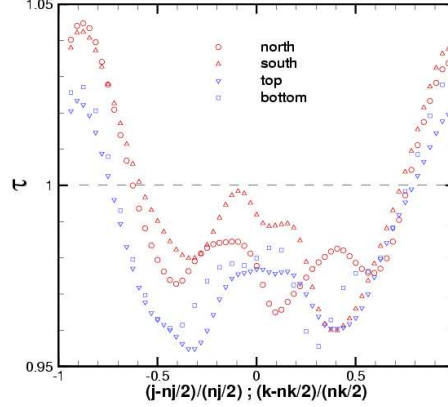


Figure B.6: Turbulent pipe: wall shear stress

Figure B.6 shows the wall shear stress in computational coordinates, for the "four walls" in which the tube is divided computationally, using the Smagorinsky model (other models give similar results). Symmetry would predict similar variations, as indeed occur. A perfect result would be a constant shear stress. It turns out that a $\pm 5\%$ variation can be observed. This is attributed to the variations in resolution, wall distance and grid distortion that occur close to the wall. Variations up to 15% in turbulent channel flow due to varying resolution and grid distortion are reported in Armenio and Piomelli (2000).

To conclude, it is felt that general agreement is good enough to warrant the use of the code in coaxial jets studies.

B.3.0.1 Validation conclusions

An existing code was modified to obtain second order accuracy in highly non-orthogonal grids via gradient reconstruction techniques in the spatial discretization. This code was used to simulate pipe flow geometries using non orthogonal grids. The gradient computation in non-orthogonal grids was tested and concluded that one gradient correction was enough to achieve reasonable accuracy in non-orthogonal grids.

Excellent agreement was obtained in laminar pipe flow. Large-eddy simulations using three popular subgrid models show good agreement with the reference DNS, similar to typical previously published LES. The passive scalar subgrid scale model was tested in a turbulent plane channel flow and the budgets of the transport equation compared well against published LES.

Appendix C

RANS Simulations of Confined Coaxial Jets Flows

Abstract

The flow of two coaxial jets confined in a tube, studied in Lima (2000), was simulated using a RANS (Reynolds-averaged Navier-Stokes) formulation. The results are compared against the experimental measurements. The five outer to inner velocity ratios, r , presented in Lima (2000) have been simulated.

C.1 Introduction

The code used for the simulations solves the Reynolds Averaged Navier Stokes equations using the SIMPLE algorithm in a collocated grid. Pressure velocity coupling is achieved using the pressure weighted interpolation method of Rhie and Chow (1983). This is an early, Cartesian version, of the non-orthogonal code developed in Castro et al. (2003). The standard $k - \epsilon$ method is used; the scalar field is not coupled to the velocity field and is obtained solving a transport equation with $Sc^{sgs} = 1$. The measurement at $x/D_{i,i} = 0.14$ is used as the inlet condition.

Dianat et al. (2006) and Jahnke et al. (2005) also present RANS simulations, that do not reproduce $\langle \phi \rangle$ accurately. This flow has always proved hard to RANS methods, that compute mean values only. In fact, in a recent review of turbulent combustion (Pitsch, 2006) it is stated that even though all the chemical reaction occurs at the subgrid scale (hence “there is no resolved part of the filtered reaction source term”) LES is still superior to RANS because it is more accurate in the reproduction of the mixing process and “...the scalar mixing process is of paramount importance in chemical conversion”.

C.2 Comparison between RANS and measurements

The mean velocity and passive scalar, $\langle u \rangle$ and $\langle \phi \rangle$, are available as outputs of the simulation and can be compared with the experiments. The velocity fluctuation, $\langle u'u' \rangle^{1/2}$, could have been estimated from the turbulent kinetic energy, k , but this has not been done in this work. The passive scalar fluctuation, $\langle \phi'\phi' \rangle^{1/2}$, and turbulent scalar flux, $\langle u'\phi' \rangle$, are not available nor can they be estimated. If a particular application requires them, RANS is not an adequate approach. For many applications, accurate reproduction of the mean field is enough. In this appendix the goal is to find out in which conditions are the mean profiles reasonably reproduced using RANS and which ones are not and could benefit from the LES approach.

C.2.1 Condition 1, $r = 3.2$

Analysis of figures C.1 and C.2 shows that merging of the inner and outer shear layers occurs in the entry region, *e.g.*, at $x/D_{i,i} = 2$ there is no inflection in the $\langle u \rangle$ profile, a feature that the RANS simulation only reproduces for $x/D_{i,i} = 8$. The RANS simulation requires a longer mixing region, *e.g.*, the experiments $\langle u \rangle$ profile resembles a fully developed one by $x/D_{i,i} = 32$, whereas the RANS remains undeveloped up to $x/D_{i,i} = 64$.

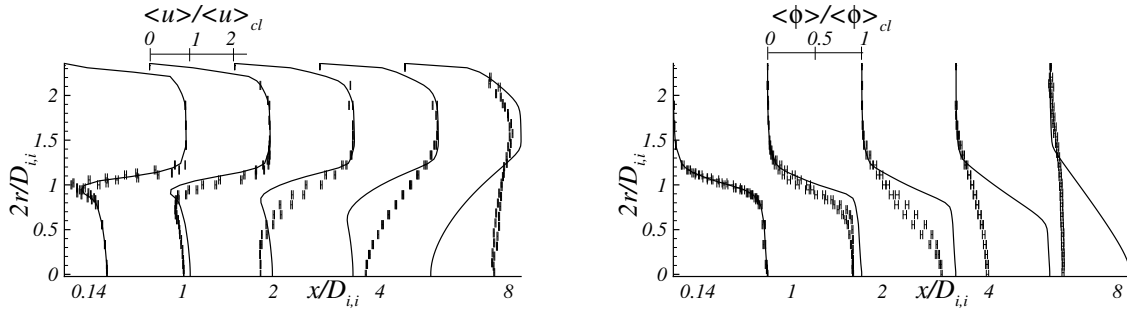


Figure C.1: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 3.2$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: RANS simulation

The mean scalar profiles show that the passive scalar mixing occurs in the entry region, as shown by the profile at $x/D_{i,i} = 4$. The mixing takes much longer in the RANS simulation, resulting in very different $\langle \phi \rangle$ profiles in the region between $x/D_{i,i} = 4$ and $x/D_{i,i} = 16$.

The conclusion is thus that RANS is unable to reproduce the strong mixing that occurs in the entry region, for this high velocity ratio condition.

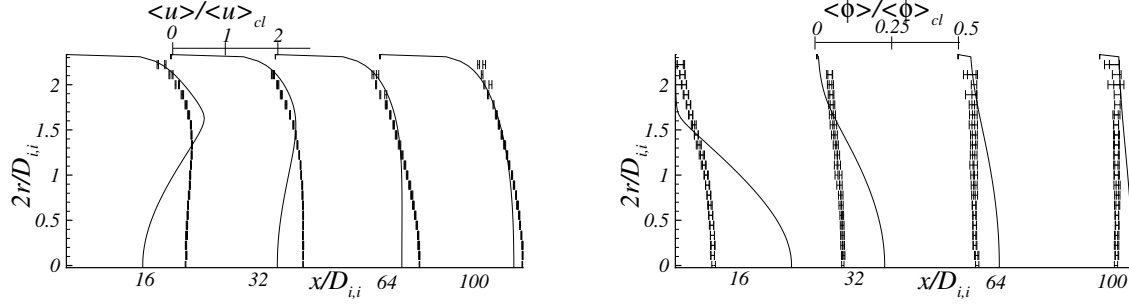


Figure C.2: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 3.2$; Far field: $x/D_{i,i} = 16, 32, 64$ and 100 ; error bars: experimental measurements; lines: RANS simulation

C.2.2 Condition 2, $r = 2.0$

This condition is compared to the experiments in figures C.3 and C.4. Compared to $r = 3.2$ this condition shows a better reproduction of the velocity $\langle u \rangle$, even though the shear layer merging is complete (no inflection) by $x/D_{i,i} = 4$ in the experiments whereas the same is observed for $x/D_{i,i} = 16$ in the RANS simulation.

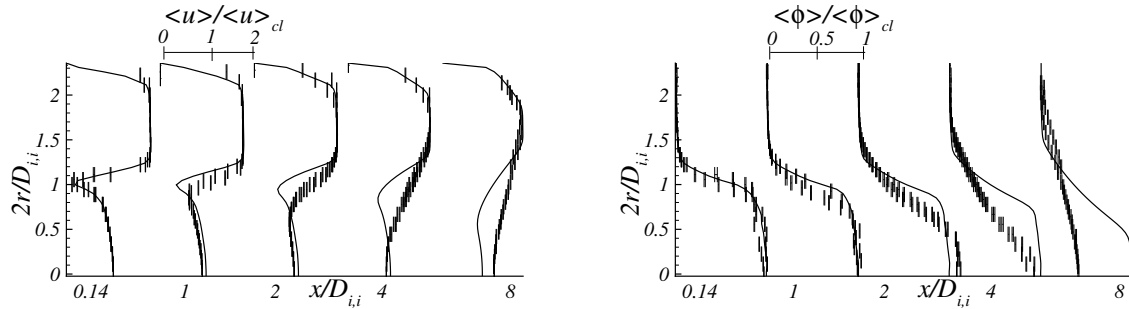


Figure C.3: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 2.0$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: RANS simulation

The scalar $\langle \phi \rangle$ has better agreement than in $r = 3.2$, but large differences between experimental and simulation profiles are still observed at $x/D_{i,i} = 8$ and $x/D_{i,i} = 16$.

We conclude that the decrease in the velocity ratio lead to a better agreement between experiment and RANS, but differences are still significant.

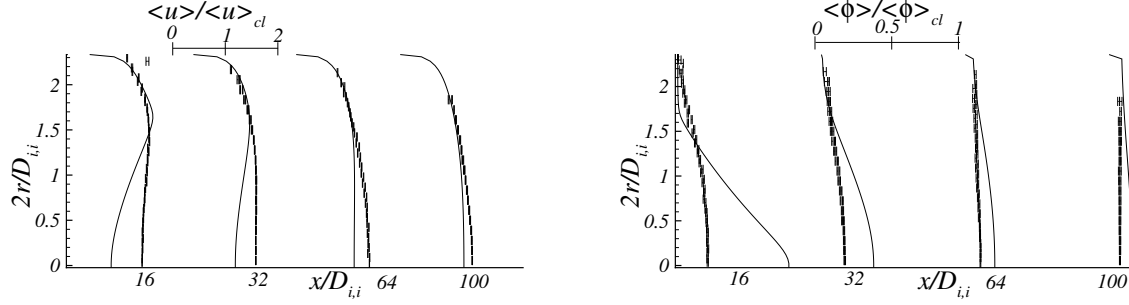


Figure C.4: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 2.0$; Far field: $x/D_{i,i} = 16, 32, 64$ and 100 ; error bars: experimental measurements; lines: RANS simulation

C.2.3 Condition 3, $r = 1.1$

This condition is compared to the experiments in figures C.5 and C.6. The velocity profiles magnitude is well reproduced, even though differences in shape are present.

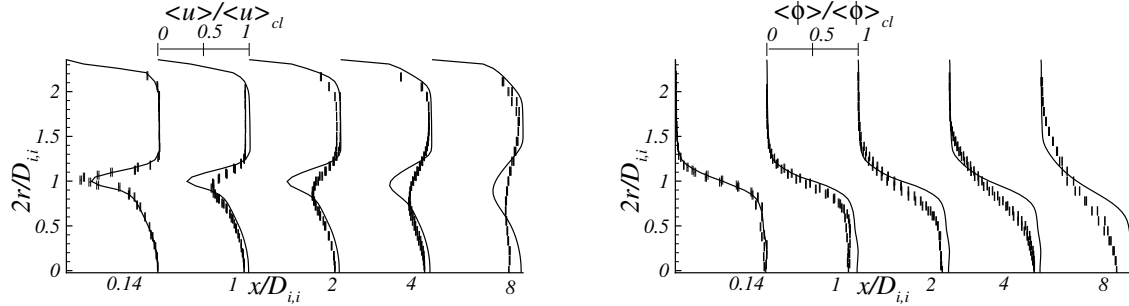


Figure C.5: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 1.1$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: RANS simulation

The passive scalar profiles are well reproduced up to $x/D_{i,i} = 8$, in the so called entry region. The final merging occurs later, in $x/D_{i,i} = 16$ and $x/D_{i,i} = 32$ and shows the larger differences between experiment and RANS.

The conclusion is that RANS is now reasonably accurate, particularly in the entry region, up to $x/D_{i,i} = 8$.

C.2.4 Condition 4, $r = 0.8$

This condition, that has the lowest velocity ratio, is compared to the experiments in figures C.7 and C.8. The mixing is much slower and the velocity and passive scalar profiles

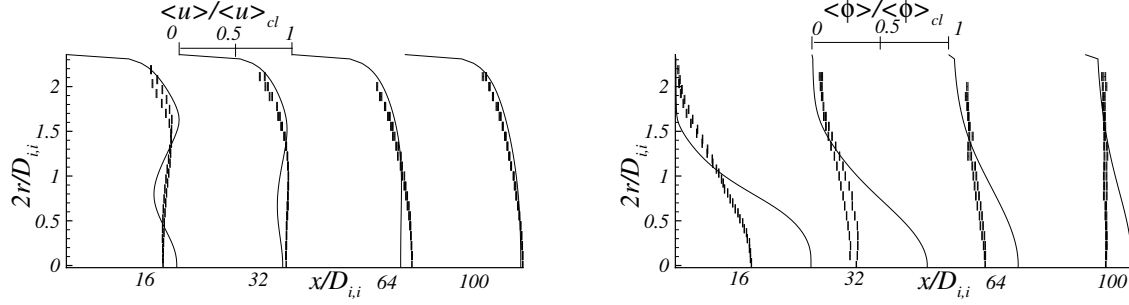


Figure C.6: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 1.1$; Far field: $x/D_{i,i} = 16, 32, 64$ and 100 ; error bars: experimental measurements; lines: RANS simulation

are well reproduced, even though the difference in shape is still present in the velocity profiles, indicating slower mixing in the simulation.

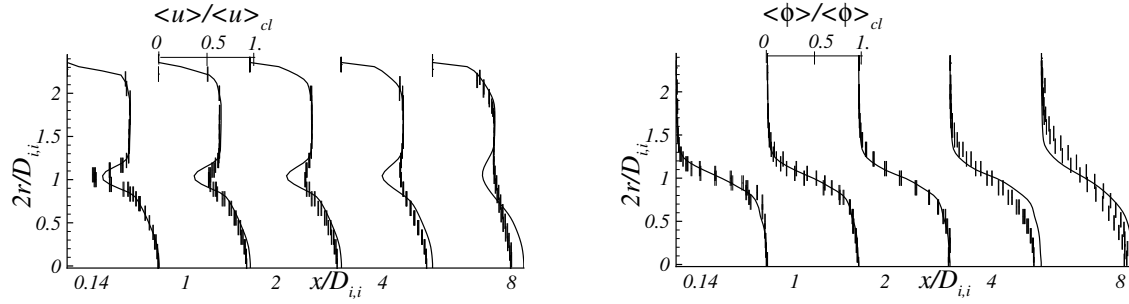


Figure C.7: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 0.8$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: RANS simulation

The conditions one to four, where the velocity ratio gradually decreased from $r = 3.2$ to $r = 0.8$, have shown that the lower the velocity ratio, the better the agreement between experiment and RANS.

C.2.5 Condition 5, $r = 6.5$

This condition, that has the highest velocity ratio, is compared to the experiments in figures C.9 and C.10. The figures show that neither shape nor magnitude is reproduced by the RANS simulation, particularly in the passive scalar $\langle \phi \rangle$ profiles.

The differences also reflect the lack of mass conservation in the experiment profiles. For this reason, even though improvement is to be expected from LES simulation, the $r = 3.2$ is likely to be a better test case.

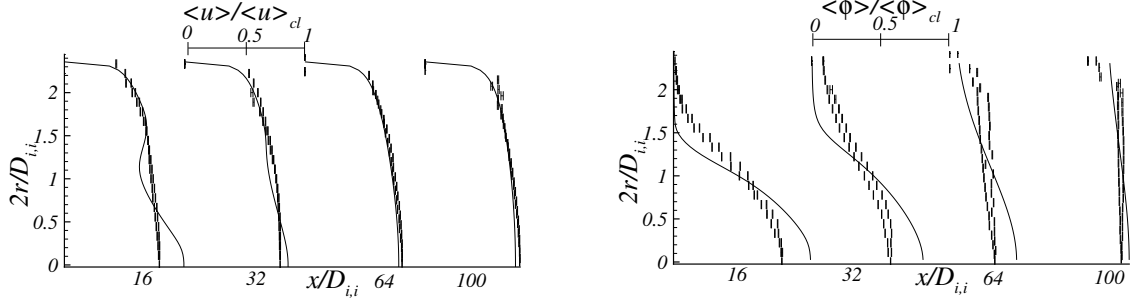


Figure C.8: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 0.8$; Far field: $x/D_{i,i} = 16, 32, 64$ and 100 ; error bars: experimental measurements; lines: RANS simulation

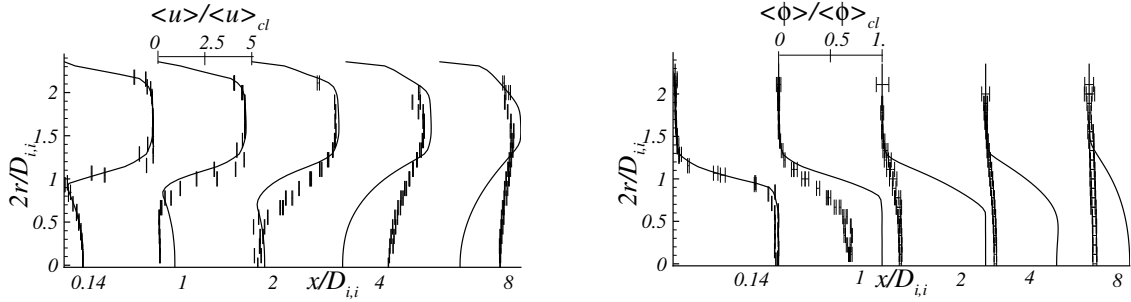


Figure C.9: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 6.5$; Near field: $x/D_{i,i} = 0.14, 1, 2, 4$ and 8 ; error bars: experimental measurements; lines: RANS simulation

C.2.6 The interior jet profile

The interior jet is very close to a fully developed turbulent profile in conditions 1 to 4. In condition 5 ($Re_i = 2134$), the inlet interior profile is approximately parabolic, but not laminar. In a previous work (Rehab et al. (1997)) a similar effect is attributed to the divergence in the interior pipe. Our measurements do not exhibit such effect in conditions 1 to 4 and its presence in condition 5, in our opinion, is due to the low Reynolds number and not to the divergence in the pipe.

C.3 Conclusions

The present study, using a standard RANS approach, has good agreement with experimental measurements for velocity ratio near unity, $r = 0.8$ and $r = 1.1$. The RANS code was unable to reproduce the experimental mean profiles for the high velocity ratio conditions, $r = 3.2$ and $r = 6.5$. The RANS simulation also highlights the lack of passive scalar mass

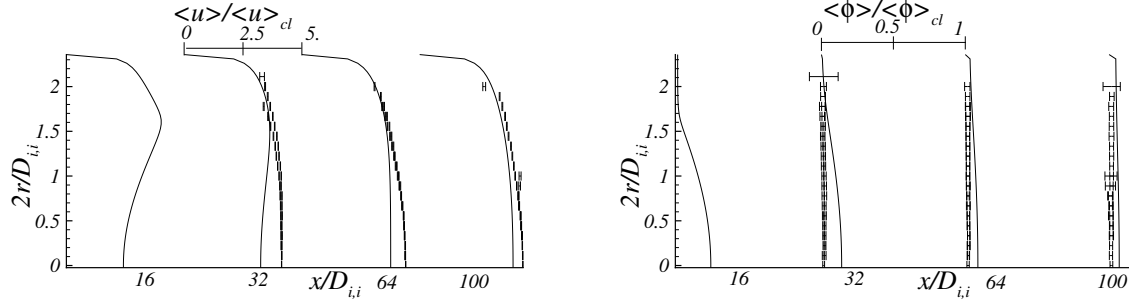


Figure C.10: Streamwise velocity mean and passive scalar mean, $\langle u \rangle$ and $\langle \phi \rangle$, for velocity ratio $r = 6.5$; Far field: $x/D_{i,i} = 16, 32, 64$ and 100 ; error bars: experimental measurements; lines: RANS simulation

conservation in $r = 6.5$, so $r = 3.2$ is pointed out as the condition where the benefits of LES in high-velocity ratio coaxial jets can be more clearly observed. This is in accordance with many published works, including recent publications on coaxial jets, such as Dianat et al. (2006) and Jahnke et al. (2005).

Appendix D

Coherent Structure Dynamics in the Entry Region of Co-annular Ducts

Abstract

Large-eddy simulations are used to study the entry region of a co-annular flow in a pipe with velocity ratio $r = 0.8$ and diameter ratio $\beta = 2.21$. Instantaneous fields of vorticity norm and Q-criteria were used to identify coherent structures and analyse their interaction. The governing frequencies are identified and its value compared to the one predicted by linear stability theory. The inner and outer shear layers interact and its vortices acquire the same crossing frequency due to a locking mechanism between the two shear layers. The value of this frequency, appearing in both shear layers, is in accordance with the value predicted by linear stability theory for the inner jet. The inner shear layer is forcing its frequency on the outer one through a vorticity inducing mechanism, *i.e.*, Biot-Savart. The analysis of turbulent kinetic energy and vorticity has shown that it is the higher vorticity interior jet that dominates the flow dynamics in the entry region. This analysis may allow the prediction of shear layer interaction in other, more complex, geometries.

D.1 Introduction

Co-annular ducts consist on two concentric pipes that discharge two flow streams in a confined region. It is a geometry frequently used in industrial applications as an effective way of mixing two fluids (Paul et al., 2004). The flow in co-annular ducts is similar to the free coaxial jets flow, to which it adds the effect of confinement. The entry region is defined as the first three diameters, a zone where the flow dynamics are little modified

by the confinement (via the pressure gradient). The dynamic of this region is therefore studied with the same jets but without confinement.

Many experimental and numerical studies have been made on free coaxial jets, going back to the 1950's (*cf.* da Silva et al., 2003, for a review). Here we focus on a recent development: DNS 3D simulations of free coaxial jets.

This was first achieved by da Silva (2001) that established a method to directly compute such a flow. It is important to note however that there are several restrictions: low Re ($Re \approx 3000$), unconfined jets (no interaction with walls) and laminar inlet profiles. The development of coherent structures occurs after ≈ 5 internal diameters, much further than in the laboratory. In the preliminary study presented in da Silva (2001) the well known connection between the inner and outer jets through a locking mechanism is verified by analysis of the coherent structures. A problem is clearly stated: "... problem ... is ... the impossibility to carry out any kind of serious validation of the results". Later (da Silva et al. (2003), Balarac and Métais (2005)) a partial validation is achieved, through comparison of $\langle u'u' \rangle^{1/2}$ in the centreline with experimental results. Of most interest to us is the application of these methods to passive scalar mixing (Balarac et al., 2007b). He uses $Sc = 1$ and a synthetic inlet scalar profile (similar to the velocity one) that is not matched to any existing experimental measurement. Therefore, the passive scalar results are not validated with experiment. Passive scalar fluctuations are presented and reach, after transition, ≈ 20 % of the maximum scalar value. Recently, two other simulations dealt with mixing control through inlet forcing; Balarac et al. (2007a) and Akihiko et al. (2007). Akihiko et al. (2007) is noticeable because $\langle \phi \rangle$ is validated with experimental data with fair agreement; no other statistics are presented.

D.2 Numerical method

A sixth-order semi-spectral code (SPECOMP), previously developed by Marcel Lesieur group, tested in canonical jets and adapted to coaxial jets by C.B. da Silva (da Silva, 2001). Since no modifications to the code were made, only a brief description is given and the reader is referred to the original work for more informations.

The finite difference code solves the Navier-Stokes equations using pseudo-spectral and compact sixth-order Lele (1992) methods for spatial discretization. Temporal discretization is ensured by a third order three sub-steps Runge-Kutta method. To achieve pressure-velocity coupling, a fractional step method is used, that solves a Poisson equation to ensure the incompressibility of the velocity field. The subgrid-scale model was the selective structure Ducros et al. (1996) function model.

The inlet velocity profile is given by $u(x_0, t) = \bar{u}(x_0) + u_{noise}(x_0, t)$ where $u(x_0, t)$ is the instantaneous velocity vector, specified in each time step. In this study, $\bar{u}(x_0)$ is based in the axial velocity profile measured in the experiments with zero mean velocity specified

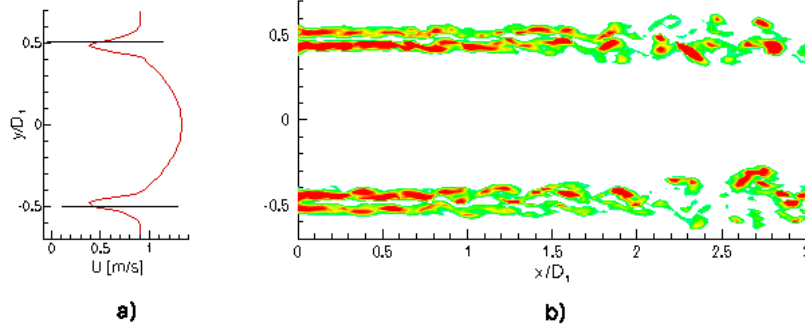


Figure D.1: a) Mean streamwise velocity at inlet b) Vorticity norm isocontours

in y and z . $u_{noise}(x_0, t)$ is the noise inlet profile, applied in the three velocity components and given by $u_{noise}(x_0, t) = A_n U_{base}(x_0) f'$. A_n is the maximum noise amplitude, $U_{base}(x_0)$ is a function that places the noise in the shear layer region and f' is random noise made to satisfy a given energy spectra $E(k) = k^s \exp(-\frac{s}{2}(k/k_0)^2)$, where $k = (k_y^2 + k_z^2)^{1/2}$ is the wave number norm in the (y, z) plane. The s exponent and k_0 wave number were chosen in order to have energy generation in the small scales and a large scale spectral behaviour typical of decaying isotropic turbulence. The maximum A_n used in the simulations was 4%. The outlet boundary condition is of the non-reflecting type. No major modifications were applied to the code for this work, therefore this level of exposition is enough. The code itself has been well validated and explained before (da Silva, 2001)

The simulations are based on the experimental data of Lima (2000) for a outer to inner mean velocity ratio of $r = 0.8$, an outer to inner diameter ratio of $\beta = 2.21$ and a mean Reynolds number of 35000.

D.3 Results and discussion

The figures D.1b and D.2 provide a general prospective on the typical fields obtained from the simulation. Downstream of the inlet section and associated with the inlet velocity profile (figure D.1a), two shear layers (inner and outer) are clearly distinguished and remain so for the whole studied region. The layers do not develop independently, they interact. After $x/D_i = 0.8$, the Kelvin-Helmholtz instability originates vortex rings in both shear layers. In figure D.2 coherent structures in the studied flow can be identified. The typical scenario of transition to turbulence is observed, with ring-shaped vortices being generated, associated to the instabilities. Between those vortex rings streamwise vortices appear ($x/D_i = 2$), which is in accordance with observations in the canonical free jet. The flow

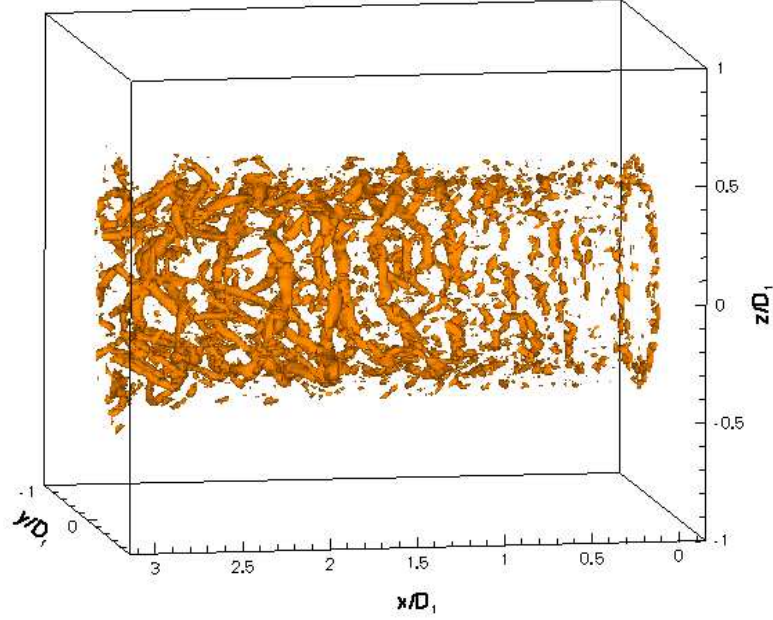


Figure D.2: Isosurfaces of positive Q-criteria

near the centreline ($|y/D_i| < .2$) and the outer flow ($|y/D_i| > 1$) remains potential up to the domain outlet, so for this potential ratio no potential core can be defined.

As noted above, in the initial transition stage the two shear layers (inner/outer) originate vortex rings due to the Kelvin-Helmholtz instability. The theoretical Strouhal number of the most unstable wave resulting from a free jet inlet profile is $St_t = f\theta/U_0 = 0.017$. This value can be compared against the values obtained by spectral analysis of timeseries located in each shear layer and summarised in table D.1. It is shown that the frequency f is the same for the inner and outer layers, *i.e.*, the vortex crossing frequency is the same for both shear layers.

	f	St_t
inner	2.4	0.018
outer	2.4	0.005

Table D.1: Most amplified frequencies and corresponding Strouhal numbers

It is also shown that the inner layer Strouhal number is close to theoretical value, showing that the inner layer behaves in accordance with linear stability theory. The visualisations showed that the inner shear layer dominates the flow dynamic and defines the most unstable frequency, transmitting it to the outer layer through a vorticity inducing

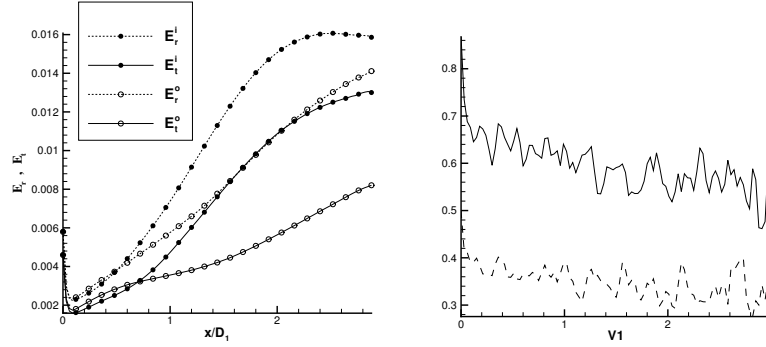


Figure D.3: a) Evolution of E_r e E_t on the inner and outer layers b) Evolution of Ω^T on the inner and outer layers

mechanism (Biot-Savart). The analysis of pressure isocontours (figure D.5) shows large structures in the inner shear layers and, locked in their intervals, smaller structures in the outer layer. This is called locking and has been observed experimentally in Dahm et al. (1992).

An explanation for the dominance of the inner shear layer may be found by studying the vorticity integrals along the two shear layers.

$$\Omega_T^o(x) = \int_{R_m}^{\infty} \langle |\mathbf{\Omega}(x, r)| \rangle dr, \Omega_T^i(x) = \int_0^{R_m} \langle |\mathbf{\Omega}(x, r)| \rangle dr, \quad (D.1)$$

The integrals are represented in figure D.3b, where it can be seen that the vorticity is always higher in the inner layer. Figure D.4 illustrates the inner jet dominance, showing vorticity concentrations in the inner layer that remain throughout the entry region.

To compare the transition evolution in the inner and outer layers the radial and tangential contributions to the turbulent kinetic energy are defined, for the inner and outer layers:

$$E_r^i = \sqrt{\frac{2\pi}{L_y L_z} \int_0^{R_m} \langle u_r'^2(x, r) \rangle r dr d\theta}, E_t^i = \sqrt{\frac{2\pi}{L_y L_z} \int_0^{R_m} \langle u_\theta'^2(x, r) \rangle r dr d\theta}, \quad (D.2)$$

$$E_r^o = \sqrt{\frac{2\pi}{L_y L_z} \int_{R_m}^{\infty} \langle u_r'^2(x, r) \rangle r dr d\theta}, E_t^o = \sqrt{\frac{2\pi}{L_y L_z} \int_{R_m}^{\infty} \langle u_\theta'^2(x, r) \rangle r dr d\theta}, \quad (D.3)$$

These quantities are represented in figure D.3a. For $x/D_i > 0.6$ the instabilities in the inner jet (filled symbols) grow faster than the outer ones, and reach higher values; this is to

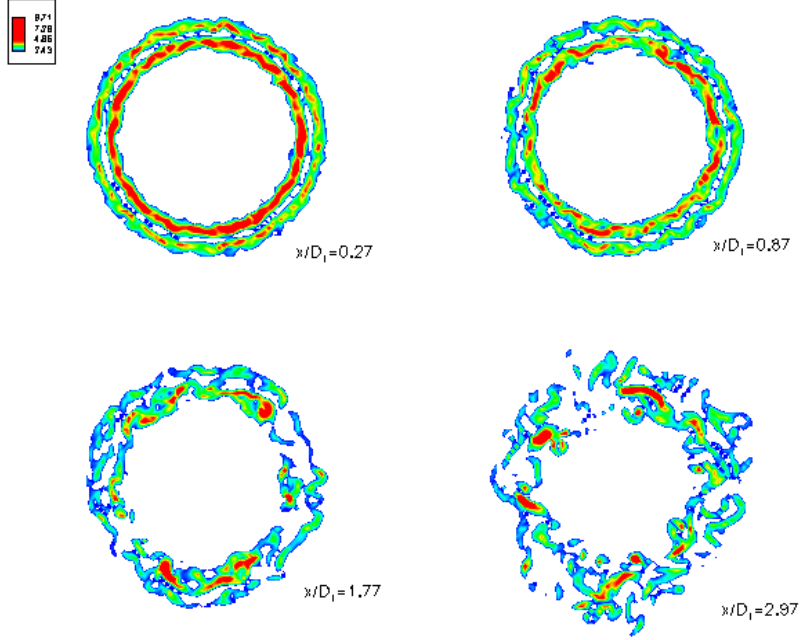


Figure D.4: Vorticity norm isocontours in 4 cross-sections

be expected, due to the dominance of the inner shear layer. More surprising is that $E_r(x)$ (dashed lines, associated with the formation of vortex rings) dominates E_θ (continuous lines, associated with the growth of azimuthal instabilities) in contrast with the behaviour for free jets, where the order of magnitude of both contributions is similar (da Silva and Métais, 2002). The interaction between the inner and outer jets therefore impacts on the instability growth.

D.4 Conclusions

The flow on the entry region of a co-annular jet is analysed, using a mean velocity profile from experimental measurements. The inner layer generates vortices with a frequency corresponding to the linear stability theory prediction, for free jet. The outer layer is dominated by the inner layer that communicates, by vorticity induction (Biot-Savart), the vortex crossing frequency. The outer layer structures are locked between the inner layer ones, a mechanism shown in previous experimental works. The dominance of the inner shear layer is connected to its higher vorticity, shown in statistics and visualisations.

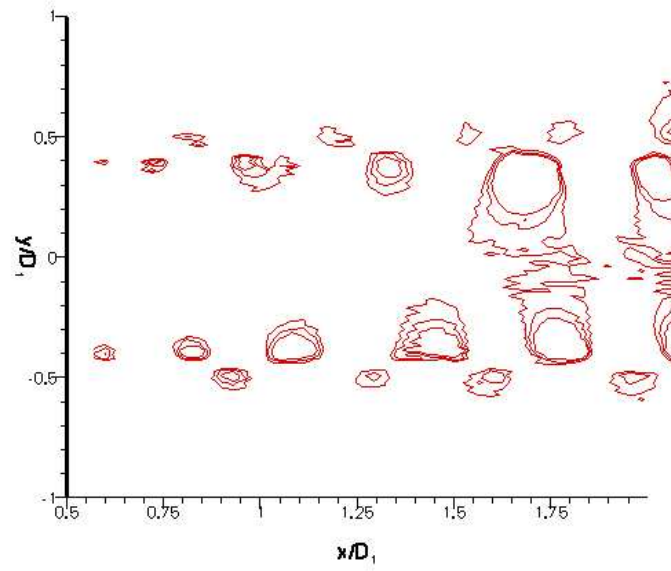


Figure D.5: Negative pressure isocontours

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