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DÉVELOPPEMENT DE LA MÉTHODE DE SIMULATION AUX GRANDES ÉCHELLES POUR LES ÉCOULEMENTS DIPHASIQUES TURBULENTS

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Résumé

La demande industrielle et l’intérêt scientifique croissants pour approfondir la connaissance des écoulements turbulents à phase dispersée est à l’origine du fort développement de la modélisation numérique de ce type d’écoulements. Ce travail de thèse se concentre sur les phénomènes physiques de dispersion et de concentration préférentielle de particules solides dans un gaz. Il vise à étendre à la Simulation aux Grandes Echelles (SGE) le formalisme Eulérien mésoscopique introduit par Février et al. (2005), et récemment mis en œuvre par Simulation Numérique Directe (SND) par Kaufmann et al. (2006).

L’extension de l’approche Eulérienne mésoscopique à la SGE soulève deux principales difficultés. En terme de modélisation tout d’abord, la subtilité de cette approche réside dans la double origine des termes à fermer : ils sont issus d’une part de la moyenne d’ensemble introduite par le formalisme mésoscopique et d’autre part du filtrage spatial au sens de la SGE. Moreau (2006) propose des modèles de fermeture pour ces différents termes fondés sur des calculs lagrangiens a priori de Turbulence Homogène Isotope (THI) décroissante chargée en particules. Ces modèles requièrent également une validation a posteriori, ce qui est l’objectif de la présente étude. La résolution numérique du système d’équations particulières constitue la deuxième difficulté du modèle SGE Eulérien mésoscopique. En effet, ces équations ne présentent pas de termes diffusifs et induisent de forts gradients difficiles à représenter sur une grille de calcul.

Dans cette étude, en premier lieu, le schéma TTGC (Colin & Rudgyard, 2000), reconnu pour ses faibles taux de dispersion et de dissipation, est étendu à la phase dispersée et couplé à une méthode de stabilisation numérique. La robustesse et la précision du modèle numérique obtenu sont ensuite démontrées en comparant les résultats d’une SND de THI décroissante chargée en particules avec des résultats de calculs lagrangiens. Finalement, le modèle SGE Eulérien mésoscopique est validé a posteriori dans deux géométries complexes pour lesquelles des données expérimentales détaillées sont disponibles. La première configuration est un jet vertical turbulent gaz-particules (Hishida et al., 1987) qui requiert le développement de conditions aux limites spécifiques pour la phase dispersée. La deuxième configuration est un jet recirculant chargé en particules (Borée et al., 2001) pour lequel des résultats lagrangiens sont également disponibles. La comparaison des SGE Eulériennes mésoscopiques avec les mesures, ainsi que les simulations lagrangiennes dans la deuxième géométrie, démontre la capacité de cette nouvelle approche à capturer la dynamique de ce type d’écoulements turbulents gaz-particules.

Mots-clés : écoulements diphasiques turbulents gaz-particules, dispersion de particules, modélisation Eulérienne mésoscopique, simulation aux grandes échelles.
Abstract

Turbulent two-phase flows occur in a wide range of industrial processes, which strongly encourages the development of numerical methods for such flows. This work focuses on the physical phenomena of dispersion and preferential concentration of solid particles in a gas flow. The main purpose is to extend to Large-Eddy Simulation (LES), the Eulerian mesoscopic formalism introduced by Février et al. (2005) and first implemented by Kaufmann et al. (2006) to perform Direct Numerical Simulation (DNS).

When extending the Eulerian mesoscopic approach to LES, two main issues arise. First, as far as modeling is concerned, two different kinds of unclosed terms appear in the transport equations for the dispersed phase, which is very specific to this approach. Those terms are due either to ensemble averaging introduced by the mesoscopic approach, or by LES spatial filtering. Several closure models are proposed and tested a priori by Moreau (2006) who performs Discrete Particle Simulation (DPS) of particle-laden Homogeneous Isotropic decaying Turbulence (HIT). A posteriori validating these models is then required, which is the aim of the present work. Second, it is delicate to handle numerically the set of transport equations for the dispersed phase. Indeed, there are no physical diffusive terms in the transport equations and strong gradients difficult to represent on the grid must be accounted for.

Consequently, first in this work, a new numerical method is proposed. The numerical scheme TTGC (Colin & Rudgyard, 2000) that is known to be few dispersive and few dissipative, is adapted to the dispersed phase and combined with a stabilising numerical method. Then, comparing Direct Numerical Simulation (DNS) of particle-laden decaying HIT flows performed with the Eulerian mesoscopic approach and the Lagrangian one shows the robustness and the accuracy of the numerical method proposed. Finally, the LES Eulerian mesoscopic modeling is validated a posteriori in two different complex geometries. For both, a detailed bank of experimental data are available. The first configuration consists of a particle-laden turbulent jet (Hishida et al., 1987). It requires to develop specific inlet Boundary Conditions (BC) for the dispersed phase. The second configuration is a particle-laden bluff body (Borée et al., 2001) where Eulerian mesoscopic and Lagrangian approaches can be evaluated. Comparing LES using the Eulerian mesoscopic approach with the experiments, and even with the DPS for the second geometry, shows that this new approach is able to accurately capture the dynamics of such particle-laden turbulent flows.

Keywords: gas-particle turbulent two-phase flows, particle dispersion, Eulerian mesoscopic modeling, large-eddy simulation.
Contents

Acknowledgements 7

Nomenclature 11

Introduction 15

1 Transport equations for dispersed two-phase flows 23
  1.1 The gas flow ............................................. 25
  1.2 Forces acting on an isolated particle .......................... 26
  1.3 Euler-Lagrange approach: Discrete Particle Simulation (DPS) .... 29
  1.4 Euler-Euler volume filtering approaches .......................... 32
  1.5 Euler-Euler mesoscopic approach .................................. 35

2 Numerical approach 47
  2.1 Cell-vertex method for the Navier-Stokes equations ................. 48
  2.2 Convective schemes ............................................. 52
  2.3 Numerical stabilization methods ..................................... 57

3 DNS of particle-laden homogeneous isotropic decaying turbulence 69
  3.1 Gas Homogeneous Isotropic Turbulence flow .......................... 71
  3.2 Two-phase flow simulations: previous work with the EE mesoscopic approach . 83
<table>
<thead>
<tr>
<th>CONTENTS</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Conclusion</td>
<td>209</td>
</tr>
<tr>
<td>Bibliography</td>
<td>213</td>
</tr>
<tr>
<td>Appendix</td>
<td>229</td>
</tr>
<tr>
<td>A  Bluffbody: additional graphs</td>
<td>229</td>
</tr>
</tbody>
</table>
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# Nomenclature

**Roman letters**

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<thead>
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<th>Symbol</th>
<th>Description</th>
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<td>$A$</td>
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</tr>
<tr>
<td>$\mathcal{F}^I_{ij}$</td>
<td>Inviscid flux tensor</td>
</tr>
<tr>
<td>$\mathcal{F}^V_{ij}$</td>
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</tr>
<tr>
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<td>$C_L$</td>
<td>Lift coefficient</td>
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<tr>
<td>$C_m$</td>
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<td>$c_{p,i}$</td>
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<tr>
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<td>Fluid heat capacity</td>
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<td>$F_{M,i}$</td>
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<td>$g_i$</td>
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<td>$P_f$</td>
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<td>$Q_{f,i}$</td>
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<td>$q_{fp}$</td>
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<td>$S_{p,ij}$</td>
<td>Particle Boussinesq tensor</td>
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<tr>
<td>$T_{f,ij}$</td>
<td>Fluid SGS Reynolds tensor</td>
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<tr>
<td>$T_f$</td>
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**NOMENCLATURE**

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<tr>
<th>Symbol</th>
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<td>$T_{p,ij}$</td>
<td>Particle SGS tensor</td>
</tr>
<tr>
<td>$u_{f,i}$</td>
<td>Instantaneous fluid velocity vector</td>
</tr>
<tr>
<td>$u_{p,i}$</td>
<td>Instantaneous Eulerian particle velocity vector</td>
</tr>
<tr>
<td>$v_{p,i}^{(m)}$</td>
<td>Instantaneous Lagrangian velocity vector of particle $(m)$</td>
</tr>
<tr>
<td>$x_{p,i}$</td>
<td>Particle coordinate vector</td>
</tr>
<tr>
<td>$V_k$</td>
<td>Nodal volume of node $k$</td>
</tr>
<tr>
<td>$V_{Ω_j}$</td>
<td>Volume of cell $j$</td>
</tr>
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<td>$x_i$</td>
<td>Node coordinate vector</td>
</tr>
<tr>
<td>$G$</td>
<td>Filter function</td>
</tr>
<tr>
<td>$w$</td>
<td>Vector of conservative variables</td>
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**Greek letters**

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<th>Symbol</th>
<th>Definition</th>
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<tbody>
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<td>$α_{1...n}$</td>
<td>Runge-Kutta coefficients</td>
</tr>
<tr>
<td>$α_p$</td>
<td>Particle volume fraction</td>
</tr>
<tr>
<td>$δθ_p$</td>
<td>Instantaneous particle uncorrelated energy</td>
</tr>
<tr>
<td>$δM_{p,ijkl}$</td>
<td>Particle 4th order uncorrelated velocity correlation tensor</td>
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<tr>
<td>$δq_p^2$</td>
<td>Mean particle uncorrelated energy</td>
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<td>$δR_{p,ij}$</td>
<td>Particle 2nd order uncorrelated velocity correlation tensor</td>
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<td>$δS_{p,ijk}$</td>
<td>Particle 3rd order uncorrelated velocity correlation tensor</td>
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<td>$Δt$</td>
<td>Time step</td>
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<td>$δu_{p,i}^{(m)}$</td>
<td>Instantaneous uncorrelated velocity vector of particle $(m)$</td>
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<td>$Δx$</td>
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<td>$Δ$</td>
<td>Filter characteristic length</td>
</tr>
<tr>
<td>$δ$</td>
<td>Dirac function</td>
</tr>
<tr>
<td>$δ_{ij}$</td>
<td>Kronecker symbol</td>
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<tr>
<td>$η_f,κ$</td>
<td>Kolmogorov length scale</td>
</tr>
<tr>
<td>$γ$</td>
<td>Fluid compressibility coefficient</td>
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<td>$κ_{p,RUM}$</td>
<td>Particle uncorrelated diffusivity</td>
</tr>
<tr>
<td>$λ_f$</td>
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</tr>
<tr>
<td>$μ_f$</td>
<td>Fluid dynamic viscosity</td>
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<td>$ν_f$</td>
<td>Fluid kinematic viscosity</td>
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<tr>
<td>$ν_{p,RUM}$</td>
<td>Particle uncorrelated viscosity</td>
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<tr>
<td>$Ω_j$</td>
<td>Computational cell $j$</td>
</tr>
<tr>
<td>$Ω_{f,i}$</td>
<td>Fluid vorticity vector</td>
</tr>
<tr>
<td>$Π_p$</td>
<td>Particle SGS production term of RUE</td>
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<tr>
<td>$ρ_f$</td>
<td>Fluid density</td>
</tr>
<tr>
<td>$ρ_p$</td>
<td>Particle density</td>
</tr>
<tr>
<td>$τ_{f,ij}$</td>
<td>Instantaneous fluid stress tensor</td>
</tr>
<tr>
<td>$τ_{f,t}$</td>
<td>Fluid Lagrangian turbulent time scale</td>
</tr>
<tr>
<td>$τ_p$</td>
<td>Particle relaxation time</td>
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<tr>
<td>$ε_f$</td>
<td>Fluid dissipation</td>
</tr>
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</table>

**Non-dimensional numbers**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Pr_f$</td>
<td>Fluid molecular Prandtl number</td>
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<tr>
<td>$Re_p$</td>
<td>Particle Reynolds number</td>
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<tr>
<td>$Re_t$</td>
<td>Fluid turbulent Reynolds number</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Levy number</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
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<tr>
<td>Re</td>
<td>Fluid Reynolds number</td>
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<td>St</td>
<td>Stokes number</td>
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**Operators**

- $\langle \cdot \rangle_f$: Fluid Reynolds averaging
- $\langle \cdot \rangle_p$: Particle or dispersed phase
- $\hat{\cdot}$: Favre volume filtering
- $\tilde{\cdot}$: Mesoscopic quantity
- $\bar{\cdot}$: Volume filtering

**Subscripts**

- $f$: Fluid or carrier phase
- $p$: Particle or dispersed phase

**Shortcuts**

- AV: Artificial Viscosity
- BC: Boundary Condition
- CFD: Computational Fluid Dynamics
- DNS: Direct Numerical Simulation
- DPS: Discrete Particle Simulation
- EE: Euler-Euler
- EL: Euler-Lagrange
- FE: Finite Element
- FL: Flux Limiter
- FV: Finite Volume
- HIT: Homogeneous Isotropic Turbulence
- LDA: Laser Doppler Anemometry
- LES: Large Eddy Simulation
- LIF: Laser Induced Fluorescence
- LW: Lax-Wendroff
- NS: Navier-Stokes
- NSCBC: Navier-Stokes Characteristic Boundary Condition
- PDA: Particle Doppler Anemometry
- PDF: probability density function
- RANS: Reynolds Averaged Navier-Stokes
- RMS: Root Mean Square
- RUE: Random Uncorrelated Energy
- RUM: Random Uncorrelated Motion
- RUV: Random Uncorrelated Velocity
- SGE: Simulation aux Grandes Echelles
- SGS: Sub-Grid Scale
- SND: Simulation Numrique Directe
- THI: Turbulence Homogene Isotrope
- TTGC: Two-step Taylor-Galerkin Colin
Introduction

La présente étude a été soutenue par une Bourse de Doctorat pour Ingénieurs (BDI) du CNRS co-financée par le Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS). Dans ce cadre, j’ai pu collaborer tant avec les membres du groupe Ecoulements Et Combustion (EEC) à l’Institut de Mécanique des Fluides de Toulouse (IMFT) qu’avec les membres du groupe Computational Fluid Dynamics (CFD) du CERFACS.

Les domaines de recherche de ces deux groupes recouvrent plusieurs champs disciplinaires que sont la turbulence monophasique, la combustion turbulente et les écoulements multiphasiques à phase dispersée. Dans ce dernier domaine, de nombreux mécanismes restent à comprendre : atomisation, dispersion et évaporation d’un jet liquide dans un gaz, phénomène de concentration préférentielle des inclusions, modulation de la turbulence par ces inclusions, interaction gouttes-gouttes et gouttes-parois et modification de la combustion par la phase dispersée pour ne citer qu’eux.

Approfondir la connaissance de ces différents phénomènes est également motivé par la forte demande des groupes industriels du secteur énergétique, notamment ceux de l’automobile, de l’aéronautique et de la production d’électricité. En effet, tant dans les moteurs diesel ou à Injection Directe Essence (IDE) que dans les moteurs aéronautiques, l’injection de carburant se fait sous la forme d’un spray de gouttelettes liquides. Le principal intérêt de cette technologie réside dans la forte capacité de stockage de l’énergie sous forme chimique dans un combustible liquide, qui dépasse le pouvoir calorifique de la plupart des autres moyens de stockage chimique. Ce sont d’une part les normes toujours plus restrictives sur l’émission de polluants et d’autre part, la volonté d’augmenter l’efficacité des processus de combustion qui justifient la participation industrielle au financement de la recherche dans le domaine de la combustion diphasique turbulente.

Pour améliorer la compréhension des différents mécanismes mis en jeu dans ces procédés industriels, il est nécessaire d’accéder à un nombre considérable de grandeurs (champs de vitesse, fractions massiques, température, pression, diamètres de goutte,...). Les mesures expérimentales permettent en principe d’accéder à cet ensemble de données. Pourtant, leur coût élevé, la difficulté d’accéder à l’ensemble des grandeurs caractérisant les écoulements diphasiques réactifs et les conditions opératoires de pression et de température rendent ces mesures délicates, sinon impossibles, à mener. Elles sont ainsi de plus en plus supplantées...
par les simulations numériques, au fur et à mesure que la puissance des calculateurs croît. Il faut néanmoins préciser que la simulation numérique n’est pas, à l’heure actuelle, utilisée en tant qu’outil prédictif pour les écoulements diphasiques réactifs turbulents. Les deux approches sont complémentaires et ce sont le plus souvent les données expérimentales qui permettent aujourd’hui d’évaluer la pertinence des calculs.

Ce travail de thèse a pour principal objectif de développer et d’appliquer une nouvelle approche dans le cadre restreint des écoulements diphasiques turbulents non réactifs. Les gouttes de fuel peuvent donc être traitées comme des particules solides, indéformables, sphériques et identiques. Dans ce cas particulier, Fede (2004) s’appuie sur les travaux d’Elghobashi & Truesdell (1993) et propose une classification des écoulements gaz-particules en fonction de la fraction volumique en particules $\alpha_p$, et la fraction massique en particules $M_p$ :

- $\alpha_p < 10^{-4}$ et $M_p < 10^{-2}$ : les particules ne sont pas suffisamment inertielles pour que les collisions inter-particulaires et le couplage inverse des particules sur le gaz soient pris en compte. La dispersion des particules constitue le mécanisme prépondérant dans ce type d’écoulements diphasiques.

- $\alpha_p < 10^{-4}$ et $M_p > 10^{-2}$ : le couplage inverse, qui se traduit principalement par une réduction de l’agitation de la phase porteuse, est à considérer.

- $10^{-4} < \alpha_p < 10^{-1}$ : les collisions particules-particules et le transport par la turbulence fluide prédominent.

- $\alpha_p > 10^{-1}$ : les collisions inter-particulaires pilotent majoritairement la trajectoire des particules.

Dans cette étude, on se limite à des fractions volumique et massique en particules telles que le phénomène de dispersion domine et que le couplage inverse est à prendre en compte.

Il existe différents niveaux de résolution numérique des écoulements gaz-particules. La “vraie” Simulation Numérique Directe (SND, ou DNS en anglais) d’un écoulement diphasique à phase dispersée consiste à résoudre les équations de Navier-Stokes (NS) autour de chaque particule, en considérant toutes les échelles de la turbulence gazeuse, ainsi que les équations des milieux continus à l’intérieur de chaque particule (Hu, 1996; Cate et al., 2004; Massol, 2004). Le diamètre des particules doit ainsi être de l’ordre d’une dizaine de mailles de calcul, ce qui réduit considérablement le nombre de particules (une centaine au maximum actuellement) que l’on peut traiter. Considérant la puissance actuelle des calculateurs, la “vraie” DNS n’est par conséquent pas encore envisageable pour des géométries complexes mettant en jeu des milliards de particules. Dans ce travail, l’appellation “DNS” sera utilisée de manière abusive puisqu’elle fera uniquement référence à la résolution des équations de NS pour la phase
gazeuse sans recours aux modèles de turbulence.

Pour les applications dont les inclusions sont de diamètre inférieur à l’échelle de longueur de Kolmogorov, d’autres approches numériques sont envisageables, qui sont détaillées ci-dessous.

Dans l’approche Euler-Lagrange (EL) ou Lagrangienne, la trajectoire de chaque particule est calculée séparément (en anglais, Discrete Particle Simulation ou DPS) en effectuant un bilan des forces sur chaque particule. Tant les interactions entre les particules (loi de rebond après collision) que les interactions entre le fluide et les particules (modèles de forces, transferts de masse, quantité de mouvement, chaleur) doivent être traitées. Le gaz quant à lui, est traité par simulation eulérienne des équations de NS et plusieurs méthodes existent :

- La moins coûteuse est indéniablement la modélisation Reynolds Averaged Navier-Stokes (RANS) qui est aujourd’hui encore l’approche la plus fréquemment employée dans l’industrie. Elle repose sur une décomposition de Reynolds du champ turbulent fluide instantané suivie d’une moyenne sur l’ensemble des réalisations possibles de ce champ fluide. Les termes non fermés qui en résultent doivent ainsi rendre compte de l’ensemble des échelles du spectre turbulent. Ainsi, cette approche perd les informations relatives aux structures turbulentes instationnaires, ce qui constitue un inconvénient majeur pour l’étude des écoulements diphasiques réactifs.

- À l’extrême inverse, la DNS permet de résoudre toutes les échelles du spectre turbulent fluide, et donc de représenter de manière précise l’ensemble des structures turbulentes. Cependant, de telles simulations requièrent des maillages dont la taille de maille est inférieure à la plus petite échelle de longueur turbulente du fluide, ce qui réduit considérablement le nombre de Reynolds et limite les applications traitables par cette approche.

- La puissance actuelle des calculateurs rend la Simulation aux Grandes Echelles (SGE, ou LES en anglais) beaucoup plus accessible et permet d’étendre le champ d’applications calculables. Elle consiste à résoudre explicitement les plus grandes échelles de la turbulence et à modéliser l’effet des plus petites échelles à l’aide de modèles de sous-maille. Cette approche est aujourd’hui largement répandue pour la simulation d’écoulements monophasiques réactifs et montre une capacité manifeste à prédire des phénomènes fortement instationnaires tels que les instabilités de combustion ou les extinctions de flamme.

Considérant les écoulements diphasiques, il est indispensable d’évaluer l’impact des petites échelles de la turbulence fluide sur la trajectoire des particules. Fede & Simonin (2006) montrent que pour des particules suffisamment lourdes, les échelles plus petites que la longueur de coupure du filtre LES ont une influence mineure sur les principales caractéristiques de la
phase particulaire comme l’énergie cinétique, la dispersion et la distribution préférentielle des inclusions. L’approche LES pour la phase porteuse est alors totalement justifiée, ce qui n’est pas aussi direct pour des particules plus légères. Ainsi, de nombreux travaux sont actuellement dédiés à la modélisation de l’effet des petites échelles gazeuses sur la trajectoire des particules (Armenio et al., 1999; Pozorsky et al., 2004; Fede & Simonin, 2006). La principale limitation de l’approche EL reste son coût numérique. En effet, si une LES de la phase gazeuse est aujourd’hui réalisable dans de véritables configurations complexes, le nombre considérable de particules mis en jeu dans la phase dispersée rend l’approche EL bien trop coûteuse pour la simulation de l’écoulement diphasique. Une alternative consiste alors à considérer des particules numériques (ou parcels en anglais) qui regroupent un certain nombre de particules physiques. Des efforts de modélisation sont dans ce cas nécessaires, ce qui réduit l’intérêt de l’approche DPS qui réside dans sa faible dépendance aux modèles.


Afin de réduire le coût des simulations numériques des écoulements gaz-particules, il est possible de résoudre les équations de transport pour les premiers moments de la pdf jointe (nombre de particules par unité de volume, vitesse, énergie d’agitation,...), et non l’équation de type Boltzmann elle-même. L’inconvénient majeur de cette approche dite “modèle à deux fluides” introduite par Simonin (1996) réside dans la nécessité de disposer d’un modèle pour le moment d’ordre (n+1) afin de résoudre l’équation de transport pour le moment d’ordre (n).

Février et al. (2005) introduisent le formalisme EE (ou Eulérien) mésoscopique qui permet de coupler une description statistique de la phase particulaire à une approche DNS ou
LES de la phase gazeuse. L’introduction d’un opérateur de moyenne sur l’ensemble des réalisations particulières conditionné par une seule réalisation fluide conduit à la décomposition de la vitesse de chaque particule en une vitesse mésooscopique, ou spatialement corrélée aux vitesses des particules proches, et une vitesse décorrélée propre à chaque particule. La pdf conditionnée par la réalisation fluide suit une équation de type Boltzmann. En pratique comme pour la méthode à deux fluides, cette équation est intégrée dans l’espace des phases pour obtenir les équations de transport pour les premiers moments de la pdf conditionnée. Comme pour la méthode à deux fluides, des modèles de fermeture sont requis (Simonin et al., 2002; Kaufmann et al., 2006). Le principal avantage de cette méthode réside dans le faible coût de calcul de ces simulations puisqu’un seul et même algorithme est employé pour résoudre les équations de transport régissant les deux phases, qui sont modélisées par deux phases continues. L’inconvénient majeur de l’approche EE mésooscopique réside dans l’écriture de modèles de fermeture. Par ailleurs, l’information sur la trajectoire individuelle de chaque particule est perdue. Néanmoins, les grandeurs moyennes telles que l’entraînement de particules par une structure tourbillonnaire fluide, restent accessibles. Ces grandeurs moyennes fournissent ainsi une quantité d’information suffisante pour la compréhension des mécanismes mis en jeu dans les applications industrielles qui cadrent cette étude.

Les premières simulations numériques avec ce formalisme EE mésooscopique ont été réalisées par Kaufmann (2004) dans une Turbulence Homogène Isotrope (THI) décroissante chargée en particules solides. Le champ fluide a été simulé par DNS. Le calcul a été effectué avec une version antérieure du code AVBP_TPFEE et les résultats ont été comparés avec les résultats de simulations DNS-DPS résultant du code NTMIX-3D. Dans la perspective d’une mise en œuvre de l’approche Eulérienne mésooscopique dans des configurations industrielles type chambres de combustion aéronautiques ou moteurs à pistons, il est nécessaire d’étendre cette approche à la LES. C’est dans ce contexte que s’inscrit ce travail de thèse qui s’est effectué en étroite collaboration avec Mathieu Moreau, chercheur en thèse dans le groupe EEC de l’IMFT. L’extension à la LES de l’approche EE mésooscopique jusqu’alors développée pour la DNS.

La dérivation des équations LES eulériennes mésooscopiques s’effectue en appliquant un filtre spatial LES classique aux équations de transport DNS EE mésooscopiques de la phase dispersée. La spécificité de cette approche réside dans l’apparition de deux types de termes non fermés, ceux issus classiquement du filtrage spatial d’une part, et ceux dus à la moyenne d’ensemble d’autre part. Pour proposer des modèles de fermeture pour l’ensemble de ces termes, la méthodologie traditionnellement mise en œuvre pour modéliser des termes de sous-maille est adoptée : des modèles de fermeture sont obtenus a priori dans des configurations académiques avant d’être évalués a posteriori dans des configurations plus complexes. Les tests a priori ont été menés par Moreau (2006) qui a effectué des DPS de THI décroissantes chargées en particules avec le code NTMIX-3D. Il a par la suite filtré deux fois (moyenne d’ensemble puis filtrage volumique) les champs lagrangiens et déterminé le degré d’adéquation de différents modèles de fermeture avec la véritable mesure des termes non fermés. La présente
étude est dévolue aux tests *a posteriori* de ces modèles de fermeture dans des configurations à géométrie complexe. Les modèles proposés par Moreau (2006) sont implantés dans le code AVBP_TPF-EE pour démontrer la capacité de l’approche Eulérienne mésoscopique LES à capter les mécanismes diphasiques turbulents (en particulier les phénomènes de dispersion et de distribution préférentielle des particules) dans des géométries complexes.

Dans cette optique, le mémoire s’articule comme suit. Le premier chapitre récapitule les équations DNS résolues pour la phase porteuse et propose un panorama des diverses descriptions existantes pour la phase particulaire. La présentation de l’approche DPS insiste sur la difficulté d’implanter cette méthode dans des configurations mettant en jeu un grand nombre de particules. Les différentes approches eulériennes existantes sont ensuite présentées et l’accent est finalement mis sur l’approche Eulérienne mésoscopique. Le système d’équations régi par l’approche EE mésoscopique est difficile à mettre en œuvre numériquement non seulement parce qu’il n’existe pas de diffusion moléculaire pour les particules, mais également parce que la phase dispersée est fortement compressible, générant par conséquent de forts gradients difficiles à représenter sur une grille de calcul. Dans le deuxième chapitre, la méthode de calcul “cell-vertex” utilisée dans le code de calcul AVBP_TPF est rappelée et les deux principaux schémas numériques convectifs disponibles sont décrits. Un cas test monodimensionnel met en évidence les propriétés dispersives des deux schémas. Enfin, deux méthodes de stabilisation de ces schémas pour la phase dispersée (dissipation artificielle et limiteur de flux) sont proposées dans ce chapitre. La validation de la méthode numérique fait l’objet du troisième chapitre. Le cas test considéré est une THI décroissante chargée en particules déjà calculée par Kaufmann *et al.* (2006) avec l’approche EE mésoscopique. L’apport de la méthode numérique développée dans ce travail est mis en évidence et les champs eulériens ainsi obtenus sont comparés avec les résultats lagrangiens obtenus par Moreau (2006) avec le code NTMIX-3D.

Le quatrième chapitre est dédié à la dérivation des équations Eulériennes mésoscopiques pour l’approche LES. Le filtrage au sens LES des équations de transport pour la phase dispersée conduit à l’apparition de termes non fermés issus du filtrage spatial (comme pour la phase porteuse) et de la moyenne d’ensemble (spécificité de l’approche EE mésoscopique). Les modèles de fermeture testés *a priori* par analogie avec les écoulements monophasiques compressibles par Moreau (2006) sont présentés et les principaux résultats sont rappelés. Le premier calcul de validation de l’approche eulérienne mésoscopique étendue à la méthode LES est effectué sur un jet turbulent confiné chargé en particules (Hishida *et al.*, 1987). Dans le cinquième chapitre, les résultats pour la phase gazeuse sont tout d’abord analysés et comparés aux données expérimentales. Différentes modélisations de la condition aux limites d’entrée pour les particules sont ensuite proposées. Leur impact sur la dispersion des particules dans le jet gazeux est finalement mis en évidence. Le sixième et dernier chapitre est consacré au calcul d’un jet recirculant confiné (ou “bluff body”) chargé en particules (Borée *et al.*, 2001), plus proche d’une configuration type chambre.
de combustion aéronautique. La précision du solveur gazeux d’AVBP_TPF-EE est évaluée par comparaison avec le code de calcul CDP développé par l’université de Stanford et les données expérimentales. Enfin, l’approche LES EE mésoscopique est comparée avec l’approche DPS des codes CDP et AVBP_TPF-EL ainsi qu’avec les expériences.
Chapter 1

Transport equations for dispersed two-phase flows

Today, Reynolds-Averaged Navier-Stokes (RANS) methods are routinely solved to design industrial devices (see Jameson (1991); Lathouwers & Bellan (2001); Andreux et al. (2002)), and especially in piston engines (Boudier et al., 1992) and aeronautical combustion chambers (Montazel et al., 1992). The main advantage of these methods is their relatively low computational cost, which explains that they are used in most commercial codes. There main drawback, however, is the effort of modelisation required to capture most physical phenomena involved in such devices. Indeed, transport equations are solved only for the mean variables, and some turbulent statistical quantities (typically the turbulent kinetic energy and the dissipation rate for the $k-\varepsilon$ model). Consequently, all the unsteady and non-deterministic phenomena require modeling, which makes the results greatly dependent on the models used. This is the main reason why much work is now devoted to the development of Large-Eddy Simulation (LES) methods (Caraeni et al., 2000; Forkel & Janicka, 2000; Mahesh et al., 2004; Moureau et al., 2005) that give access to the unsteady large scales of the gas flow in such industrial devices. In comparison with Direct Numerical Simulation where all the scales of turbulence are resolved, only the large turbulent scales are resolved in LES while the small ones are modeled. Thus, LES is less CPU-consuming than DNS and the importance of modeling is reduced compared to RANS methods. Their potential of LES is illustrated when predicting combustion instabilities (Selle et al., 2006) or pollutant emissions (Schmitt et al., 2007) for instance.

Extension of LES to reactive two-phase flows still remains a challenge. Indeed, additional computational cost due to the resolution of the dispersed phase is not negligible. Therefore, RANS methods are still commonly used because resolution of the two phases can be done in a weak procedure. This means that these methods first bring the gas flow to convergence, then the solid particles and finally iterate until both phases converge. Focusing on combustion chambers, modeling the dispersed phase accurately is however of great importance since it notably
influences the flame structure as well as the combustion mode. Considering the success of LES of gaseous flows and flames, it is interesting to extend this method to two-phase flows. It is a difficult task for two main reasons. First, the number of droplets involved in such devices is considerable (the typical order of magnitude is $10^8$ in a combustion chamber) and requires the use of an accurate numerical method which maintains the efficiency of the solver used. Then, the physics of a liquid fuel spray are of a very complex nature and are not yet well understood. Among them, atomization of the liquid fuel jet, turbulent dispersion of the resulting droplets, their interaction with each other and with the walls, their evaporation and finally combustion are essential phenomena that often occur at subgrid scales and so, require modeling. These two points influence the method chosen to numerically solve two-phase flows and work has still to be done for DNS of two-phase flows before performing LES of two-phase flows.

In the Lagrangian approach described in Section 1.3, the individual trajectory of million of droplets created by standard injectors is followed. It is the most intuitive method and besides, it requires few modeling. Efforts of modelisation however increase when the number of droplets required to predict accurately the physical phenomena involved is very large. In this case, the stochastic Lagrangian approach is preferred (Sankaran & Menon, 2002; Apte et al., 2003a; Ham et al., 2003). Each tracked particle is only a “numerical” one and actually represents a statistically homogeneous group of real particles that requires modeling. Still, difficulty of the Lagrangian approach is its numerical implementation for parallel computers (García et al., 2005).

An alternative is the Eulerian approach where the dispersed phase is treated as a continuous phase. Thus, the gas phase algorithm may be used on the dispersed phase with the same numerical accuracy and computational efficiency. For this approach, modeling remains the main challenge. Nevertheless, for very low-inertia particles, modeling effort is low since such particles behave nearly as passive scalars, and so nearly follow the fluid flow. Ferry & Balachandar (2002) and Rani & Balachandar (2003) show that very accurate results can be obtained using the Equilibrium approach (see Section 1.4), only by solving a transport equation for the particle number density and using a Taylor extension of the fluid velocity to predict the particle one. When the particles become heavier, their response time to turbulent fluctuations increases and this method reaches its limits. It becomes then necessary to also solve a transport equation for the particle velocity. The first approach consists in volume averaging (Whitaker (1999)) and is described in Section 1.4. The second one is based on ensemble averaging (Simonin, 1991; Février et al., 2005) and referred in the manuscript as the Euler-Euler (EE) mesoscopic approach. Since this approach has been chosen for this work, it is described in details in Section 1.5.

As this work is devoted to the modeling of particle dispersion, all the approaches presented hereafter are restricted to this specific case. Extension to evaporating colliding droplets is however possible. In Section 1.2, a brief review of the forces acting on a particle is given. In this chapter, only the transport equations for Direct Numerical Simulation (DNS) are focused on. Before dealing with the dispersed phase, the fluid transport equations limited to non reactive gas flows that remain the same for all the approaches are focused on in Section 1.1.
1.1 The gas flow

In this section the compressible Navier-Stokes equations are quickly described (as found in fundamental CFD text books such as Anderson (1990) or Hirsch (1988)). Transport equations used for DNS are focused on.

The set of conservation equations describing the evolution of a compressible fluid flow without any chemical reaction reads:

\[ \frac{\partial}{\partial t} \rho_f + \frac{\partial}{\partial x_m} \rho_f u_{f,m} = 0 \] (1.1)

\[ \frac{\partial}{\partial t} \rho_f u_{f,i} + \frac{\partial}{\partial x_m} \rho_f u_{f,i} u_{f,m} = -\frac{\partial}{\partial x_m} [P_f \delta_{im} - \tau_{f,im}] \] (1.2)

\[ \frac{\partial}{\partial t} \rho_f E_f + \frac{\partial}{\partial x_m} \rho_f E_f u_{f,m} = -\frac{\partial}{\partial x_m} [u_{f,i} (P_f \delta_{im} - \tau_{f,im}) + q_{f,m}] \] (1.3)

In Eqs. (1.1) – (1.3) respectively corresponding to the conservation laws for fluid density, momentum and total energy, the following symbols, \( \rho_f, u_{f,i}, E_f \) denote respectively the fluid density, velocity vector and total energy.

It is usual to decompose the flux tensor into an inviscid \( \mathcal{F}_I \), and a viscous component \( \mathcal{F}_V \). They are respectively noted for the three conservation equations:

\[ \mathcal{F}_I = \begin{pmatrix} \rho_f u_{f,i} u_{f,m} + P_f \delta_{im} \\ \rho_f E_f + P_f \delta_{im} u_{f,m} \\ \rho_f u_{f,m} \end{pmatrix} \] (1.4)

\[ \mathcal{F}_V = \begin{pmatrix} -\tau_{f,im} \\ -(u_{f,i} \tau_{f,im}) + q_{f,m} \end{pmatrix} \] (1.5)

where the hydrostatic pressure \( P_f \), is given by the equation of state for a perfect gas:

\[ P_f = \rho_f \frac{\mathcal{R}}{W_f} T_f, \] where \( \mathcal{R} = 8.3143 \text{ J/mol.K} \) is the universal gas constant and \( W_f \) is the fluid molecular weight.

The fluid stress tensor \( \tau_{f,im} \) is given by the following relations:

\[ \tau_{f,im} = 2 \mu_f \left( S_{f,im} - \frac{1}{3} \delta_{im} S_{f,ll} \right) \] with \( S_{f,im} = \frac{1}{2} \left( \frac{\partial u_{f,m}}{\partial x_i} + \frac{\partial u_{f,i}}{\partial x_m} \right) \) (1.6)

where \( \mu_f \) is the fluid dynamic viscosity.

Finally, the heat flux vector \( q_{f,m} \) follows the classical Fourier law,

\[ q_{f,m} = -\lambda_f \frac{\partial T_f}{\partial x_m}, \] (1.7)
where $\lambda_f$ is the fluid heat conduction coefficient that can be computed by introducing the fluid molecular Prandtl number $P_{r,f}$, as:

$$\lambda_f = \frac{\mu_f C_p}{P_{r,f}}$$  \hspace{1cm} (1.8)

with $P_{r,f} = 0.7$ supposed as constant in time and space and $C_p$ the fluid heat capacity.

## 1.2 Forces acting on an isolated particle

The first analytical work on particle motion in a turbulent field was performed by Tchen (1947), who took the equation for particle motion derived by Boussinesq (1885), Basset (1888) and Oseen (1927) and applied it to a particle in a homogeneous turbulent field. The analysis accounted for Stokes drag, pressure gradient force, added mass, and Basset force. More recently, Maxey & Riley (1983) brought some corrections to the transport equation proposed by Tchen (1947). In Section 1.2.1, a brief review of the forces acting on an isolated particle is presented, according to the two main works quoted above. Section 1.2.2 summarises the forces accounting for in this work.

### 1.2.1 Review of the different forces

The study is restricted to spherical and rigid particles with constant diameter $d_p$, and constant density $\rho_p$. Since cold dilute flows are focused on in this work, neither inter-particle collisions nor evaporation are accounted for hereafter. Following Maxey & Riley (1983) (who assumed that the particle diameter and the fluid smallest turbulent length scales are of the same order of magnitude) and Gatignol (1983) (who did not restrict the particle size), the equation for particle $k$ animated with velocity $v^{(k)}_p$ reads:

$$\frac{\pi d^3_p}{6} \frac{d v^{(k)}_p}{dt} = F^{unp}_{p,i} + F^p_{p,i},$$  \hspace{1cm} (1.9)

where $d/dt$ is the local derivative following the moving particle. The force acting on the particle $k$ is decomposed into two contributions: $F^{unp}_{p,i}$ stands for the force that would act on the fluid if it were to exist in the volume occupied by the particle whereas $F^p_{p,i}$ represents the perturbation of the fluid velocity field due to the presence of the solid particle.

- **$F^{unp}_{p,i}$ force term**

The $F^{unp}_{p,i}$ force term implies that the acceleration that would have been given to the gas,
because of the pressure and the viscous stresses transferred from the neighboring gas, is transmitted as a force on the particles. It also accounts for buoyancy effects. Maxey & Riley (1983) and Gatignol (1983) suggested:

$$ F_{ unp}^{p} = \frac{\pi d_p^3}{6} \left[ \rho_f \frac{Du_{f@p}}{Dt} + (\rho_p - \rho_f) g i \right], \quad (1.10) $$

where the first term accounts for pressure and viscous stresses and the second one stands for buoyancy effects. \( u_{f@p} \) is the fluid velocity sampled along particle trajectories and satisfies the fluid Navier-Stokes equations given by Eqs. (1.1)–(1.3).

- **\( F_{ p,i}^{p} \) force term**

The \( F_{ p,i}^{p} \) force term stands for the aerodynamic forces that are detailed below:

- **Drag force**

The drag force noted \( F_D \), accounts for pressure and viscous stresses that exercise on the particle surface and yields:

$$ F_D = \frac{3}{4} \rho_f \frac{\pi d_p^3}{6} \frac{1}{d_p} C_D | u_{f@p} - v_p | \left( u_{f@p} - v_p \right) \quad (1.11) $$

Determination of the drag coefficient \( C_D \) in Eq. (1.11) depends on the particle Reynolds number that reads:

$$ Re_p = \frac{d_p | u_{f@p} - v_p |}{\nu} \quad (1.12) $$

where \( \nu \) is the fluid kinematic viscosity.

Another way to write the drag force consists in introducing the particle response time \( \tau_p \), defined as:

$$ \tau_p = \frac{4 \rho_p d_p}{3 \rho_f C_D} | u_{f@p} - v_p | \quad (1.13) $$

Then, the drag force yields:

$$ F_D = \frac{m_p}{\tau_p} \left( u_{f@p} - v_p \right) \quad (1.14) $$

where \( m_p \) is the particle mass.
The three main relations used for the drag coefficient are summarised in Table 1.1. For very small particle Reynolds numbers $Re_p << 1$, Stokes (1851) developed an analytical solution given by Eq. (1.15). For larger particle Reynolds numbers $Re_p < 1000$, Clift et al. (2004) proposed a semi-empirical extension of Eq. (1.15) detailed in Eq. (1.16). Finally, for even larger particle Reynolds numbers $Re_p > 1000$, the drag coefficient is unaffected by the wake shape behind the particle, leading to a constant value given by Eq. (1.17).

<table>
<thead>
<tr>
<th>$Re_p$</th>
<th>Equation</th>
<th>$C_D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re_p &lt;&lt; 1$</td>
<td>$\frac{24}{Re_p}$ (1.15)</td>
<td>24</td>
</tr>
<tr>
<td>$Re_p &lt; 1000$</td>
<td>$\frac{24}{Re_p} \left(1 + 0.15Re_p^{0.687}\right)$ (1.16)</td>
<td>0.44</td>
</tr>
<tr>
<td>$Re_p &gt; 1000$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1.1 - Relations for the drag coefficient $C_D$, depending on the particle Reynolds number $Re_p$.

– Added-mass force

Acceleration of the particle is at the origin of the added-mass force, noted $F_{AM}$. It accounts for the fluid inertia in the boundary layer and wake of the particle, which makes the fluid accelerate in the neighboring of the particle that accelerates itself. Many studies have focused on expliciting the added-mass force term (see Magnaudet et al. (1995) for instance) that usually reads:

$$F_{AM} = \frac{\pi d_p^3}{6} \rho_f C_m \left(\frac{Du_f @ p}{Dt} - \frac{dv_p}{dt}\right) \quad \text{with} \quad C_m = 0.5$$

(1.18)

– History (or Basset) force

The History, or Basset force $F_H$, is linked to the memory of the particle, that is to say the history of its past accelerations. It reads:

$$F_H = \frac{\pi d_p^3 \rho_f}{6} \int_0^\infty \frac{d}{d\tau} (u_f @ p - v_p) \frac{d\tau}{\sqrt{t-\tau}}$$

(1.19)

– Lift force

The lift force $F_L$, must be accounted for when the particle is big enough to see a velocity field with a velocity gradient from one side to the other. This can occur in a shear layer for instance. The lift force is due to the fluid vorticity $\Omega_f$, and yields:

$$F_L = \frac{\pi d_p^3}{6} \rho_f C_L (u_f @ p - v_p) \times \Omega_f$$

(1.20)

Note that another lift force must be considered when the particle shows a rotating motion. The Magnus effect can for instance be non-negligible in a turbulent channel flow when inter-particle collisions play a significant role.
1.2.2 Forces accounting for in this study

Hinze (1975) and Desjonqueres et al. (1986) among others have studied the influence of the above forces (pressure gradient, drag, added-mass and Basset forces more exactly) on the particle motion. Particularly, they have shown that for $\rho_p/\rho_f > 1000$, the pressure gradient and the added-mass forces as well as the History force are negligible compared to the particle agitation and dispersion mechanisms. More recently, Elghobashi & Truesdell (1993) showed that these two mechanisms are mainly due to drag force and gravity performing DNS of particle-laden HIT flows.

In this work, solid spherical particles with diameter equal or smaller than the Kolmogorov length scales and density much larger than the fluid one are considered. Consequently, only the drag force and the gravity are accounted for in the rest of the manuscript. Concerning the drag force, either the correlation introduced by Stokes (1851) (see Eq. (1.15)) or the correction proposed by Schiller & Nauman (1935) is used, depending on the dispersed phase characteristics.

1.3 Euler-Lagrange approach: Discrete Particle Simulation (DPS)

The Euler-Lagrange (EL) approach, also referred as Discrete Particle Simulation (DPS), has been widely used to study gas-solid flows (Tchen, 1947; Hinze, 1975; Desjonqueres et al., 1986; Squires & Eaton, 1990; Deutsch & Simonin, 1991; Druzhinin, 1995; Boivin et al., 1998; Février et al., 2005; Moreau, 2006) in academic configurations. The main reason is that it requires few modeling efforts, as shown when presenting the equations to solve in Section 1.3.1. Numerical handling of these equations can however become difficult when high-order statistics are analysed. Indeed, a large amount of particle trajectories must then be solved, which considerably increases the computational cost of the EL approach. Application to more complex geometries showing complex coupling between both phases is even less frequent (Ham et al., 2003; Riber et al., 2006). Not only the number of particles required but also numerical aspects linked to the use of massively parallel machines arise. Section 1.3.2 summarises the main difficulties.

1.3.1 Particle transport equations and definition of useful quantities

Restricting to drag and gravity (see Section 1.2.1), the coordinate $\mathbf{x}_p^{(k)}$ and the Lagrangian velocity $\mathbf{v}_p^{(k)}$ of the individual particle with index $k$ are advanced in time with the following set of
TRANSPORT EQUATIONS FOR DISPERSED TWO-PHASE FLOWS

equations:
\[ \frac{d\mathbf{x}_p^{(k)}}{dt} = \mathbf{v}_p^{(k)} \] (1.21)
\[ \frac{d\mathbf{v}_p^{(k)}}{dt} = \frac{1}{\tau_p \left(1 + 0.15 R_{\text{e}_p}^{0.687}\right)} \left( \mathbf{u}_{f,p} - \mathbf{v}_p^{(k)} \right) + \mathbf{g} \] (1.22)

Equation (1.22) requires the fluid velocity at the location of the particle \( k \), although it is an Eulerian field computed at the computational nodes of the domain. Special care has to be taken to evaluate \( u_{f,p} \) and high order interpolation methods are necessary to ensure a minimal error (Pope, 1994).

- **Useful lagrangian quantities**

The averaging operator associated with particle-phase is noted \( < \cdot >_p \) and defined for the Lagrangian quantity \( \Phi \) as:

\[ < \Phi^{(k)} >_p = \frac{1}{N_p} \sum_{k=1}^{N_p} \Phi^{(k)} \] (1.23)

where \( N_p \) is the total number of particles.

Then, the particle kinetic energy \( q_{p}^2 \), and the fluid-particle correlation \( q_{f,p} \), yield:

\[ q_{p}^2 = \frac{1}{2} \left< \mathbf{v}_p^{(k)} \cdot \mathbf{v}_p^{(k)} \right>_p \] (1.24)
\[ q_{f,p} = \left< \mathbf{v}_p^{(k)} \cdot \mathbf{u}_{f,p} \left( \mathbf{x}^{(k)} \right) \right>_p \] (1.25)

As for the gas phase, the fluid turbulent kinetic energy \( q_f^2 \) can be defined using the classical Reynolds averaging (Hinze, 1975) noted \( < \cdot >_f \):

\[ q_f^2 = \frac{1}{2} \left< \mathbf{u}_f' \cdot \mathbf{u}_f' \right>_f \] (1.26)

where \( \mathbf{u}_f' \) is the fluctuating part of the fluid velocity \( \mathbf{u}_f \).

- **Tchen’s theory**

When studying stationnary particle-laden HIT flows, Tchen (1947) proposed to link the three previous quantities through the two following relations:

\[ q_{f,p} = \frac{2}{1 + St} q_f^2 \] (1.27)
\[ 2q_p^2 = q_{f,p} \] (1.28)
1.3 Euler-Lagrange approach: Discrete Particle Simulation (DPS)

with $St = \tau_p / \tau_f'$ and $\tau_f'$ the Lagrangian turbulent time-scale (Haworth & Pope, 1986). The establishment of Eqs. (1.27) & (1.31) requires two main assumptions. First, the aerodynamic force acting on the particles must consist of Stokes drag given by Eq. (1.15) only. Second, the relative velocity between the particle and the fluid must be very small.

**Deutsch & Simonin’s extended theory**

This second assumption is restrictive and Deutsch & Simonin (1991) proposed an extension of Tchen’s theory using the fluid velocity along particle trajectories $\mathbf{u}_{f@p}$ introduced in Section 1.2.1. Consequently, the fluid turbulent kinetic energy sampled along particle trajectories, $q^2_{f@p}$, is defined as:

$$q^2_{f@p} = \frac{1}{2} \left\langle \mathbf{u}'_{f@p} \cdot \mathbf{u}'_{f@p} \right\rangle_p$$  \hspace{1cm} (1.29)

$$q_{fp} = \frac{2}{1 + St'} q^2_{f@p}$$  \hspace{1cm} (1.30)

$$2 q^2_p = q_{fp}$$  \hspace{1cm} (1.31)

where $St' = \tau_p / \tau_{f@p}'$ is a modified Stokes number accounting for the time-scale $\tau_{f@p}'$. Note that in the limit of very small Stokes numbers ($St \rightarrow 0$), the two time-scales, $\tau_{f@p}'$ and $\tau_f'$, tend to the same value. Since $\tau_{f@p}'$ and $q^2_{f@p}$ are still difficult to quantify, Eqs. (1.27) & (1.31) are often used as a first approximation to evaluate $q^2_p$.

1.3.2 Numerical implementation

As shown above, the EL approach requires few modeling efforts in the restricted case of the present work. Actually, the main issue is its numerical implementation. Indeed, most of the time, a large number of particle trajectories must be solved to accurately predict the dispersed phase. This is true both for academic configurations and for more complex geometries. In the first case, the EL approach is mainly used either to understand complex phenomena (preferential concentration, modification of the turbulence by the particles for instance) or to propose models for Eulerian formulations (Février et al., 2005; Vance et al., 2006; Moreau, 2006). This requires accurate quantification of high-order statistics. Therefore, a great number of particles are required in the domain to obtain meaningful averaged quantities. For instance, Moreau (2006) shows than 80 millions of particles are required in a particle-laden decreasing HIT flow performed on a $64^3$ cells grid to obtain accurate particle velocity spectrum. This increases dramatically both the computational cost of DPS and the size of the data files to
Performing DPS in industrial devices such as aeronautical combustion chambers is even more difficult and only few work (Ham et al., 2003; García et al., 2005; Riber et al., 2006) has been published up to now. There are at least two main issues. First, the particles are often not real particles but parcels that contain thousands of real particles because present computers cannot handle the millions of droplets that emerge from real fuel injectors. Therefore, models are required for these parcels, which sometimes makes modeling more delicate (Moin, 2004). Secondly, calculations of these complex geometries require parallel computers because of the considerable number of grid points.

In terms of parallelisation, the complexity of the implementation of the EL approach significantly increases because the method requires the coupling of two very different solvers. Two methods may be used (García et al., 2005). The first one consists in task parallelisation where some processors are devoted to the gas phase and others to the dispersed phase. Droplets must then be exchanged between processors when they leave a subdomain for an adjacent one. The second method is domain partitioning where all the processors compute both phases on a smaller subdomain and then exchange information on the subdomain frontier for both phases. With combustion devices in prospect, only domain decomposition can be considered because task parallelisation would require the exchange of very large three-dimensional data sets at each iteration between all the processors. Considering domain decomposition, the main difficulties lie in the location of the droplets and their distribution varying with space and time in the domain. Indeed, most of the droplets remain close to the injector tip due to large fluid recirculation zones and those traveling farther in the chamber quickly evaporate. As a result, dynamic load balancing strategies must be worked on to redecouple the domain depending on the particle distribution to keep a reasonable speedup.

Despite the development of powerful and massively parallel computers, performing DPS is still challenging and very expensive. It is one reason why some authors focus on Euler-Euler methods that exhibit conservation equations for the dispersed phase very similar to the Navier-Stokes equations for the gas phase. One possibility consists in volume filtering a two-phase flow realization. This Euler-Euler volume filtering approach presented in Section 1.4 shows very good results for particles with low inertia that follow almost the fluid. On the contrary, when the inertia of the particles is much higher, the particle motion is much more independent of the gas phase and two motions described as correlated and uncorrelated by Février et al. (2005) are exhibited. An ensemble averaging is introduced to account for this decomposition and EE mesoscopic transport equations are derived for the dispersed phase. Those are detailed in Section 1.5.
1.4 Euler-Euler volume filtering approaches

The Euler-Euler volume filtering approach assumes the existence of Navier-Stokes equations (see Eqs. (1.1)–(1.3)) for both the gas and the dispersed phases. It is based on spatial filtering of a two-phase flow realization and is therefore close to spatial filtering in the sense of Large-Eddy Simulation (LES) detailed in Chapter 4. The principle of this approach is quickly presented in Section 1.4.1. Druzhinin & Elghobashi (1998) are the first authors using the resulting set of equations, refered as the two-fluid model. The equations to solve for the dispersed phase as well as the assumptions required to derive them are summarised in Section 1.4.2. A variant of the two-fluid approach was proposed by Ferry & Balachandar (2001) and is summarised in Section 1.4.3. The so-called Eulerian equilibrium approach considers a transport equation for the particle number density only and uses a Taylor expansion of the fluid velocity to determine the particle velocity.

1.4.1 Principle

A convolution product of the unfiltered quantity, \( \Phi \), with the spatial filter function, \( G_\Delta \), in the whole domain, leads to the filtered quantity, \( \bar{\Phi} \):

\[
\bar{\Phi}(x) = \int G_\Delta(x-x') \Phi(x') \, dx',
\]  

(1.32)

where the filter characteristic length is \( \Delta \). To simplify, the following averaging properties are assumed:

- **Linearity:**
  \[
  \bar{\Phi + \lambda \Psi} = \bar{\Phi + \lambda \Psi},
  \]  
  (1.33)

where \( \Phi \) and \( \Psi \) are two quantities varying in space and time, and \( \lambda \) is a constant. Note that to ensure \( \bar{\lambda} = \lambda \), the filter kernel must satisfy: \( \int G_\Delta(x) \, dx = 1 \).

- **Idempotence:**
  \[
  \bar{\Phi \Psi} = \bar{\Phi} \bar{\Psi}
  \]  
  (1.34)

- **Commutation with derivative operators:**
  \[
  \frac{\partial \bar{\Phi}}{\partial t} = \frac{\partial \bar{\Phi}}{\partial t}
  \]  
  (1.35)

\[
\frac{\partial \bar{\Phi}}{\partial x_i} = \frac{\partial \bar{\Phi}}{\partial x_i}
\]  

(1.36)
All the variations of $\phi$ that occur at a length scale smaller than $\Delta$ are contained in the quantity $\phi'$ defined as:

$$\phi' = \phi - \bar{\phi} \quad (1.37)$$

As a consequence, if the smallest scales of variations of $\phi$ are much larger than the filter length $\Delta$, the quantity $\phi'$ is zero and the separation of scales is total. On the contrary, $\phi'$ is non-zero and unclosed terms due to the non-linear terms arise in the transport equations.

### 1.4.2 Two-fluid approach

The two-fluid approach was originally developed by Druzhinin & Elghobashi (1998) when performing a DNS of bubble-laden isotropic decaying turbulence. The set of equations is obtained by spatially averaging the instantaneous equations of the carrier flow and bubble (or particle) phase over a scale of the order of the Kolmogorov length scale. Thus, the filter length is much larger than the particle diameter. This is the main assumption in this formulation: the filter length must be not only significantly larger than the particle diameter so that the averaging is meaningful, but also smaller than the smallest length scale in the particle velocity field to ensure unicity of the particle velocity in the filtering volume. Note that one-way coupling between the two phases is not a necessary assumption to derive the set of equations.

The transport equations for the gas phase used by Druzhinin & Elghobashi (1998) are very similar to Eqs. (1.1)–(1.3). The only difference is the two-way coupling term through drag force in the gas momentum equation. As for the dispersed phase, two transport equations for particle number density and particle velocity are considered:

$$\frac{\partial}{\partial t} n_p + \frac{\partial}{\partial x_j} n_p u_p,j = 0 \quad (1.38)$$

$$\frac{\partial}{\partial t} u_{p,i} + u_{p,j} \frac{\partial}{\partial x_j} u_{p,i} = g_i - \frac{1}{\tau_p} (u_{p,i} - u_{f,i}) \quad (1.39)$$

The computational cost of such simulations is low compared to DPS because the same algorithms are used to solve the transport equations for both phases. In terms of results, the two-fluid approach shows good results for particles with small Stokes numbers moving in the decaying HIT flow considered. Especially, the phenomenon of preferential accumulation of bubbles in the high-enstrophy regions of the fluid flow is accurately predicted, as shown by comparisons with analytical solutions. Nevertheless, the method fails for larger Stokes numbers when particles are more inertial and more independant of the gas phase.
1.4.3 Eulerian equilibrium approach

Ferry & Balachandar (2001) introduced the Eulerian equilibrium approach that reduces the number of transport equations to be solved. Indeed, only the transport equation for particle number density (see Eq. (1.38)) is solved while the particle velocity is given by the expansion in $\tau_p$ of the local fluid quantities (velocity and its spatial and temporal derivatives) proposed first by Maxey (1987):

$$u_{p,i} = u_{f,i} - \tau_p \frac{D u_{f,i}}{Dt} + O\left(\tau_p^2\right), \quad (1.40)$$

where $D/Dt = \partial/\partial t + u_{f,j} \partial/\partial x_j$ is the local derivative following the fluid element. Thus, the particle velocity field approaches a unique, equilibrium field, independent of the initial conditions. Eq. (1.40) was then extended by Druzhinin (1995) to second-order, and even later by Ferry & Balachandar (2001) to mass-added, rotational lift and Basset forces. Only the mass-added force was shown necessary to account for in the first order approximation.

The computational cost of the Eulerian equilibrium approach is even lower than for the two-fluid approach since only one transport equation for the particle number density has to be solved. For small particle relaxation times, this method presents good agreements with DPS results when focusing on preferential concentration. This was shown in a HIT flow with or without accounting for gravity (Maxey, 1987), as well as in a turbulent channel flow (Rani & Balachandar, 2003). However, the errors in the predictions of the particle field increase with the particle response time (Rani & Balachandar, 2004), which is due to the Taylor expansion in $\tau_p$ of the particle velocity.

1.5 Euler-Euler mesoscopic approach

A reason why the simulations performed with the EE volume filtering approaches failed for high-inertia particles was first proposed by Février et al. (2005). The authors suggested to split the motion of the particles into a correlated and an uncorrelated motion, this latter becoming non-negligible for very inertial particles. A definition of both motions is given in Section 1.5.1 following Février et al. (2005). The mesoscopic formalism based on a conditional ensemble averaging is presented in Section 1.5.2 before the transport equations for the dispersed phase are derived in Section 1.5.3. The ensemble averaging leads to unclosed terms whose modeling is focused on in Section 1.5.4. Finally, the system of transport equations considered in the present work is summarised in Section 1.5.5.
Figure 1.1 - Instantaneous fluid and particle velocity vectors in a single plane of a DNS of forced isotropic turbulence for increasing Stokes numbers (based on the fluid Lagrangian integral time scale) : a. $St = 0.13$, b. $St = 2.17$. (Février et al., 2005)

1.5.1 Definitions of correlated and uncorrelated motions

Numerous studies in gas-solid turbulent flows have focused on preferential concentration of particles into regions of low vorticity and/or high strain rate (Squires & Eaton, 1991b; Rouson & Eaton, 2001; Rani & Balachandar, 2004; Picciotto et al., 2005a). Interactions between the dispersed and the continuous phases are at the origin of such a specific structure in the particle number density field. However, these interactions also induce correlations in the velocities of neighboring particles and two asymptotic behaviors emerge. Those are illustrated by Février et al. (2005) when carrying out DPS of particle-laden isotropic turbulence.

In practice, there is a delay noted $\tau_p$, before the particles react towards fluid variations. When this relaxation time is small compared to a characteristic time scale of the fluid variations (the ratio defines the Stokes number $St$ already introduced by Tchen (1947), see Section 1.3.1), velocities of neighboring particles are correlated through the same fluid velocity field. This is illustrated by Fig. 1.1a, where the particle and fluid velocity vectors are very similar. In contrast, Fig. 1.1b. shows particle and fluid velocity vectors for very inertial particles. In this case, the correlation between neighboring velocities is much smaller because particles take more time to react to the fluid variations and so, come from very distant and independant fluid regions. Consequently, very different spatial features can be observed in the particle velocity field as well as in the particle number density field, depending on the Stokes number.

Another way to put forward such a behavior is to consider the particle-particle spatial velocity correlation. For a stationnary homogeneous isotropic turbulence, Février et al. (2005) plots the
normalised longitudinal component (see Fig. 1.2) defined as:

\[
F_{pp}^p(r) = \frac{\left\langle v_{p,i}^{(m)}(t) v_{p,i}^{(n)}(t) \mid x = x_p^{(m)}(t); x + re_i = x_p^{(n)}(t) \right\rangle}{\frac{2}{5}q_p^2},
\]

(1.41)

where \(q_p^2\) is the macroscopic particle kinetic energy and \(< \cdot >\) is the averaging operator defined over a large number of two-phase flow realizations. For low-inertia particles, the particle two-point spatial velocity correlation is very close to the one describing fluid turbulence (Hinze, 1975). It can therefore be accurately modeled by a decaying exponential. In contrast, large-inertia particle motion is statistically equivalent to a Brownian motion with independant random velocities (Abrahamson, 1975) and can then be described using kinetic theory (Reeks, 1991). Consequently, the particle field is not spatially-continous in this limit.

Figure 1.2 - Influence of particle inertia on the longitudinal Eulerian spatial correlation function (See Eq. (1.41)) of particles suspended in isotropic turbulence. Curves in the figure correspond to different Stokes numbers (based on the fluid Lagrangian integral time scale): \(\circ\): \(St = 0.05\); \(+\): \(St = 0.3\); \(\Box\): \(St = 1.47\); \(\triangle\): \(St = 3.4\); \(*\): \(St = 4.83\). (Février et al., 2005)

Such observations are at the origin of the Eulerian mesoscopic formalism developed by Février et al. (2005).
1.5.2 Conditional averaging procedure and mesoscopic quantities

The starting point is the introduction of the function $W_p$, that describes the dynamics of particles with respect to time in the phase space. In this work, only the position and velocity of the particle are considered. Nevertheless, this formalism can be extended to other particle quantities, such as temperature or mass for instance (Simonin, 1996).

\[ W_p^{(k)}(x, c_p, t) = \delta \left( x - x_p^{(k)}(t) \right) \delta \left( c_p - u_p^{(k)}(t) \right), \]  

where $\delta$ is the Dirac function. The originality comes from the specific ensemble averaging of this function $W_p$. Indeed, the Eulerian mesoscopic formalism is based on the chaotic behaviour of inertial particles in a given turbulent fluid flow. Thus, for a given fluid flow realization $\mathcal{H}_f$, a large number of particulate flow realizations can be initialised slightly differently, yielding the same statistics at finite time. Applying the ensemble averaging over this large number of particulate flow realizations $\mathcal{H}_p$, conditioned by the fluid flow realization $\mathcal{H}_f$, to the function $W_p$ defines the particle probability density function (pdf), $\tilde{f}_p$:

\[ \tilde{f}_p(c_p, x, t|\mathcal{H}_f) = \lim_{N_p \to \infty} \left[ \frac{1}{N_p} \sum_{N_p} \sum_{k=1} W_p^{(k)}(x, c_p, t, \mathcal{H}_p|\mathcal{H}_f) \right]. \]  

Then, the probable number of particles, whose center of mass at time $t$ is located in the volume $[x, x + dx]$, and with a translation velocity $u_p$ in $[c_p, c_p + dc_p]$, is: $\tilde{f}_p(c_p, x, t|\mathcal{H}_f) dx dc_p$.

Integration of the conditioned pdf $\tilde{f}_p$, over particle velocity space gives access to the moments of the pdf that are particle Eulerian mesoscopic quantities. The first five moments are the particle number density, $\bar{n}_p$, the particle mesoscopic velocity, $\bar{u}_p$, and the particle 2nd, 3rd and 4th order random uncorrelated velocity correlations, respectively noted $\delta\bar{R}_{p,ij}$, $\delta\bar{S}_{p,ij}$ and $\delta\tilde{M}_{p,ijkl}$. They read:

\[ \bar{n}_p(x, t|\mathcal{H}_f) = \int \tilde{f}_p(c_p, x, t|\mathcal{H}_f) dc_p, \]  

\[ \bar{u}_{p,i}(x, t|\mathcal{H}_f) = \frac{1}{\bar{n}_p} \int c_{p,i} \tilde{f}_p(c_p, x, t|\mathcal{H}_f) dc_p, \]  

\[ \delta\bar{R}_{p,ij}(x, t|\mathcal{H}_f) = \frac{1}{\bar{n}_p} \int \delta c_{p,i} \delta c_{p,j} \tilde{f}_p(c_p, x, t|\mathcal{H}_f) dc_p, \]  

\[ \delta\bar{S}_{p,ijk}(x, t|\mathcal{H}_f) = \frac{1}{\bar{n}_p} \int \delta c_{p,i} \delta c_{p,j} \delta c_{p,k} \tilde{f}_p(c_p, x, t|\mathcal{H}_f) dc_p, \]  

\[ \delta\tilde{M}_{p,ijkl}(x, t|\mathcal{H}_f) = \frac{1}{\bar{n}_p} \int \delta c_{p,i} \delta c_{p,j} \delta c_{p,k} \delta c_{p,l} \tilde{f}_p(c_p, x, t|\mathcal{H}_f) dc_p, \]

where the notation $\delta c_{p,i} = c_{p,i} - \bar{u}_{p,i}$ is introduced.
1.5 Euler-Euler mesoscopic approach

As a consequence, the Lagrangian velocity of each individual particle \( k \), can be split into two contributions:

\[
\mathbf{u}_p^{(k)}(t) = \bar{\mathbf{u}}_p(x_p^{(k)}(t), t) + \delta \mathbf{u}_p^{(k)}(t) \tag{1.49}
\]

where \( \delta \mathbf{u}_p^{(k)}(t) \) is the residual velocity component, or Random Uncorrelated velocity (RUV), of the particle \( k \). As the particle mesoscopic velocity is defined in the Eulerian framework, it can be considered as a velocity shared by all the particles in the system. Therefore, it provides a description of the spatial structure of the velocity field and is often called “correlated” velocity. On the contrary, \( \delta \mathbf{u}_p^{(k)}(t) \) is a Lagrangian quantity, like \( \mathbf{u}_p^{(k)}(t) \), and therefore is defined for each individual particle along trajectories.

The definition of the total turbulent kinetic energy \( q_p^2 \), the correlated kinetic energy \( \bar{q}_p^2 \) and the Random Uncorrelated Energy (RUE) \( \delta q_p^2 \), is then straightforward. \( \bar{q}_p^2 \) accounts for the correlated velocity only while \( \delta q_p^2 \) is due to the uncorrelated velocity only. As for \( q_p^2 \), it accounts for the total particle velocity.

Using the properties of the statistical operator \( \langle \cdot \rangle \), several relations can be formulated for the Eulerian mesoscopic formalism:

- The ensemble averaging of the particle residual velocity component is zero: \( \langle \delta \mathbf{u}_p^{(k)} \rangle = 0 \).
- The particle residual velocity component \( \delta \mathbf{u}_p^{(k)} \) is spatially decorrelated from the fluid velocity: \( \langle \mathbf{u}_f \cdot \delta \mathbf{u}_p^{(k)} \rangle = 0 \).
- The particle residual velocity component \( \delta \mathbf{u}_p^{(k)} \) is spatially decorrelated from the particle mesoscopic velocity: \( \langle \bar{\mathbf{u}}_p \cdot \delta \mathbf{u}_p^{(k)} \rangle = 0 \).

Using these properties and the definition of the different energies \( q_p^2, \bar{q}_p^2 \) and \( \delta q_p^2 \), the relation between all three can be written:

\[
q_p^2 = \bar{q}_p^2 + \delta q_p^2 \tag{1.50}
\]

A first attempt to evaluate the two contributions was made by Février et al. (2005). DPS of a particle-laden statistically stationary HIT were carried out to quantify the effects of particle inertia on the total kinetic energy distribution. In Fig. 1.3, it is shown that the ratio of the kinetic energy of the RUV field to the total particle kinetic energy increases with inertia. More recently, Vance et al. (2006) showed the same trend in a fully-developped channel flow for both non-colliding and colliding particles. Figure 1.4 presents the wall-normal component...
profiles of the total mean-square particle velocity fluctuations in addition to the variance of the correlated and uncorrelated particle velocities for increasing Stokes numbers (based on the half-height of the channel and the fluid friction velocity). Most turbulent kinetic energy is contained in the correlated part for $\St = 0.1625$ whereas the uncorrelated contribution is as important as the correlated one for a bigger Stokes number. Such behaviour was also confirmed by Khalitov & Longmire (2003) by experimental work in a turbulent channel flow.

Note that Vance et al. (2006) proposed a correlation linking the particle uncorrelated contribution to the particle correlated contribution and the fluid-particle correlation. It is explicit in Eq. (1.51) and will be used further in this work to evaluate the uncorrelated motion.

$$\langle \delta u_{p,i} \delta u_{p,i} \rangle = \langle \hat{u}_{p,i} \hat{u}_{p,i} \rangle \frac{\langle u'_{f,i} u'_{f,i} \rangle}{\langle u'_{f,i} u'_{f,i} \rangle} - \langle \hat{u}_{p,i} \hat{u}_{p,i} \rangle$$  \hspace{1cm} (1.51)

Figure 1.3 - Effect of particle inertia on the kinetic energy of the particle Eulerian mesoscopic velocity and the Random Uncorrelated Velocity. The Stokes number $\St'$ is defined in Section 1.3.1. The test case is a particle-laden stationnary HIT computed by Février et al. (2005). $\circ$: $Re_t = 110$; $x$: $Re_t = 140$; $\triangle$: $Re_t = 700$. 

42
1.5 Euler-Euler mesoscopic approach

1.5.3 Particle mesoscopic transport equations

At this point, the dependence on the fluid flow realization $\mathcal{H}_f$ is no longer made explicit when quoting the pdf $\tilde{f}_p$.

Local instantaneous Eulerian mesoscopic equations for the particulate phase can be derived from the kinetic transport equation satisfied by the pdf $\tilde{f}_p$:

$$\frac{\partial}{\partial t} \tilde{f}_p + \frac{\partial}{\partial x_j} \left[ c_{p,j} \tilde{f}_p \right] + \frac{\partial}{\partial c_{p,j}} \left[ \frac{F_{p,j} f_p}{m_p} \right] = \left( \frac{\partial f_p}{\partial t} \right)_{\text{coll}},$$

(1.52)

where $F_p$ represents the external force acting on the particle with mass $m_p$ and the RHS term is the pdf modification by inter-particle collisions. The transport equation for any moment of the pdf $\tilde{f}_p$ is obtained by multiplying Eq. (1.52) with the corresponding function $\Psi_p$ depending on particle velocity $c_p$, and then integrating the resulting equation over particle velocity phase.

Note first that this procedure requires to assume that the product $(\Psi_p \tilde{f}_p)$ is finite and tends to zero when any velocity component $c_{p,j}$ tends to infinity. Second, as detailed in Section 1.2.2, the collisions are not accounted for in the present work and the external forces acting on the particle are limited to gravity and drag. In the Stokes regime (see Section 1.2.1), the drag force depends linearly on the particle-to-fluid relative velocity divided by a constant particle relaxation time $\tau_p$. Thus, the ensemble-averaging of the fluid force term in Eq. (1.52) can be explicitly written in terms of the mesoscopic particle properties. In contrast, when $Re_p < 1000$, the drag force is not linear due to the particle response time that depends on the
particle Reynolds number. This dependence is however omitted when deriving the mesoscopic equations.

Also, the fluctuations of particle Reynolds number and fluid-to-particle relative velocity must be neglected. Under these assumptions, the Eulerian mesoscopic transport equations can be written for the four first moments defined in Eqs. (1.44) – (1.47):

\[
\begin{align*}
\frac{\partial}{\partial t} \hat{n}_p + \frac{\partial}{\partial x_m} \hat{n}_p \hat{u}_{p,m} &= 0 \quad (1.53) \\
\frac{\partial}{\partial t} \hat{n}_p \hat{u}_{p,i} + \frac{\partial}{\partial x_m} \hat{n}_p \hat{u}_{p,j} \hat{u}_{p,m} &= -\hat{n}_p \frac{\tau_p}{\tau_p} (\hat{u}_{p,i} - u_{f,p,i}) - \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{R}_{p,im} \quad (1.54) \\
\frac{\partial}{\partial t} \hat{n}_p \delta \hat{R}_{p,ij} + \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{R}_{p,ij} \hat{u}_{p,m} &= -\frac{\hat{n}_p}{\tau_p} \delta \hat{R}_{p,im} \frac{\partial}{\partial x_m} \hat{u}_{p,i} - \hat{n}_p \delta \hat{R}_{p,im} \frac{\partial}{\partial x_m} \hat{u}_{p,j} - 2 \frac{\hat{n}_p}{\tau_p} \delta \hat{R}_{p,ij} - \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{S}_{p,ijm} \quad (1.55) \\
\frac{\partial}{\partial t} \hat{n}_p \delta \hat{S}_{p,ijk} + \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{S}_{p,ijk} \hat{u}_{p,m} &= -\frac{\hat{n}_p}{\tau_p} \delta \hat{S}_{p,ikm} \frac{\partial}{\partial x_m} \hat{u}_{p,i} - \hat{n}_p \delta \hat{S}_{p,ikm} \frac{\partial}{\partial x_m} \hat{u}_{p,j} - \hat{n}_p \delta \hat{S}_{p,ikm} \hat{u}_{p,k} \bigg( \delta \hat{R}_{p,ij} + \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{R}_{p,im} \bigg) + \delta \hat{R}_{p,ik} \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{R}_{p,jm} + \delta \hat{R}_{p,ij} \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{R}_{p,km} - 3 \frac{\hat{n}_p}{\tau_p} \delta \hat{S}_{p,ijk} - \frac{\partial}{\partial x_m} \hat{n}_p \delta \hat{M}_{p,ikm} \quad (1.56)
\end{align*}
\]

The spatio-temporal evolution of the dispersed phase can be described in terms of particle number density \( \hat{n}_p \), and particle correlated velocity \( \hat{u}_p \), which requires to solve Eqs. (1.53) and (1.54). However, the momentum conservation equation requires to model the particle 2\textsuperscript{nd} order uncorrelated velocity correlations \( \delta \hat{R}_{p,ij} \).

1.5.4 Modeling the second order unclosed term

Several closures have been proposed by Simonin et al. (2002) and Kaufmann et al. (2006) for the particle 2\textsuperscript{nd} order uncorrelated velocity correlations \( \delta \hat{R}_{p,ij} \). They are summarised hereafter, from the highest to the lowest computational cost.

- 2\textsuperscript{nd} order model

The 2\textsuperscript{nd} order model introduced by Simonin et al. (2002) consists in resolving Eq. (1.55) for the six components of the particle 2\textsuperscript{nd} order uncorrelated velocity correlations \( \delta \hat{R}_{p,ij} \). However, this shifts the difficulty to model the particle 3\textsuperscript{rd} order uncorrelated velocity correlations.
\[ \delta \tilde{S}_{p,ijk} \] that appear in Eq. (1.55). When assuming equilibrium of \( \delta \tilde{S}_{p,ijk} \) and neglecting besides the deformation terms, Eq. (1.56) reduces to:

\[
3 \frac{\bar{n}_p}{\tau_p} \delta \tilde{S}_{p,ijk} = \delta \tilde{R}_{p,ik} \frac{\partial}{\partial x_m} \bar{n}_p \delta \tilde{R}_{p,im} + \delta \tilde{R}_{p,jk} \frac{\partial}{\partial x_m} \bar{n}_p \delta \tilde{R}_{p,jm} + \frac{\partial}{\partial x_m} \bar{n}_p \delta \tilde{M}_{p,ijkm} \]

(1.57)

At this point, it is necessary to model the particle 4th order uncorrelated velocity correlations \( \delta \tilde{M}_{p,ijkm} \). Simonin (1996) proposed to consider the gaussian value of \( \delta \tilde{M}_{p,ijkm} \). This suggestion is used hereafter, neglecting the inter-particles collision influence:

\[
\delta \tilde{M}_{p,ijkm} = \delta \tilde{R}_{p,ij} \delta \tilde{R}_{p,km} + \delta \tilde{R}_{p,ik} \delta \tilde{R}_{p,jm} + \delta \tilde{R}_{p,im} \delta \tilde{R}_{p,jk} \]

(1.58)

Finally, combining Eqs. (1.57) and (1.58) leads to replace \( \delta \tilde{S}_{p,ijm} \) by the following term in Eq. (1.55):

\[
\delta \tilde{S}_{p,ijm} = \frac{\tau_p}{3} \left( \delta \tilde{R}_{p,ml} \frac{\partial}{\partial x_l} \delta \tilde{R}_{p,ij} + \delta \tilde{R}_{p,jl} \frac{\partial}{\partial x_l} \delta \tilde{R}_{p,im} + \delta \tilde{R}_{p,il} \frac{\partial}{\partial x_l} \delta \tilde{R}_{p,jm} \right) \]

(1.59)

Due to its expensive computational cost, the 2nd order model can be simplified, as described above.

**Viscosity model and equation for particle Random Uncorrelated Energy (RUE)**

Simonin et al. (2002) introduced the particle RUE as a half of the trace of \( \delta \tilde{R}_{p,ij} \):

\[
\delta \tilde{\theta}_p = \frac{1}{2} \delta \tilde{R}_{p,ll} \]

(1.60)

Then, the transport equation for particle mesoscopic velocity (see Eq. (1.54)) can be rewritten as:

\[
\frac{\partial}{\partial t} \bar{n}_p \tilde{u}_{p,i} + \frac{\partial}{\partial x_m} \bar{n}_p \tilde{u}_{p,i} \bar{u}_{p,m} = - \frac{\bar{n}_p}{\tau_p} \left( \tilde{u}_{p,i} - u_{f@p,i} \right) - \frac{\partial}{\partial x_i} \frac{2}{3} \bar{n}_p \delta \tilde{\theta}_p - \frac{\partial}{\partial x_m} \bar{n}_p \delta \tilde{R}^*_{p,im} \]

(1.61)

where \( \delta \tilde{R}^*_{p,im} \) is the deviatoric part of \( \delta \tilde{R}_{p,im} \):

\[
\delta \tilde{R}^*_{p,im} = \delta \tilde{R}_{p,im} - \frac{2}{3} \delta \tilde{R}_{p,kk} \delta_{im} \]

(1.62)

Quoting the pdf \( \tilde{f}_p \) and the corresponding moments, \( \delta \tilde{R}^*_{p,im} \) can be modeled assuming local equilibrium of the particle 2nd order uncorrelated velocity correlations. Neglecting the term due to the particle 3rd order uncorrelated velocity correlations, Eq. (1.55) finally reduces to:

\[
\delta \tilde{R}^*_{p,im} = - \frac{\tau_p}{2} \left[ \delta \tilde{R}_{p,ik} \frac{\partial}{\partial x_k} \tilde{u}_{p,m} + \delta \tilde{R}_{p,jk} \frac{\partial}{\partial x_k} \tilde{u}_{p,i} - \frac{2}{3} \delta \tilde{R}_{p,kl} \frac{\partial}{\partial x_l} \delta_{im} \right] \]

(1.63)
Assuming besides equilibrium of the anisotropic tensor defined as $a_{p,ij} = (\delta R^*_{p,ij} - 2/3 \delta \hat{\theta}_p \delta_{ij})/2/3 \delta \hat{\theta}_p$ and that the anisotropy is small ($a_{p,ij} a_{p,ij} << 1$), $\delta R^*_{p,im}$ follows a viscosity model (Simonin et al., 2002):

$$\delta R^*_{p,im} = -v_{p,RUM} \left[ \frac{\partial \hat{u}_{p,i}}{\partial x_m} + \frac{\partial \hat{u}_{p,m}}{\partial x_i} - \frac{2}{3} \frac{\partial \hat{u}_{p,l}}{\partial x_l} \delta_{im} \right],$$

(1.64)

where the particle uncorrelated viscosity $v_{p,RUM}$, reads:

$$v_{p,RUM} = \frac{\tau_p}{3} \delta \hat{\theta}_p$$

(1.65)

A transport equation for particle RUE can finally be deduced from the transport equation for particle 2nd order uncorrelated velocity correlation (see Eq. (1.55)) and above assumptions:

$$\frac{\partial}{\partial t} \tilde{n}_p \delta \hat{\theta}_p + \frac{\partial}{\partial x_m} \tilde{n}_p \delta \hat{\theta}_p \hat{u}_{p,m} = -2 \tilde{n}_p \delta \hat{\theta}_p \frac{\partial}{\partial x_m} \frac{1}{2} \tilde{n}_p \delta \hat{\theta}_p \hat{u}_{p,m}$$

$$- \tilde{n}_p \left[ \delta R^*_{p,im} + \frac{2}{3} \delta \hat{\theta}_p \delta_{im} \right] \frac{\partial \hat{u}_{p,i}}{\partial x_m}$$

(1.66)

with $\delta R^*_{p,im}$ given by Eqs. (1.64) and (1.68). Apart from the first term on the RHS of Eq. (1.66) that is linked to the drag force, the transport equation for particle RUE is very similar to the transport equation for fluid temperature. In Eq. (1.66), the last term to model is the particle 3rd order uncorrelated velocity correlation. Kaufmann et al. (2005) suggested to model $\delta \tilde{S}^*_{p,im}$ in analogy with the Fick’s law for the fluid temperature:

$$\frac{1}{2} \delta \tilde{S}^*_{p,im} = -\kappa_{p,RUM} \frac{\partial \delta \hat{\theta}_p}{\partial x_m}$$

(1.67)

In Eq. (1.67), $\kappa_{p,RUM}$ stands for the uncorrelated diffusion coefficient and is modeled in analogy with the RANS two-fluid approach (Simonin, 1996):

$$\kappa_{p,RUM} = \frac{5}{3} \tau_p \delta \hat{\theta}_p$$

(1.68)

Note that Eqs. (1.67) and (1.68) are directly derived from Eq. (1.59) replacing $\delta R^*_{p,ij}$ by $2/3 \delta \hat{\theta}_p \delta_{ij}$.

- **Isentropic pressure model**

The computational cost of a simulation using the Eulerian mesoscopic approach is even lower when no transport equation has to be resolved for the particle 2nd order uncorrelated velocity correlation. This is the case for the isentropic pressure model introduced by Kaufmann et al. (2006). The starting point is the analogy with compressible gaseous flows. There, compression
1.5 Euler-Euler mesoscopic approach

(most of the time) leads to an increase in temperature. When translating this phenomenon to the dispersed phase, it comes that an isentropic compression leads to an increase in particle RUE in the regions where preferential concentration of particles occurs.

To account for this mechanism, Kaufmann et al. (2006) considered the transport equations for particle number density and for particle RUE, respectively Eqs. (1.53) and (1.66). When neglecting the effects due to drag force, shear production and diffusion yields, Eq. (1.66) reduces to:

$$\frac{\partial}{\partial t} \tilde{n}_p \delta \tilde{\theta}_p + \frac{\partial}{\partial x_m} \tilde{n}_p \delta \tilde{\theta}_p \tilde{u}_{p,m} = -\frac{2}{3} \tilde{n}_p \delta \tilde{\theta}_p$$

(1.69)

When combining Eq. (1.53) multiplied by $\frac{2}{3} \tilde{n}_p^{-5/3} \delta \tilde{\theta}_p$ and Eq. (1.69), the product $\tilde{n}_p^{-2/3} \delta \tilde{\theta}_p$ appears as a conserved quantity. This means that the particle RUE can be directly determined by:

$$\delta \tilde{\theta}_p = A \tilde{n}_p^{-\frac{2}{3}}$$

(1.70)

where the coefficient $A$ is determined in HIT flows using the correlation given by Février et al. (2005) (see Section 1.5.2).

1.5.5 Summary of the set of equations tested in this work

The present work is motivated by the promising results obtained by Kaufmann et al. (2006) when predicting the motion of high-inertia particles in a decaying HIT flow with the Euler-Euler mesoscopic approach. In the rest of the manuscript, the EE mesoscopic approach is worked on. The second order term appearing in the particle momentum equation is chosen to be modeled by the viscosity model and the equation for particle RUE detailed is then also resolved. The final set of equations considered for the dispersed phase reduces to Eqs. (1.53), (1.54) and (1.66) with the viscosity and diffusivity models and reads:

$$\frac{\partial}{\partial t} \tilde{n}_p + \frac{\partial}{\partial x_m} \tilde{n}_p \tilde{u}_{p,m} = 0 ,$$

$$\frac{\partial}{\partial t} \tilde{n}_p \tilde{u}_{p,i} + \frac{\partial}{\partial x_m} \tilde{n}_p \tilde{u}_{p,i} \tilde{u}_{p,m} = -\frac{\tilde{n}_p}{\tau_p} \left( \tilde{u}_{p,i} - u_{f@p,i} \right) - \frac{\partial}{\partial x_m} \frac{2}{3} \tilde{n}_p \delta \tilde{\theta}_p - \frac{\partial}{\partial x_m} \tilde{n}_p \delta \tilde{K}_{p,im} ,$$

$$\frac{\partial}{\partial t} \tilde{n}_p \delta \tilde{\theta}_p + \frac{\partial}{\partial x_m} \tilde{n}_p \delta \tilde{\theta}_p \tilde{u}_{p,m} = -\frac{\tilde{n}_p}{\tau_p} \delta \tilde{\theta}_p + \frac{\partial}{\partial x_m} \kappa_{RUM} \frac{\partial \delta \tilde{\theta}_p}{\partial x_m} - \frac{\partial}{\partial x_m} \tilde{n}_p \delta \tilde{K}_{p,im} ,$$

$$-\tilde{n}_p \left[ \delta \tilde{K}_{p,im} + \frac{2}{3} \delta \tilde{\theta}_p \delta_{im} \right] \frac{\partial \tilde{u}_{p,i}}{\partial x_m} .$$
with $\delta \tilde{R}_{p,im} = -V_{p,RUM} \left[ \frac{\partial \tilde{u}_{p,i}}{\partial x_m} + \frac{\partial \tilde{u}_{p,m}}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_{p,l}}{\partial x_l} \delta_{lm} \right]$, 

$V_{p,RUM} = \frac{\tau_p}{3} \delta \tilde{\theta}_p$, 

$\kappa_{p,RUM} = \frac{5}{3} \tau_p \delta \tilde{\theta}_p$

Furthermore when introducing the mesoscopic formalism, it was pointed out that the approach was developed assuming one-way coupling. In the bluff body configuration however, the influence of the particles on the gas flow is non-negligible. As a consequence, for this configuration only, the two-way coupling term is roughly added to the transport equation for the gaseous momentum. Theoretically, there are two main issues to extend the mesoscopic formalism to two-way coupling. First, the ensemble averaging operator is conditioned by a fluid flow realization. Second, defining the fluid velocity locally unperturbed by the particle is not straightforward. This second point can be dealt with in analogy with the work of Vermorel et al. (2003) who performed DPS of a particle laden slab flow to model the turbulence modulation by the particles. Following the RANS methods, extending the mesoscopic formalism to two-way coupling may require the introduction of a drift velocity. Consequently, the field of application of the method may be more limited. The first point is more delicate and some additional work is required.
Chapter 2

Numerical approach

The code AVBP_TPF is an extension of AVBP to two-phase flows. AVBP is devoted to LES of gaseous reactive flows in combustion chamber devices. It is explicit in time and based on a cell-vertex method which allows to handle unstructured as well as hybrid meshes. Extension to two-phase flows using the Euler-Euler mesoscopic approach developed in Section 1.5 was first made by Kaufmann et al. (2006). Only DNS was performed. The Eulerian mesoscopic equations describing the particle motion are difficult to treat numerically, especially because the dispersed phase shows high compressibility effects. As a consequence, strong gradients appear on the particle number density and particle velocity fields, delicate to handle on LES grids and even more on DNS ones. Therefore, performing LES of two-phase flows requires some previous work on numerical methods.

In this chapter, the cell-vertex method used in AVBP_TPF for the spatial discretisation of the equations as well as the temporal discretisation are presented in Section 2.1. Section 2.2 describes the two schemes commonly used in AVBP_TPF. Kaufmann’s work was limited to the use of Lax-Wendroff scheme which is second order accurate in time and space. Another scheme, TTGC (Colin & Rudgyard, 2000), already available for the gas phase, is however more adapted to high compressibility effects in the dispersed phase because it is less dispersive and offers third order spatial accuracy. It has been integrated in AVBP_TPF and a simple test case compares the dispersion errors for both schemes. Still, both schemes are spatially centered and show small-scale oscillations in the vicinity of steep gradients. Numerical treatments such as Artificial Viscosity models and flux limitors are therefore required and are presented in Section 2.3.
2.1 Cell-vertex method for the Navier-Stokes equations

The flow solver used for the discretization of the governing equations is based on the finite volume (FV) method. There are three common techniques for implementing FV methods: the so called cell-vertex, vertex-centered and cell-centered formulations. In the two latter, not used in AVBP_TPF, discrete solution values are stored at the center of the control volumes (or grid cells), and neighbouring values are averaged across cell boundaries in order to calculate fluxes. In the alternative cell-vertex technique, the discrete values of the conserved variables are stored at the vertices (or grid nodes) of the control volume. The mean values of the fluxes are then obtained by averaging along the cell edges.

2.1.1 The Euler equations

Formulation

For the description of the weighted cell-residual approach the laminar equations are considered in their conservative formulation:

\[
\frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \mathbf{F} = 0 \quad (2.1)
\]

where \( \mathbf{w} \) is the vector of conservative variables (taking account the gas and dispersed phase variables) and \( \mathbf{F} \) is the corresponding flux tensor. For convenience, the latter is divided into an inviscid and a viscous part, \( \mathbf{F} = F^I(\mathbf{w}) + F^V(\mathbf{w}, \nabla \mathbf{w}) \).

For a better understanding, it is useful to follow the discretisation of Eq. (2.1) in an example. Figure 2.1 shows a regular triangular mesh. The conservative variables are stored at the nodes which are marked by numbers and normally referenced to by the index \( k = 1, 2, \ldots, k_t \). The cells that define the control volumes are marked by letters and normally referenced to by the symbol \( \Omega \) with the index \( j = A, B, \ldots, n_j \). The nodes associated to a cell, also called vertices, are referenced to by the index \( i = (1, A), (2, A), \ldots, (k_t, n_j) \).

The node-normal vectors defined for each face are associated to the nodes. In the example of Fig. (2.1), nodes \((1, A), (2, A)\) and \((3, A)\) each have a normal \( \mathbf{dS}_i \) as shown by the arrows. These normals are in fact normal to the opposed faces. They contain all the information of the cell geometry. Their length is such, that the result of Eq. (2.2) corresponds to the cell volume \( V_{\Omega_j} \):

\[
V_{\Omega_j} = -\frac{1}{N_d} \sum_{i \in \Omega_j} \mathbf{x}_i \cdot \mathbf{dS}_i \quad (2.2)
\]

where \( N_d \) is the number of dimensions and \( \mathbf{x}_i \) are the node coordinates.
2.1 Cell-vertex method for the Navier-Stokes equations

Figure 2.1 - Control volume for the divergence of the Euler fluxes. The involved node-normals are shown only for cell A.

The FV method in AVBP_TPF is based on this cell-vertex approach. The two terms of Eq. (2.1) are integrated over the mesh cell, $\Omega_j$, so that:

$$\int_{\Omega_j} \frac{\partial \mathbf{w}}{\partial t} dV + \int_{\Omega_j} \nabla \cdot \mathbf{\vec{F}} dV = 0$$

(2.3)

We can then define the cell residual, $\mathbf{R}_{\Omega_j}$, that is proportional to the time variation of $\mathbf{w}$:

$$\mathbf{R}_{\Omega_j} = \frac{1}{V_{\Omega_j}} \int_{\partial \Omega_j} \mathbf{\vec{F}} \cdot d\mathbf{S}$$

(2.4)

It is calculated in AVBP_TPF as proposed by Roe (1987), Rudgyard (1990) or Crumpton et al. (1993) for instance:

$$\mathbf{R}_{\Omega_j} = -\frac{1}{N_d V_{\Omega_j}} \sum_{i \in \Omega_j} \mathbf{\vec{F}}_i \cdot d\mathbf{S}_i$$

(2.5)

where the Euler fluxes $\mathbf{\vec{F}}_i$ are constructed from the conservative variables at the nodes. To be able to determine the time variation $d\mathbf{w}_k/dt$, which is needed to advance Eq. (2.1) in time, the nodal volume $V_k$ is defined as:

$$V_k = \sum_{j|k \in \Omega_j} \frac{V_{\Omega_j}}{n_v(\Omega_j)}$$

(2.6)
NUMERICAL APPROACH

where \( n_v \) is the number of vertices for each cell. For example in Fig. 2.1, the volume associated with node \( I \) is a third of the sum of cells’ \( A - F \) volumes.

Then, writing the nodal residual, \( \mathbf{R}_k \), at node \( k \) becomes the main difficulty of the cell-vertex method. It reads:

\[
\mathbf{R}_k(w) = \frac{d\mathbf{w}_k}{dt} = \frac{1}{V_k} \sum_{j|k \in \Omega_j} D_{\Omega_j}^{k} V_{\Omega_j} R_{\Omega_j}
\]  

(2.7)

where \( D_{\Omega_j}^{k} \) is a distribution matrix that weights the cell residual from cell center \( \Omega_j \) to node \( k \). The control volume used for this residual is shown hatched in Fig. 2.1 and is actually called the dual cell. Conservation is guaranteed if \( \sum_{k \in \Omega_j} D_{\Omega_j}^{k} = I \), where \( I \) is the unit matrix.

Taking \( D_{\Omega_j}^{k} = \frac{I}{n_v(\Omega_j)} \) defines the central-differences scheme.

Finally, the conservative variables can be updated for the new iteration \( (n+1) \) from the preceding one \( (n) \):

\[
\mathbf{w}_k^{(n+1)} = \mathbf{w}_k^{(n)} - \Delta t \mathbf{R}_k(w^{(n)})
\]  

(2.8)

with \( \Delta t \) the time step. It is fixed by the gas phase and then used to advance in time the equations for both phases. It is determined by the Courant condition with states that for stability, information must not travel further than across one cell. As the Euler equations include acoustics, information travels at fluid sound speed \( c_f \) plus the fluid convective speed \( u_f \):

\[
\Delta t = \frac{CFL \cdot \Delta x}{|u_f \pm c_f|}
\]  

(2.9)

where \( \Delta x \) is the characteristic length of the cell and \( CFL \) number is a stability parameter which is often lower than one. The sound speed \( c_f \) is:

\[
c_f = \sqrt{\gamma r T_f}
\]  

(2.10)

This is the simplest possible way to integrate the Euler equations in time. The resulting Euler time-stepping scheme is first order accurate in time and second order accurate in space. It is unconditionally unstable. However, it becomes neutrally stable when combined with Runge-Kutta time-stepping.

Multi-stage Runge-Kutta

Runge-Kutta time-stepping is the extension of the simple explicit Euler time-stepping. An
2.1 Cell-vertex method for the Navier-Stokes equations

$m$-stage (low-storage) Runge-Kutta scheme simply writes:

\[
\begin{align*}
  w_k^{(0)} &= w_k^{(n)} \\
  w_k^{(1)} &= w_k^{(0)} - \alpha_1 \Delta t \, R_k(w^{(0)}) \\
  & \vdots \\
  w_k^{(n)} &= w_k^{(0)} - \alpha_m \Delta t \, R_k(w^{(m-1)}) \\
  w_k^{(n+1)} &= w_k^{(m)}
\end{align*}
\]

(2.11)

where \((\alpha_i)_{i=1}^{m}\) are the Runge-Kutta coefficients. Unfortunately, the two-stage scheme is unstable, so the first additional, useful scheme is the three-step one. It is third order accurate in time (spatial accuracy stays second order). However it is also three times more expensive than the explicit Euler time-stepping.

2.1.2 The diffusive part

The extension of the described solution procedure to the Navier-Stokes equations can be done by constructing as for the convective terms a flux tensor for the diffusive terms \(\vec{G}\) of Eqs. (1.2) and (1.3). This requires the gradients of the conserved variables. They are obtained by a similar approach as used for the computation of the divergence of the Euler fluxes:

\[
(\nabla w)_{\Omega_j} = -\frac{1}{N_d V_k} \sum_{i \in \Omega_j} w_i \cdot \vec{d}S_i
\]

(2.12)

So, the gradients are calculated at the cells, but not scattered back to the nodes. This is done to keep the control volume as small as possible. The viscous flux tensor is then assembled at the cells, using cell-averaged values of the conservative variables where necessary. Then the Green-Gauss integration is carried out by using all the normals attached to one node and the corresponding cell-fluxes:

\[
\frac{d w_k}{dt} = \frac{1}{N_d V_k} \sum_{j[k \in \Omega_j]} \vec{G}_{\Omega_j} \cdot \vec{d}S_{(i=k)}
\]

(2.13)

The contribution to the residual of node 1 from cell A would only be the normal at node (1,A) multiplied with \(\vec{G}_{\Omega_A}\). This is seen in Fig. 2.2 where all involved normals are shown. Additionally the control volume is shown in grey. As the total residual at a node is now influenced by nodes just one edge away, this diffusive operator is called a 2\(\Delta\)-operator. This compact diffusive operator recognises the highest frequency mode, which is an important property for LES calculations. The extension of this approach to bilinear control volumes (such as quadrilaterals) involves some additional considerations which will not be treated here.
2.2 Convective schemes

The RK3 scheme described in Section 2.1 which is second order accurate in space and third order accurate in time is not always used because of its computational cost. A useful alternative scheme, the Lax-Wendroff (LW) one, is presented in Section 2.2.1. It is a second order accurate in time and space, one-step scheme and so, less expensive. Nevertheless, it shows a very oscillating behaviour when dealing with very strong gradients, which is often the case for the dispersed phase. This may lead to negative values of particle number density or particle Random Uncorrelated Energy for instance. It is nearly impossible to develop schemes of high order in space on unstructured meshes with a compact stencil in a finite volume context. Fortunately, the cell-vertex formulation is closely linked to the Galerkin finite element approach, where high order schemes can be developed for the convective terms. The Taylor-Galerkin family of schemes is thus a natural extension of the cell-vertex LW scheme. Colin & Rudgyard (2000) developed a two-step Taylor-Galerkin scheme (TTGC) summarised in Section 2.2.2. This scheme is third accurate in space and time. Although it is approximatively 2.5 times more expensive than LW, it is useful for the dispersed phase because it is much less dispersive than LW. In Section 2.2.3, the dispersion errors introduced by both schemes are compared in a simple purely convective test case.
2.2 Convective schemes

2.2.1 Lax-Wendroff scheme

The starting point is a 2\textsuperscript{nd} order Taylor expansion in time which directly links the conservative variables for the iteration \((n + 1)\) to the ones for the iteration \((n)\):

\[
\frac{w^{n+1} - w^n}{\Delta t} = \left( \frac{\partial w}{\partial t} \right)^n + \frac{\Delta t}{2} \left( \frac{\partial^2 w}{\partial t^2} \right)^n + \mathcal{O}(\Delta t^2)
\]  

(2.14)

The idea of Lax & Wendroff (1960) consists in replacing the time derivatives in Eq. (2.14) by space derivatives using Eq. (2.1):

\[
\frac{\partial w}{\partial t} \rightarrow - \nabla \cdot F
\]

(2.15)

\[
\frac{\partial^2 w}{\partial t^2} \rightarrow - \nabla \cdot \left( A \nabla \cdot F \right)
\]

(2.16)

where \(A\) is the Jacobian of the flux tensor. Using Eqs. (2.15) and (2.16) in Eq. (2.14) yields:

\[
\frac{w^{n+1} - w^n}{\Delta t} = \left( - \nabla \cdot F \right)^n + \frac{\Delta t}{2} \left( - \nabla \cdot \left[ A \nabla \cdot F \right] \right)^n + \mathcal{O}(\Delta t^2)
\]  

(2.17)

Now, this temporal expansion is projected onto the grid, for instance at point \(k\) which belongs to a certain amount of cells \(\Omega_j\). Making use of Eq. (2.17) gives:

\[
\delta w^n_{k \in \Omega_j} = \frac{1}{V_k} \left( R^n_{\Omega_j} \frac{V_{\Omega_j}}{n_v(\Omega_j)} + LW^n_{k \in \Omega_j} \right) \quad \text{and} \quad R^n_{k}(w) = \sum_{j|k \in \Omega_j} \delta w^n_{k \in \Omega_j}
\]  

(2.18)

The 2\textsuperscript{nd} derivative in time in the Taylor expansion is at the origin of the Lax-Wendroff term \(LW^n_{k \in \Omega_j}\) which reads:

\[
LW^n_{k \in \Omega_j} = - \frac{1}{2} \Delta t \int_{\Omega_j \cap \Omega_k} \nabla \cdot \left( A \nabla \cdot F \right) dV
\]

\[
= - \frac{1}{2} \Delta t \int_{\Omega_j \cap \partial \Omega_k} \left( A \nabla \cdot F \right) \cdot dS
\]

\[
= - \frac{1}{2} \Delta t \left( A \nabla \cdot F \right)_{\Omega_j} \cdot \frac{1}{N_d} dS_k
\]  

(2.19)

The LW term in Eq. (2.18) is replaced by Eq. (2.19) and the residual at node \(k\) in cell \(\Omega_j\) becomes:

\[
\delta w^n_{k \in \Omega_j} = \frac{1}{V_k} D^n_{\Omega_j} V_{\Omega_j} R^n_{\Omega_j}
\]  

(2.20)
where \( D^k_{\Omega_j} \) is the distribution matrix already introduced in Section 2.1, see Eq. (2.7). For LW scheme, it reads:

\[
D^k_{\Omega_j} = \frac{1}{n_v(\Omega_j)} \left[ I - \frac{\Delta t}{2N_d} \frac{n_v(\Omega_j)}{V_{\Omega_j}} A_{\Omega_j} \cdot dS_k \right] \tag{2.21}
\]

Finally, the residual at node \( k \) takes all the contributions of neighbouring cells \( \Omega_j \) into account so that:

\[
R_k(w) = \frac{dw_k}{dt} = \frac{1}{V_k} \sum_{j|k \in \Omega_j} D^k_{\Omega_j} V_{\Omega_j} R_{\Omega_j} \tag{2.22}
\]

Thus, comparing Eqs. (2.7) and (2.22), it is the distribution matrix that makes the difference between explicit Euler time-stepping and Lax-Wendoff schemes.

2.2.2 TTGC scheme

Second order convection schemes such as LW are known to be dispersive. As far as the dispersed phase is concerned, their oscillating behaviour can create negative values of number density or RUE. Therefore, higher order schemes must be used for the convective terms. The choice has been made to use Taylor-Galerkin schemes (very low diffusion and dispersion). Those are based on a finite element (FE) method which is straightforward to develop in AVBP, TPF thanks to the cell-vertex approach.

The first difference between TTGC and LW schemes is the use of a 3rd order Taylor expansion in time. Euler-Taylor-Galerkin (ETG) schemes use the classical one but they show a restricted stability criterion. Therefore, Selmin (1987) proposed a family of two-step Taylor Galerkin schemes (TTG) which are based on a two-step Taylor expansion. The TTGC scheme proposed by Colin & Rudgyard (2000) is one of them and uses the following two-step approximation:

\[
\frac{\bar{w}^n - w^n}{\Delta t} = \left[ \frac{1}{2} - \gamma \right] \left( \frac{\partial \bar{w}}{\partial t} \right)^n + \frac{\Delta t}{6} \left( \frac{\partial^2 \bar{w}}{\partial t^2} \right)^n + O(\Delta t^2) \tag{2.23}
\]

\[
\frac{w^{n+1} - w^n}{\Delta t} = \left( \frac{\partial \bar{w}}{\partial t} \right)^n + \gamma \Delta t \left( \frac{\partial^2 \bar{w}}{\partial t^2} \right)^n + O(\Delta t^2) \tag{2.24}
\]

Then, the time derivatives are replaced by the spacel ones, following Lax and Wendroff’s idea (see Eqs. (2.15) and (2.16)). The two-step Taylor expansion then reads:

\[
\frac{\bar{w}^n - w^n}{\Delta t} = - \left[ \frac{1}{2} - \gamma \right] \left( \bar{\nabla} \cdot \bar{F} \right)^n + \frac{\Delta t}{6} \left( \bar{\nabla} \cdot \left[ \bar{A} \bar{\nabla} \cdot \bar{F} \right] \right)^n + O(\Delta t^2) \tag{2.25}
\]

\[
\frac{w^{n+1} - w^n}{\Delta t} = \left( - \bar{\nabla} \cdot \bar{F} \right)^n + \gamma \Delta t \left( \bar{\nabla} \cdot \left[ \bar{A} \bar{\nabla} \cdot \bar{F} \right] \right)^n + O(\Delta t^2) \tag{2.26}
\]
Now comes the second main difference with Lax-Wendroff scheme. Spatial discretisation of Eqs. (2.25) and (2.26) uses the FE method. It consists in writing the conserved variables \( w(\vec{x}) \) as a sum of test functions \( \Phi(\vec{x}) \):

\[
w^n(\vec{x}) = \sum_{k=1,N_n} w^n_k \Phi_k(\vec{x})
\]

where \( w_k \) is the value of \( w \) at node \( k \) and \( N_n \) the total number of nodes of the mesh. The time advancement of each step is noted \( \tilde{R} \) and reads:

\[
\tilde{R}^n = \frac{\tilde{w}^n - w^n}{\Delta t} = \sum_{k=1,N_n} \tilde{R}^n_k \Phi_k
\]

\[
R^{n+1} = \frac{w^{n+1} - w^n}{\Delta t} = \sum_{k=1,N_n} R^{n+1}_k \Phi_k
\]

These test functions must be piecewise linear functions satisfying:

\[
\Phi_j(\vec{x}^i) = \delta_{ij}
\]

\[
\sum_{k=1,N_n} \Phi_k(\vec{x}) = 1 \text{ for every } \vec{x} \in \Omega_j
\]

Finally, Eqs. (2.25) and (2.26) are first multiplied by \( \Phi_i \) and then integrated over the whole domain \( \Omega \). They become:

\[
\sum_{k=1,N_n} M_{ik} \tilde{R}^n_k = -\left[ \frac{1}{2} - \gamma \right] L_i(w^n) - \frac{1}{6} \Delta t \; LL_i(w^n)
\]

\[
\sum_{k=1,N_n} M_{ik} R^{n+1}_k = -L_i(\tilde{w}^n) - \gamma \Delta t \; LL_i(w^n)
\]

where \( M_{ik} \) is the mass matrix defined as \( M_{ik} = \int_{\Omega} \Phi_i \Phi_k dV \).

\( L_i \) and \( LL_i \) are two operators coming from the FE approach. The cell-vertex approach is used to explicit both of them on linear elements. Some corrections are however required on bi- or tri-linear elements. Their most general definition is:

\[
L_i(w^n) = \int_{\Omega} \left( \nabla \cdot \vec{f} \right)^n \Phi_i dV
\]

\[
LL_i(w^n) = \int_{\Omega} \left( \nabla \cdot \vec{A} \; \nabla \cdot \vec{f} \right) \cdot \nabla \Phi_i dV - \int_{\partial \Omega} \Phi_i \left( \vec{A} \; \nabla \cdot \vec{f} \right) \cdot \vec{n} dS
\]
2.2.3 Comparison of the dispersion errors for LW and TTGC schemes.

To highlight the dispersive behaviour of both schemes, the pure convection of a gaussian profile of particle RUE in a periodic domain is studied. Thus, all the source terms and diffusion terms are set to zero in the transport equations of particle correlated velocity and particle RUE (see Section 1.5.5). The system of equations which characterize this test case then reduces to:

\[
\frac{\partial}{\partial t} \tilde{n}_p + \frac{\partial}{\partial x_j} \tilde{n}_p \tilde{u}_{p,j} = 0 \tag{2.36}
\]

\[
\frac{\partial}{\partial t} \tilde{n}_p \tilde{u}_{p,i} + \frac{\partial}{\partial x_j} \tilde{n}_p \tilde{u}_{p,i} \tilde{u}_{p,j} = 0 \tag{2.37}
\]

\[
\frac{\partial}{\partial t} \tilde{n}_p \tilde{\theta}_p + \frac{\partial}{\partial x_j} \tilde{n}_p \tilde{\theta}_p \tilde{u}_{p,j} = 0 \tag{2.38}
\]

Numerical dispersion is critical in the Homogeneous Isotropic Turbulence (HIT) configuration presented in Chapter 3, not only the length of the domain and the kind of resolution but also the order of magnitude of the different quantities in this two-dimensional test case are close to the HIT ones. Therefore, a one-dimensional domain with length \(L_D = 2\pi \cdot 10^{-3} \text{ m}\) is used. The left and right faces are defined as periodic boundaries. Three meshes with increasing resolution are tested. Table 2.1 details the three spatial resolutions:

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Type</th>
<th>Number of cells</th>
<th>Grid spacing (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>meshDisp32</td>
<td>Structured</td>
<td>32</td>
<td>196.10^{-6}</td>
</tr>
<tr>
<td>meshDisp64</td>
<td>Structured</td>
<td>64</td>
<td>98.10^{-6}</td>
</tr>
<tr>
<td>meshDisp128</td>
<td>Structured</td>
<td>128</td>
<td>49.10^{-6}</td>
</tr>
</tbody>
</table>

Table 2.1 - Characteristics of the three meshes used for the dispersion test case.

Initially, the particle number density and particle correlated velocity are uniform in the domain: \(\tilde{n}_p = 10^{13}\); \(\tilde{u}_p = 80 \text{ m.s}^{-1}\). Only the particle RUE shows a gaussian profile in the middle of the domain (see Fig. 2.3). Depending on the spatial resolution, there are respectively 5, 10 and 20 points in the gaussian.

Results

Figures 2.4 – 2.6 compare the behaviour of both schemes, from the lowest resolution to the highest one. Spatial profiles of particle RUE, particle number density and particle correlated velocity are plotted for four increasing times.
2.3 Numerical stabilization methods

2.3.1 Artificial viscosity models

Section 2.2.3 highlights the dispersive behaviour of both LW and TTGC schemes, due to their spatially centered discretization. To avoid the small-scale oscillations (also known as “wiggles”) in the vicinity of steep variations and in order to smooth very strong gradients, it
is common practice to add a so-called artificial viscosity (AV) term to the discrete equations. Such a method avoids accumulation of energy in these non-physical modes without altering the quality of the solution. These AV models are based on a combination of a “shock capturing” term (called 2\textsuperscript{nd} order AV) which smoothes under-resolved gradients and a “background dissipation” term (called 4\textsuperscript{th} order AV) which dissipates the wiggles. They are characterized by the “linear preserving” property which leaves unmodified a linear solution on any type of element.
2.3 Numerical stabilization methods

![Graphs showing temporal evolution of particle RUE, particle number density, and particle velocity for LW scheme (left) and TTGC scheme (right).](image)

Figure 2.5 - Temporal evolution of particle RUE (a. & b.), particle number density (c. & d.) and particle velocity (e. & f.) for LW scheme (left side) and TTGC scheme (right side). $t_{\text{conv}}$ is the convective time based on the initial velocity and the length of the domain. The mesh “mesh disp 64” was used.

The introduction of AV is done in two steps. First, a sensor detects if AV is necessary, as a function of the flow characteristics. In LES, the sensor must be active only in spatially limited zones to avoid interacting with the subgrid stresses. Then, a certain amount of 2nd and 4th AV is applied, depending on the sensor value and on user-defined parameters.

For the gas phase, the sensors are based on the pressure. Indeed, it is assumed that the pressure is most sensitive to any perturbation of the flow. For the dispersed phase, considering only one variable to detect the wiggles and the strong gradients in the whole particle field is not
sufficient. Therefore, both the particle density number and the particle correlated velocity are used to detect such behaviours. This requires a slight modification of the sensors for the dispersed phase. Then, the AV operators are the same for both phase.

The sensors
2.3 Numerical stabilization methods

A sensor $\zeta_{\Omega_j}$ is a scaled parameter which is defined for every cell $\Omega_j$ of the domain that takes values from zero to one. $\zeta_{\Omega_j} = 0$ means that the solution is well resolved and that no AV should be applied while $\zeta_{\Omega_j} = 1$ signifies that the solution has strong local variations and that AV must be applied. This sensor is obtained by comparing different evaluations (on different stencils) of the gradient of a given scalar (pressure, total energy, mass fractions, ...). If these estimations are identical, then the solution is locally linear and the sensor is zero. On the contrary, if these estimations are different, local non-linearities are present, and the sensor is activated. The key point is to find a suitable sensor-function that is non-zero only at places where stability problems effectively occur.

Two sensors are available for the gas phase in AVBP_TPF: the so-called ‘Jameson-sensor’ ($\zeta_{Jf,\Omega_j}$) (Jameson et al., 1981) and the ‘Colin-sensor’ ($\zeta_{Cf,\Omega_j}$) (Colin, 2000) which is an upgrade of the previous one.

- **The fluid ‘Jameson-sensor’**

  For every cell $\Omega_j$, the fluid ‘Jameson cell-sensor’ $\zeta_{Jf,\Omega_j}$ is the maximum over all cell vertices of the fluid ‘Jameson vertex-sensor’ $\zeta_{Jf,i}$:

  \[
  \zeta_{Jf,\Omega_j} = \max_{i \in \Omega_j} \zeta_{Jf,i}
  \]  

  (2.39)

  Denoting $S_f$ the fluid scalar quantity the sensor is based on, the fluid ‘Jameson vertex-sensor’ is:

  \[
  \zeta_{Jf,i} = \frac{|\Delta_i^1 - \Delta_i^2|}{|\Delta_i^1| + |\Delta_i^2| + |S_{f,i}|}
  \]  

  (2.40)

  with the $\Delta_i^1$ and $\Delta_i^2$ functions defined as:

  \[
  \Delta_i^1 = S_{f,\Omega_j} - S_{f,i} \quad \Delta_i^2 = (\vec{\nabla} S_f)_i \cdot (\vec{x}_{\Omega_j} - \vec{x}_i)
  \]  

  (2.41)

  where a $i$ subscript denotes vertex values while $\Omega_j$ is the subscript for cell-averaged values. $(\vec{\nabla} S_f)_i$ is the gradient of $S_f$ at vertex $i$ as computed in AVBP_TPF. $\Delta_i^1$ measures the variation of $S_f$ inside the cell $\Omega_j$ (using only quantities defined on this cell). $\Delta_i^2$ is an estimation of the same variation but on a wider stencil (using all the neighbouring cells of the vertex $i$).

  For non-reactive flows, the only quantity $S_f$ to consider is the fluid pressure $P_f$.

  It is important to note that this sensor varies smoothly: it is roughly proportional to the amplitude of the deviation from linearity.

- **The fluid ‘Colin-sensor’**

  The ‘Jameson-sensor’ was initially derived for steady-state computations. For most unsteady turbulent computations it is however necessary to have a sharper sensor, which is very small...
when the flow is sufficiently resolved, and which is nearly maximum when a certain level of non-linearities occurs.

This is the aim of the so-called ‘Colin-sensor’ proposed by Colin (2000), whose properties can be summarized as follows:

- $\xi_{f, \Omega_j}^C$ is very small when both $\Delta_1^i$ and $\Delta_2^i$ are small compared to $S_{f, \Omega_j}$. This corresponds to low amplitude numerical errors (when $\Delta_1^i$ and $\Delta_2^i$ have opposite signs) or smooth gradients that are well resolved by the scheme (when $\Delta_1^i$ and $\Delta_2^i$ have the same sign).

- $\xi_{f, \Omega_j}^C$ is small when $\Delta_1^i$ and $\Delta_2^i$ have the same sign and the same order of magnitude, even if they are quite large. This corresponds to stiff gradients well resolved by the scheme.

- $\xi_{f, \Omega_j}^C$ is big when $\Delta_1^i$ and $\Delta_2^i$ have opposite signs and one of the two term is large compared to the other. This corresponds to a high-amplitude numerical oscillation.

- $\xi_{f, \Omega_j}^C$ is big when either $\Delta_1^i$ or $\Delta_2^i$ is of the same order of magnitude as $S_{f, \Omega_j}$. This corresponds to a non-physical situation that originates from a numerical problem.

The exact definition of the fluid ‘Colin-sensor’ is:

$$\xi_{f, \Omega_j}^C = \frac{1}{2} \left( 1 + \tanh \left( \frac{\Psi_f - \Psi_{f,0}}{\delta} \right) \right) - \frac{1}{2} \left( 1 + \tanh \left( \frac{-\Psi_{f,0}}{\delta} \right) \right)$$

(2.42)

with:

$$\Psi_f = \max_{i \in \Omega_j} \left( 0, \frac{\Delta^i}{|\Delta^i| + \epsilon_1 S_{f,i} \epsilon_f^j} \right)$$

(2.43)

$$\Delta^i = |\Delta_1^i - \Delta_2^i| - \epsilon_f^j \max(|\Delta_1^i|, |\Delta_2^i|)$$

(2.44)

$$\epsilon_f^j = \epsilon_2 \left( 1 - \epsilon_3 \max \left( \frac{|\Delta_1^i|, |\Delta_2^i|}{|\Delta_1^i| + |\Delta_2^i| + S_{f,i}} \right) \right)$$

(2.45)

The numerical values used in AVBP_TPF are fixed by Colin (2000) to:

$$\Psi_{f,0} = 2.10^{-2} \quad \delta = 1.10^{-2} \quad \epsilon_1 = 1.10^{-2} \quad \epsilon_2 = 0.95 \quad \epsilon_3 = 0.5$$

(2.46)

- **The sensors for the dispersed phase**

For the carrier phase, the fluid sensor is based on pressure. Considering the particle flow, it is much more difficult to determine or to reconstruct a similar unique variable, able to detect
2.3 Numerical stabilization methods

efficiently dangerous oscillations. Indeed, gradients of particle number density and particle correlated velocity can appear independently and remain strongly uncorrelated (preferential concentration is a relevant example, see Chapter 3). Consequently, it has been decided to adapt the fluid ‘Jameson-sensor’ to the dispersed phase in order to calculate two sensors, one based on the particle number density $\zeta_{p,\Omega_j}$, and another based on the particle correlated velocity $\zeta_{\bar{u}_p,\Omega_j}$. Another difficulty arises when conditioning the value of the sensor. Indeed, in the case of the carrier phase, cell-to-cell pressure variations remain several order of magnitude lower than the pressure itself. As far as particle number density or particle correlated velocity are concerned, this is not true anymore. Variations can be indeed of the same order of the variable itself (for instance, at the borders of a jet for injection of particles, see Chapter 5). Therefore the normalisation used for the fluid cannot be used, otherwise rapid saturation of the sensors is observed, and the sensor no longer acts as it should. Eqs. (2.47) and (2.48) define the two sensors used for the dispersed phase:

$$\zeta_{\bar{u}_p,\Omega_j} = \frac{|\Delta_{i}^{\bar{u}_p} - \Delta_{j}^{\bar{u}_p}|}{|\Delta_{i}^{\bar{u}_p}| + |\Delta_{j}^{\bar{u}_p}| + c_i}$$ (2.47)

$$\zeta_{p,\Omega_j} = \left[\frac{|\Delta_{i}^{p} - \Delta_{j}^{p}|}{|\Delta_{i}^{p}| + |\Delta_{j}^{p}| + \bar{n}_{p,j}}\right]^2$$ (2.48)

where $c_i$ is a local measure of the sound speed roughly defined as: $c_i = (V_{\Omega_j})^{1/3} / \Delta t$.

The node-to-node variations of particle correlated velocity remain small compared to this local sound speed, except if strong oscillations appear. As a consequence, the sensor $\zeta_{\bar{u}_p,\Omega_j}$ remains small, except if strong local gradients of particle correlated velocity are detected.

The particle number density cannot be related to any reference value and the normalization is not helpful to sharpen the sensor. Therefore, as the sensor takes values from zero to one, another simple way to prevent from saturation is to square the function itself.

The operators

There are two AV operators in AVBP_{TPF}: a 2nd order operator and a 4th order operator. All AV models in AVBP_{TPF} are a blend of these two operators. These operators have the following properties:

- 2nd order operator: it acts just like a “classical” viscosity. It smoothes gradients, and introduces artificial dissipation. It is thus associated to a sensor which determines where it must be applied. Doing this, the numerical scheme keeps its order of convergence in the zones where the sensor is inactive, while ensuring stability and robustness in the critical regions. The viscosity coefficient associated to this operator is noted $\nu_{2}^{AV}$.
– 4th order operator: it is a less common operator. It acts as a bi-Laplacian and is mainly used to control spurious high-frequency wiggles. The viscosity coefficient associated to this operator is noted $\nu_A^4$.

It can be shown that $\nu_A^2$ can be seen as an artificial viscosity (it has the same units as a physical viscosity), which is controlled by the user-defined parameter $\beta_A^2$. The $\beta_A^2$ parameter is therefore dimensionless and is a Fourier number for the AV. Likewise, $\nu_A^4$ can be seen as an artificial 4th order hyper-viscosity, which is controlled by the user-defined parameter $\beta_A^4$ (also dimensionless). Equation (2.49) gives the definition of the two viscosity coefficients on a one-dimensional regular mesh:

$$\nu_A^2 = \frac{\beta_A^2 \Delta x^2}{2 \Delta t} \quad \nu_A^4 = \frac{\beta_A^4 \Delta x^4}{16 \Delta t} \quad (2.49)$$

The artificial viscosity models

When performing Direct Numerical Simulation or Large-Eddy Simulation, it is essential to handle artificial viscosity with care in order to minimize its influence on the quality of the numerical schemes and the models used. Therefore, the AV models combine:

– the choice of the sensor and the variable which is used for the sensor,

– the way the 2nd order and the 4th order operators are combined,

– the choice of variables on which the operators are applied.

• The fluid ‘Jameson-model’

The fluid ‘Jameson-sensor’ $\zeta_{f,\Omega_j}$, based on pressure is used in this case. The amount of 2nd and 4th order AV applied is directly proportional to this sensor. Actually, the input parameter $\beta_{A,f}^4$ is replaced by:

$$\beta_{A,f}^4 = \max(0, \beta_{A,f}^4 - \zeta_{f,\Omega_j} \cdot \beta_{A,f}^2) \quad (2.50)$$

This formulation allows to put 4th order AV only where the sensor is small. On the other hand, if the sensor is large, it is no use to put 4th order AV, because the 2nd order AV operates fully and overcomes most of the problems. Both operators are applied to all fluid variables (density, momentum and energy).

This model was originally proposed by Jameson et al. (1981). It is very well suited for unconfined aerodynamics, with possible shocks and without combustion.
2.3 Numerical stabilization methods

- The fluid ‘Colin-model’

In this model, the fluid ‘Colin-sensor’ \( \zeta_C^{jf,\Omega_j} \), also based on pressure, is used. It acts more locally and more suddenly than the fluid ‘Jameson-sensor’. The operators are unchanged, see Eq. (2.50), but they are applied differently. The 2\textsuperscript{nd} order AV operates on all the variables but the 4\textsuperscript{th} order one is not applied to momentum, allowing to keep more small scale structures.

- The ‘Jameson-model’ for the dispersed phase

As the fluid ‘Jameson-model’ is well adapted to shocks, the same model is used for the dispersed phase, where the gradients are often strong. The only difference comes from the particle ‘Jameso-sensor’ defined as:

\[
\zeta_{p,\Omega_j}^J = \max \left( \zeta_{p,\Omega_j}^{\tilde{a}_p}, \zeta_{p,\Omega_j}^{\tilde{n}_p} \right)
\]  

(2.51)

Application of 2\textsuperscript{nd} and 4\textsuperscript{th} order AV on all the variables of the dispersed phase (number density, correlated velocity and RUE) is done the same way as in the fluid ‘Jameson-model’.

2.3.2 Particle RUE flux limiter

The AV models described in Section 2.3.1 are essential for all simulations using centered schemes. The particle AV model is efficient in most geometries, avoiding in particular negative values of particle number density. A very specific case is the decaying Homogeneous Isotropic Turbulence described in Chapter 3 where preferential concentration effects are very strong. Those lead to steep gradients, not only on particle number density and correlated velocity, but also on particle RUE. That can locally take negative values, which is unphysical.

The transport equations for particle RUE is difficult to handle numerically, especially because the source terms on the RHS of Eq. (2.2.3) are often big. Nevertheless, it has been verified that these source terms are not the origin of the problem. To overcome negative values of particle RUE, a so-called flux limiter (FL) is used on the Euler flux in the transport equation for particle RUE.

Unlike the limiters that have been defined in the context of Total Variation Diminishing (TVD) schemes (Van Leer, 1977; Roe, 1984; Chakravarthy & Osher, 1977), the target here is just to avoid negative values of particle RUE (and not the oscillations of particle RUE).

As an example, the test case described in Section 2.2.3 is used again to show the impact of the FL on the particle fields. Only the intermediate resolution showing 64 cells in the box is used in this case. Figure 2.7 compares the particle RUE, number density and correlated velocity calculated with the TTGC scheme, with and without the RUE FL. As expected, negative values of particle RUE disappear with the flux limiter while neither the shape nor the maximum values
of RUE, number density and correlated velocity are modified. Tables 2.2 and 2.3 show the minimum, maximum and mean values for particle RUE after two and five convective times \( t_{\text{conv}} \), based on the initial velocity and the length of the domain. The RUE flux limiter has very little influence on the extrema and the loss of energy in the domain is less than 6% after five convective times.

\[
\delta \theta_p^{\text{max}}\quad \delta \theta_p^{\text{min}}\quad \delta \theta_p^{\text{mean}}
\]

\[
\begin{array}{ccc}
\text{without FL} & 0.4525 & -0.0469 & 0.0744 \\
\text{with FL} & 0.4515 & 0.0069 & 0.0763 \\
\end{array}
\]

Table 2.2 - Statistics of the particle RUE field with and without the RUE flux limiter for \( t = 2 t_{\text{conv}} \)

\[
\begin{array}{ccc}
\text{without FL} & 0.3989 & -0.0596 & 0.0744 \\
\text{with FL} & 0.4025 & 0.0038 & 0.0789 \\
\end{array}
\]

Table 2.3 - Statistics of the particle RUE field with and without the RUE flux limiter for \( t = 5 t_{\text{conv}} \)
2.3 Numerical stabilization methods

Figure 2.7 - Temporal evolution of particle RUE (a. & b.), particle number density (c. & d.) and particle correlated velocity (e. & f.) without RUE flux limiter (left side) and with RUE flux limiter (right side). The TTGC scheme was used on the mesh 'meshDisp64'.
Chapter 3

DNS of particle-laden homogeneous isotropic decaying turbulence

Gaseous Homogeneous Isotropic Turbulence (HIT) flows have been considered for a long time to analyse characteristics of turbulence and to propose turbulence models. The pioneers are undoubtedly Taylor (1921) and Batchelor (1949) who conducted theoretical studies about the diffusion of passive scalars in stationary HIT. Since then, a large amount of theoretical work has been achieved to increase the knowledge in turbulence structures, and in mechanisms of turbulence dissipation and production. Numerical investigations of HIT flows are more recent (1970’s), and closely linked to the development and availability of powerful computers. Conceptually, the simplest numerical approach to solve the Navier-Stokes equations is Direct Numerical Simulation (DNS) that consists in resolving all the scales of motion. First DNS of HIT flow was carried out by Orszag & Patterson (1972) implementing a pseudo-spectral method.

The dynamics of particles in HIT flows has been theoretically studied for a while. Although it is an academic problem, mechanisms induced in such two-phase flows arise in a wide variety of industrial applications. In dilute flows ($\alpha_p < 10^{-4}$), the mechanism of transport of particles interacting with the fluid are dominating. Tchen (1947) and Hinze (1975) extended the diffusion of passive scalars in stationary HIT to inertial particles. Numerous theoretical, experimental and numerical studies allowed to characterise more precisely the mechanisms of transport of particles in a turbulent flow (Snyder & Lumley, 1971; Riley & Paterson, 1974). Moreover, the effects of preferential concentration have been widely investigated (Maxey, 1987; Squires & Eaton, 1991a; Wang et al., 2000; Février et al., 2005). When increasing the volume fraction ($\alpha_p > 10^{-4}$), modification of the turbulence by particles must be accounted for. Several authors have been working on this phenomenon (Squires & Eaton, 1990; Elghobashi & Truesdell, 1993; Pan & Banerjee, 1997; Boivin et al., 1998; Druzhinin, 2001;
Focusing on the study of particle dispersion and preferential concentration effects, DNS have been performed by several authors using the Lagrangian transport equations (Deutsch, 1992; Elghobashi & Truesdell, 1993; Février et al., 2005; Moreau, 2006), the equilibrium Eulerian approach (Rani & Balachandar, 2004) or the EE mesoscopic approach (Février et al., 2005). Obviously, the Lagrangian results are the most accurate, provided a large number of particle trajectories are calculated to ensure reliable statistics. As a consequence, the computational cost of the Eulerian simulations are usually much cheaper, especially when accounting for complex interphase couplings (mass and momentum for instance). Calculating the motion of low-inertia particles in a HIT flow with either the equilibrium Eulerian approach or the EE mesoscopic formalism gives very accurate results. However, when increasing particle inertia, both methods face difficulties, respectively due to modeling and to numerical implementation.

With two-phase reactive flow modeling in prospect, it has been decided to carry on the work of Kaufmann et al. (2006) in order to improve the numerical resolution of the EE mesoscopic transport equations. The particle-laden decaying HIT flow from Kaufmann et al. (2006) that shows significant compressibility effects, and is difficult to handle numerically, is computed again using the transport equation for particle RUE proposed by Simonin (1996) and Kaufmann et al. (2006). The purpose is to show the impact of the numerical developments detailed in Chapter 2 on the results and to validate AVBP_TPF on this two-phase flow configuration.

The results provided by DNS using the EE mesoscopic approach are validated by comparison with the results of DPS performed by Moreau (2006). The code NTMIX3D used is a three-dimensional finite differences solver, fully parallel and using domain decomposition. The gas DNS solver of NTMIX3D has been mainly developed by Baum & Poinrot (1992); Poinrot et al. (1993); Stoessel et al. (1994); Cuenot & Poinrot (1996); Boughnem & Trouvé (1996) whereas two-phase flows have been widely investigated by Albrecht et al. (1999), Vermorel et al. (2003), Paoli et al. (2004) and Moreau (2006). For the gas phase, the fully compressible Navier-Stokes equations are solved with a non-dimensional formulation. Space discretization is performed by a sixth-order compact scheme (Lele, 1992) while time integration is performed by a three-stage Runge-Kutta method. For the dispersed phase, the transport equation for particle trajectories (see Section 1.3.1) are advanced in time with a three-stage Runge-Kutta method as the gas phase. A fourth-order interpolation of the Lagrangian polynomials provides the fluid velocity sampled along particle trajectories, that is required for drag force computation. The DPS results are interpreted in terms of EE mesoscopic results using an adequate gaussian projection procedure (Moreau, 2006).

In the present particle-laden HIT flow, the regime is dilute enough to assume one-way coupling and the fluid flow is independent of the particle motion. Therefore, the gaseous HIT
flow is presented first and the main results are analysed in Section 3.1. Then, a brief analysis of the results obtained by Kaufmann et al. (2006) is proposed in Section 3.2 to enhance the main numerical issues of the two-phase flow calculations. Finally, the results obtained with the numerical tools developed during this work are discussed in Section 3.3. Analysis of integral quantities as well as spectral properties, and comparison with the Lagrangian results from Moreau (2006) are also provided.

3.1 Gas Homogeneous Isotropic Turbulence flow

3.1.1 Theoretical basis

- The main turbulent scales

Many flows encountered in technical applications are turbulent. To be laminar, the fluid must be either very viscous or very slow. The inertia-viscous forces ratio, also called the Reynolds number, \( Re \), quantifies this observation:

\[
Re = \frac{u_f \cdot l_f}{v_f}
\]  

(3.1)

where \( u_f \) and \( l_f \) are the characteristic velocity and length scales of the flow and \( v_f \) is the kinematic viscosity of the fluid.

Laminar flows are characterised by low Reynolds numbers. They are generally steady in time and regular in space. Destabilisation of the flow happens when the Reynolds number increases, leading to turbulent flows. Those are unsteady and very irregular in space. The limit between laminar and turbulent flows is difficult to define because other parameters such as wall roughness for example may influence the transition from laminar to turbulent flow. For instance, the transition in a pipe flow occurs around \( Re \approx 2300 \), where \( Re \) is based on the bulk velocity and the diameter of the pipe (Pope, 2000).

The role of turbulence for transporting and mixing mass, momentum and heat is of great importance. The Reynolds number defined by Eq. (3.1) is not sufficient to characterize the large variety of turbulent processes. Although turbulence exhibits randomness (in the sense that the velocity at a specified position and time is never exactly the same when repeating the fluid-flow experiment), they are organised in coherent structures. Therefore, there are many different time, velocity and length scales to define.

Figure 3.1 illustrates this variety of scales showing two laser-induced fluorescence (LIF) photographs of a coaxial jet for increasing Reynolds number. Turbulence is known to be produced by mean velocity gradients. Comparing the two pictures in Fig. 3.1, it appears that
the size of the largest turbulent eddies is practically unaffected when increasing the Reynolds number, whereas the smallest scales become even smaller. The size of the largest scale turbulent eddies, also referred as integral length scale $l_{f,t}$, is mainly linked to the geometry and the boundary conditions. Introducing the kinetic energy $u_{f,t}^2$ contained in the large scales, the turbulent Reynolds number that compares turbulent inertia and viscosity effects, reads:

$$Re_{t} = \frac{\sqrt{u_{f,t}^2 \cdot l_{f,t}}}{\nu_f}$$

The turbulent time-scale of the largest scale turbulent eddies then yields:

$$\tau_{f,t} = \frac{l_{f,t}}{u_{f,t}}$$

Richardson (1922)'s notion is that the large eddies responsible for production of turbulence are unstable and break-up, transferring their energy to smaller eddies. This process referred as "energy cascade" ends when the eddies become stable and kinetic energy is dissipated by molecular viscosity. The dissipation $\varepsilon_f$ scales independently of $\nu_f$ as:

$$\varepsilon_f = \frac{u_{\varepsilon_f}^2}{\tau_{\varepsilon_f}}$$

where $\tau_{\varepsilon_f} = l_{\varepsilon_f} / u_{\varepsilon_f}^\prime$ and $u_{\varepsilon_f}^\prime$ is the velocity fluctuation of the eddies of length $l_{\varepsilon_f}$.

The Kolmogorov scales characterize the smallest and dissipative scales. Considering that they appear when turbulence is dissipated by molecular viscosity, the Reynolds number based on the Kolmogorov length scale $\eta_{f,K}$ and its corresponding velocity fluctuation $u_{f,K}^\prime$ reads:

$$Re_K = \frac{u_{f,K}^\prime \cdot \eta_{f,K}}{\nu_f} = 1$$
3.1 Gas Homogeneous Isotropic Turbulence flow

\( \tau_{f,K} \) is the turnover time of the smallest eddies with length \( \eta_{f,K} \). Combining Eqs. (3.4) and (3.5) directly links the Kolmogorov scales to the dissipation rate and the kinematic viscosity of the fluid:

\[
\eta_{f,K} = \left( \frac{\nu_f^3}{\varepsilon_f} \right)^{\frac{1}{4}}
\]  

(3.6)

The ratios of the integral scales to the smallest scales are readily determined from Eqs. (3.2), (3.4) and (3.6):

\[
\frac{l_{f,t}}{\eta_{f,K}} = \text{Re}_\nu^{\frac{3}{4}}
\]  

(3.7)

\[
\frac{\tau_{f,t}}{\tau_{f,K}} = \text{Re}_\nu^{\frac{1}{2}}
\]  

(3.8)

\[
\frac{u'_{f,t}}{u'_{f,K}} = \text{Re}_\nu^{\frac{1}{4}}
\]  

(3.9)

• Specificities of a Homogeneous Isotropic Turbulence (HIT) flow

The Homogeneous Isotropic Turbulence (HIT) test case is undoubtedly the simplest class of flows to study with Direct Numerical Simulation. It allows to quantify the numerous scales previously defined. A field is statistically homogeneous when all statistics are invariant under translations. If the field is also statistically invariant under rotations and reflexions of the coordinate axes, it is besides isotropic.

• HIT statistical analysis in physical space

The starting point is the observation that all statistics are independent of the location and orientation of the coordinate system. All the statistical quantities are therefore only a function of the distance \( r \) separating the locations observed. The correlation function of the velocity vectors at points \( A \) and \( B \) separated by the distance \( \vec{r} \) reads:

\[
Q_{f,ij} = \frac{u'_{f,j}(A) u'_{f,j}(B)}{u_f^2}
\]  

(3.10)

where \( u'_{f,i}(A) \) is the \( i^{th} \) component of the fluctuating velocity vector at the location \( A \) and the over-bar stands for the ensemble mean which is equivalent to a spatial mean under the assumption of homogeneity.

The correlation coefficient is defined as:

\[
R_{f,ij}(\vec{r}) = \frac{Q_{f,ij}(\vec{r})}{u_f^2}
\]  

(3.11)
where \( u_f' \) and \( u_f'' \) are defined as:

\[
\begin{align*}
\frac{1}{3} u_f' u_f'' &= \frac{1}{3} Q_{f,ii}(0).
\end{align*}
\]

Based on Eq. (3.11), the longitudinal, transversal and cross-stream integral length scales are respectively defined as:

\[
L_{f,11}^1 = \int_0^\infty R_{f,11}(r,0,0)dr; \quad L_{f,22}^2 = \int_0^\infty R_{f,22}(0,r,0)dr; \quad L_{f,33}^3 = \int_0^\infty R_{f,33}(0,0,r)dr
\]

\[ (3.12) \]

\( L_{f,ii}^i \) is another characteristic length of the large scale motions in the turbulent field and is of the same order as the turbulent length scale \( l_{f,t} \). The Reynolds number based on \( L_{f,ii}^i \) reads:

\[
Re_{L_{f,ii}} = \frac{u_f' \cdot L_{f,ii}^i}{\nu_f}
\]

\[ (3.13) \]

For an incompressible fluid, isotropy imposes:

\[
L_{f,11}^1 = L_{f,22}^2 = L_{f,33}^3
\]

\[ (3.14) \]

**Numerical restrictions**

After introducing all these scales, the question of accurate spatial resolution when performing a Direct Numerical Simulation (DNS) naturally arises. It is directly linked to the resolution of turbulence which requires:

- **Accurate description of the biggest eddies of the turbulence.**
  The domain length must be bigger than the integral length scale \( l_{f,t} \). This guarantees that spatial averaging is the same as converged ensemble averaging.

\[
L_{f,ii}^i(t) < \frac{L_D}{C_1} \quad \text{with} \quad C_1 \simeq 15
\]

\[ (3.15) \]

\( L_D \) is the length of the domain. As the current test is a decaying HIT, it is important to ensure that Eq. (3.15) is verified during the whole simulation.

- **Good resolution of the most dissipative scales.**
  If the most dissipative scales are not well resolved, the energy is not dissipated but accumulates in the smallest resolved structures, leading to numerical instabilities.

\[
l_{ef}(t) > C_2 \Delta x \quad \text{with} \quad C_2 \simeq 5
\]

\[ (3.16) \]

\( \Delta x \) the grid spacing.
Combining Eqs. (3.15) and (3.16) with classical turbulent approximations, \( L_{f,i} \simeq l_{f,i}/2 \) and \( \eta_{f,K} \simeq l_{f,1}/10 \), leads to restrictions on the integral and Kolmogorov length scales, and so on the turbulent Reynolds number:

\[
l_{f,t} < \frac{2L_D}{15} \tag{3.17}
\]
\[
\eta_{f,K} > \frac{\Delta x}{2} \tag{3.18}
\]
\[
Re_t < \left( \frac{4N_x}{15} \right)^{\frac{1}{4}} \tag{3.19}
\]

where \( N_x \) is the number of grid points in the x-direction. Therefore, accurate resolution is ensured for turbulent Reynolds numbers smaller than 44 and 111 when the numerical grid respectively consists in \( 64^3 \) and \( 128^3 \) cells.

- **Turbulent kinetic energy temporal decaying**

  Equation (3.20) defines the turbulent kinetic energy \( q_f^2 \) and the dissipation rate \( \varepsilon_f \).

  \[
  q_f^2 = \frac{1}{2} u_{f,i}^2 \quad \varepsilon_f = \nu_f \left( \frac{\partial u_{f,i}'}{\partial x_j} \frac{\partial u_{f,i}'}{\partial x_j} \right) \tag{3.20}
  \]

  If the Navier-Stokes equations are restricted to incompressible flows, those quantities verify two exact equations. For this study, the exact equation, Eq. (3.21), is used for \( q_f^2 \) whereas a modeled one, Eq. (3.22), is considered for \( \varepsilon_f \).

  \[
  \frac{dq_f^2}{dt} = -\varepsilon_f \tag{3.21}
  \]

  \[
  \frac{d\varepsilon_f}{dt} = -C_{\varepsilon_f} \frac{\varepsilon_f^2}{q_f^2} \tag{3.22}
  \]

  There is an analytical solution to this system. The change of variable \( \tau_{\varepsilon_f} = q_f^2/\varepsilon_f \) determines the temporal evolution of \( \tau_{\varepsilon_f} \) itself, \( q_f^2 \) and \( \varepsilon_f \) among others:

  \[
  \tau_{\varepsilon_f} = \tau_{\varepsilon_f,0} \left[ 1 + \left( C_{\varepsilon_f} - 1 \right) \frac{t}{\tau_{\varepsilon_f,0}} \right]^{-\frac{1}{C_{\varepsilon_f} - 1}} \tag{3.23}
  \]

  \[
  q_f^2 = q_{f,0}^2 \left[ 1 + \left( C_{\varepsilon_f} - 1 \right) \frac{t}{\tau_{\varepsilon_f,0}} \right]^{\frac{c_{\varepsilon_f}}{C_{\varepsilon_f} - 1}} \tag{3.24}
  \]

  \[
  \varepsilon_f = \varepsilon_{f,0} \left[ 1 + \left( C_{\varepsilon_f} - 1 \right) \frac{t}{\tau_{\varepsilon_f,0}} \right]^{\frac{c_{\varepsilon_f}}{C_{\varepsilon_f} - 1}} \tag{3.25}
  \]
where the subscript 0 denotes the initial field. \( C_{\varepsilon_f} \) is a constant whose value was determined experimentally: \( C_{\varepsilon_f} = 1.92 \).

- HIT statistical analysis in spectral space

In the Fourier space, a wave number \( k \) is associated to each length scale \( l (k = 2\pi/l) \). The turbulent kinetic energy then depends on wave number and time, and is usually referred as the fluid turbulent kinetic energy spectrum \( E_f(k) \). Its temporal evolution is described by Eq. (3.26):

\[
\frac{\partial}{\partial t} E_f(k,t) = T_f(k,t) - 2\nu_f k^2 E_f(k,t)
\]

(3.26)

\( T_f \) represents the energy transfer from the largest scales to the smallest scales. It neither products nor dissipates energy. Therefore, its integral over the spectral space is zero.

For Homogeneous Isotropic Turbulence, \( E_f(k,t) \) is sufficient to reconstruct \( \sqrt{\overline{q^2_f}} \), \( \varepsilon_f \) and \( L_{ii}^t \):

\[
\sqrt{\overline{q^2_f}}(t) = \int_0^\infty E_f(k,t)dk
\]

(3.27)

\[
\varepsilon_f(t) = \int_0^\infty D_f(k,t)dk = 2\nu_f \int_0^\infty k^2 E_{f,t}(k)dk
\]

(3.28)

\[
L_{ii}^t(t) = \frac{\pi}{2u_f^2} \int_0^\infty \frac{E_f(k,t)}{k}dk \text{ in the 3D case.}
\]

(3.29)

### 3.1.2 HIT test case parameters and initialisation

All the simulations are computed on a square box with an edge length \( L_D = 2\pi \times 10^{-3} \text{ m} \). The computational grid is periodic in all directions. A structured mesh (cubic hexahedra cells) is used and two resolutions are considered. The first one called \( \text{hit\_mesh64} \), contains 64\(^3\) cells with a cell size of \( \Delta x = 98 \times 10^{-3} \text{ m} \). The second one \( \text{hit\_mesh128} \), exhibits a grid spacing two times smaller \( \Delta x = 49 \times 10^{-3} \text{ m} \) and so, contains 128\(^3\) cells. Table 3.1 summarizes this information.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Type</th>
<th>Number of cells</th>
<th>Number of nodes</th>
<th>Grid spacing (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{hit_mesh64} )</td>
<td>Structured</td>
<td>262,144</td>
<td>274,625</td>
<td>98 \times 10^{-6}</td>
</tr>
<tr>
<td>( \text{hit_mesh128} )</td>
<td>Structured</td>
<td>2,097,152</td>
<td>2,146,689</td>
<td>49 \times 10^{-6}</td>
</tr>
</tbody>
</table>

Table 3.1 - Characteristics of the two meshes used for the HIT test case.
Hereafter, the DNS performed with AVBP_TPF are validated by comparison with NT-MIX3D results. The latter uses a non-dimensional formulation with reference values for length, time and velocity (respectively \( L_{\text{ref}}, T_{\text{ref}} \) and \( c_{\text{ref}} \)) given in Table 3.2. For the sake of simplicity, all the results provided by AVBP_TPF are non-dimensionalised by the same reference values and are denoted with the superscript + later in the text.

<table>
<thead>
<tr>
<th>( c_{\text{ref}} (m.s^{-1}) )</th>
<th>( L_{\text{ref}} (m) )</th>
<th>( T_{\text{ref}} (s) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>347.0</td>
<td>( 10^{-3} )</td>
<td>2.881810^{-6}</td>
</tr>
</tbody>
</table>

Table 3.2 - Reference values used to convert to non-dimensional quantities. HIT configuration.

**Initialisation**

The DNS of a HIT flow requires the initialisation of the velocity field to a turbulent-like velocity field. This is done from the turbulent kinetic energy spectrum, used to calculate the velocity field in the spectral space. A reverse Fourier transform then gives access to the initial velocity field in the physical space. Several spectrum models are available. Most of them constitute an approximate solution of Eq. (3.26) for a specific range of wave numbers. The Passot-Pouquet (PP) (Passot & Pouquet, 1987) and the von Kármán Pao (VKP) models are the most used.

The VKP spectrum allows to represent both the biggest and the most dissipative scales of the turbulent field, and so, is rather physical. However, it is valid only for \( Re_{L_{\text{ij}}} > 100 \), or \( Re_{t} > 200 \). Considering the grid resolution of this test case, only the PP spectrum can be used to initialize the velocity field. Eq. (3.30) gives the form of the PP synthetic spectrum:

\[
E_f(k,t) = \frac{16u'_{f,t}^2}{k_e} \sqrt{\frac{2}{\pi}} \left(\frac{k}{k_e}\right)^4 e^{-2\left[\frac{k}{k_e}\right]^2}
\]

The PP spectrum depends on a characteristic wave number \( k_e \), with \( k_e = 2\pi/l_e \), and the associated velocity fluctuation \( u'_{f,t} \). Both quantities are only parameters, and not really physical. However, \( l_e \) can be linked to the integral length scale: \( L_{ij} \simeq 0.12l_e \) (Hinze, 1975).

The main drawback of this model is that it takes into account the most energetic eddies only, which means that turbulent kinetic energy is concentrated in the neighbourhood of \( k_e \). Besides, the model verifies the continuity equation but not the momentum equation. Therefore, it is necessary to run the simulation for an initial transient time to recover a true solution to the Navier-Stokes equations.

The parameters of the synthetic Passot-Pouquet spectrum used for this case are: \( l_e^+ = 2.2 \) and \( u'_{f,t}^+ = 0.1 \). The three Reynolds numbers defined in Eqs. (3.2), (3.5) and (3.13) respectively read: \( Re_{t} = 13.4 \), \( Re_K = 10.4 \) and \( Re_{L_{ij}} = 17.8 \) at \( t=0 \). About one turnover time of the initial biggest eddies (\( t_{0}^+ = 4.233 \)) is computed before collecting statistics.
Table 3.3 compares the detailed characterisation of the initial field and the field obtained at time $t_0^+$ whereas Fig. 3.2 shows the turbulent kinetic energy spectra at times $0$ and $t_0^+$. During the time interval $[0; t_0^+]$, the most energetic structures that are well modeled by the PP spectrum, transfer energy to the smallest ones, leading to a better representation of the smallest scales.

<table>
<thead>
<tr>
<th>$t^+$</th>
<th>$q_f^2$</th>
<th>$u_f'$</th>
<th>$\varepsilon_f^+$</th>
<th>$L_{11}^{1+}$</th>
<th>$L_{22}^{2+}$</th>
<th>$L_{33}^{3+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.015</td>
<td>0.1</td>
<td>0.0015</td>
<td>0.881</td>
<td>0.852</td>
<td>0.571</td>
</tr>
<tr>
<td>$t_0^+$</td>
<td>0.00945</td>
<td>0.079</td>
<td>0.0012</td>
<td>0.926</td>
<td>0.935</td>
<td>0.557</td>
</tr>
</tbody>
</table>

Table 3.3 - Statistical analysis of the turbulent field obtained numerically at time 0 and $t_0^+$. HIT configuration.

Figure 3.2 - Comparison of the turbulent kinetic energy spectra at time 0 (dotted-dashed line) and $t_0^+$ (solid line). HIT configuration.

3.1.3 Results

The HIT test case can be easily validated by comparison with theory. Except for the scheme analysis, all results shown were obtained with the TTGC scheme. First, the temporal evolution of both the Kolmogorov and the integral length scales is compared to the limits given by Boughanem & Trouvé (1996) to verify the spatial resolution accuracy. Then, the turbulent
kinetic energy decay is compared to theory. Finally, a discrete balance of turbulent kinetic energy is derived to evaluate the effect of the convective scheme. For this part only, results for both the LW and the TTGC schemes are shown. All quantities are plotted versus time non-dimensionalised by the initial turnover time of the biggest eddies, that is to say $t/\tau_{f,0}$.

Temporal evolution of the integral length scales $L_{f,ii}^i$ and Kolmogorov scales $\eta_{f,K}$

![Figure 3.3 - Temporal evolution of the integral length scales ($L_{f,11}^1$: □, $L_{f,22}^2$: △, $L_{f,33}^3$: +) (a.) and the Kolmogorov length scale, $\eta_{f,K}$ (b.). HIT configuration](image)

The first step is to check the spatial resolution criteria summarised in Eqs. (3.15) and (3.16). Figure 3.3 a. shows the temporal evolution of the integral length scales $L_{f,ii}^i$ non-dimensionalised by $L_D^+$/15 whereas Fig. 3.3 b. focuses on the temporal evolution of the Kolmogorov scale $\eta_{f,K}^+$ non-dimensionalised by $\Delta x^+$/2 so that the criteria are represented by a horizontal line at 1 in Fig. 3.3. Initially, all scales are in the limits of spatial resolution accuracy. When time increases, the smallest scales are dissipated by viscosity, which increases the Kolmogorov length scale. Consequently, the dissipative scales keep being well resolved all the simulation long. Meanwhile, the two-point correlation of velocity also increases, and so do the integral length scales. Thus, the criterion of resolution of the most energetic eddies is not well satisfied. For $t/\tau_{f,0} < 6$, the temporal evolution of $L_{f,ii}^+\approx t/\tau_{f,0}$ is all the same linear, suggesting there is no real problem of resolution. Then, the change of slope indicates that the three length scales saturate. However, there is not much turbulent kinetic energy in the box ($q_f^2/q_{f,0}^2 \leq 6\%$ for $t/\tau_{f,0} \geq 6$) (see Fig. 3.5 a.). It is to be noted that $L_{f,33}^3\approx t/\tau_{f,0}$ remains two times smaller than the two other integral length scales, suggesting a slight anisotropy of the velocity field. The length of the box, finite and not large enough compared to the integral length scales, must be at the origin of the discrepancy.
Temporal turbulent kinetic energy decay

Two validations for the temporal turbulent kinetic energy decay are proposed hereafter, comparing the results provided by AVBP_TPF with theory and with NTMIX3D results from Moreau (2006):

- Non forced HIT is decaying and the rates of decay are well known (see Eqs. (3.23), (3.24) and (3.25)). The turbulent time scale is a good candidate to evaluate the constant $C_{\epsilon_f}$. Figure 3.4 shows its evolution versus time that should be and effectively is linear. The coefficient $C_{\epsilon_f}$ in the present simulation is found to 1.45, smaller than the experimental value, $C_{\epsilon_f} = 1.92$.

![Figure 3.4 - Temporal evolution of the turbulent time scale relative to the most dissipative eddies. HIT configuration.](image)

- Figure 3.5 compares the temporal evolution of the turbulent kinetic energy computed with AVBP_TPF and NTMIX3D. It shows very good agreement although the spatial scheme is much lower order for AVBP_TPF ($2^{nd}$ order) than for NTMIX3D ($6^{th}$ order).

Discrete balance equation for turbulent kinetic energy

In a decaying HIT flow, Eq. (3.21) shows that at every instant, the dissipation due to molecular viscosity, $\epsilon_f$, theoretically balances the temporal variation of turbulent kinetic energy $dq_f^2/dt$. When performing numerical simulations, the two terms do not strictly balance, mainly due to numerical errors. Following Moureau (2004), a discrete balance equation for the turbulent kinetic energy is derived hereafter to show that the turbulent kinetic energy budget is well closed in the simulations, and to compare the dissipative properties of the Lax-Wendroff and TTGC schemes.

82
3.1 Gas Homogeneous Isotropic Turbulence flow

The variation of kinetic energy can be obtained directly from mass and momentum variations, as shown in Eq. (3.31):

$$\frac{\partial \frac{1}{2} \rho f u_{f,i}^2}{\partial t} = u_{f,i} \frac{\partial \rho f u_{f,i}}{\partial t} - \frac{u_{f,i}^2}{2} \frac{\partial \rho f}{\partial t}$$ \hspace{1cm} (3.31)

The most intuitive discrete form of Eq. (3.31) is:

$$\frac{1}{2} \rho f^{(n+1)} u_{f,i}^{(n+1)}^2 - \frac{1}{2} \rho f^{(n)} u_{f,i}^{(n)}^2 \Delta t = \left( u_{f,i}^{(n)} + u_{f,i}^{(n+1)} \right) \left( \rho f^{(n+1)} u_{f,i}^{(n+1)} - \rho f^{(n)} u_{f,i}^{(n)} \right) \left( \frac{1}{2} \right)$$

$$- \left( u_{f,i}^{(n)} \right) \left( \rho f^{(n+1)} - \rho f^{(n)} \right) \left( \frac{1}{2} \right) \Delta t$$ \hspace{1cm} (3.32)

where \( n \) stands for the \( n^{th} \) iteration. Using a Runge-Kutta time discretisation leads to the following form for mass and momentum equations:

$$\frac{\rho f^{(n+1)} - \rho f^{(n)}}{\Delta t} + \mathcal{C}(\rho f) = 0$$ \hspace{1cm} (3.33)

$$\frac{\rho f^{(n+1)} u_{f,i}^{(n+1)} - \rho f^{(n)} u_{f,i}^{(n)}}{\Delta t} + \mathcal{C}(\rho f u_{f,i}) = \mathcal{A}(\rho f u_{f,i}) + \mathcal{V}_{lam}(\rho f u_{f,i}) + \mathcal{V}_{avis}(\rho f u_{f,i})$$ \hspace{1cm} (3.34)

where \( \mathcal{C} \) stands for a convective contribution, \( \mathcal{A} \) for a pressure gradient contribution and \( \mathcal{V} \) for the viscous contributions. Eqs. (3.32), (3.34) and (3.34) allow to obtain the discrete balance.
equation of kinetic energy:

\[
\frac{1}{2} \rho_j^{(n+1)} u_{f,j,i}^{(n+1)} - \frac{1}{2} \rho_j^{(n)} u_{f,j,i}^{(n)} \left\langle \frac{\Delta q_j^2}{\Delta t} \right\rangle = - \left( u_{f,j,i}^{(n+1/2)} \mathcal{C}(\rho_j u_{f,j,i}) - \frac{u_{f,j,i}^{(n)} u_{f,j,i}^{(n+1)}}{2} \mathcal{C}(\rho_j) \right) - \mathcal{C}(q_j^2)
\]

\[+ u_{f,j,i}^{(n+1/2)} \mathcal{A}(\rho_j u_{f,j,i}) + u_{f,j,i}^{(n+1/2)} \mathcal{V}_{\text{lam}}(\rho_j u_{f,j,i}) + u_{f,j,i}^{(n+1/2)} \mathcal{V}_{\text{avis}}(\rho_j u_{f,j,i})
\]

A spatial integration over the whole computational domain leads to the global equilibrium equation:

\[
\left\langle \frac{\Delta q_j^2}{\Delta t} \right\rangle = \left\langle \mathcal{C}(q_j^2) \right\rangle + \left\langle \mathcal{A}(q_j^2) \right\rangle + \left\langle \mathcal{V}_{\text{lam}}(q_j^2) \right\rangle + \left\langle \mathcal{V}_{\text{avis}}(q_j^2) \right\rangle
\]  

(3.35)

In Eq. (3.35), \(\epsilon_{f,\text{conv}}\) is the kinetic energy dissipated or undissipated by the numerical convective scheme, \(\epsilon_{f,\text{ac}}\) is the part of kinetic energy transferred to internal energy by acoustic effects, \(\epsilon_{f,\text{vislam}}\) is the energy transferred to internal energy by molecular diffusion and \(\epsilon_{f,\text{avis}}\) is the energy dissipated by artificial viscosity effects. It is important to note that \(\epsilon_{f,\text{conv}}\) should be negligible because it is a convective term, \(\epsilon_{f,\text{avis}}\) should be small because use of artificial viscosity is very limited and \(\epsilon_{f,\text{vislam}}\) is normally small for low Reynolds number flows.

Limiting to HIT flows at low Mach number, the dissipation is only due to the viscous term \(\epsilon_{f,\text{vislam}}\) and all terms, \(\epsilon_{f,\text{conv}}, \epsilon_{f,\text{ac}}\) and \(\epsilon_{f,\text{avis}}\), should be zero. In this study, no artificial viscosity was used. The two terms \(\epsilon_{f,\text{conv}}\) and \(\epsilon_{f,\text{ac}}\) are then gathered in a numerical dissipation term, \(\epsilon_{f,\text{num}}\). As acoustic effects are negligible (they account for less than 1% of the budget in this case), quantification of the numerical dissipation \(\epsilon_{f,\text{num}}\) directly gives access to the dissipative property of the numerical convected scheme.

Dividing all the terms of Eq. (3.35) by \(\left\langle \Delta q_j^2/\Delta t \right\rangle\), the turbulent kinetic energy budget finally yields:

\[1 = \epsilon_{f,\text{vislam}}^+ + \epsilon_{f,\text{num}}^+\]  

(3.36)

The two terms of the RHS of Eq. (3.36) are evaluated for both Lax-Wendroff and TTGC schemes in Fig. 3.6. As expected, TTGC scheme is almost not dissipative whereas Lax-Wendroff scheme dissipates about 5% of the total kinetic energy in the box at the beginning of the computation before stabilising around 3%.
3.2 Two-phase flow simulations: previous work with the EE mesoscopic approach

Few studies have been devoted to the evaluation of Eulerian approaches for the simulation of an ensemble of particles interacting with a DNS of decaying Homogeneous Isotropic Turbulence. When the particle relaxation time is small compared to the Kolmogorov time-scale, Ferry & Balachandar (2001) and Rani & Balachandar (2003) showed that the equilibrium Eulerian approach (see Section 1.4.3) is well suited to predict both the particle number density and velocity fields. Such a method considers a transport equation for the particle number density and compute the particle velocity using a Taylor expansion in $\tau_p$ of the local gas quantities. Their computational cost is therefore much smaller than DPS. However, for high Stokes numbers, results are less accurate since the Taylor expansion depends on the Stokes number.

First attempt to use the Euler-Euler mesoscopic approach for high Stokes numbers was made by Kaufmann et al. (2006). In this approach, the mesoscopic formalism derived by Février et al. (2005) and presented in Section 1.5 was used to solve transport equations for particle number density, particle correlated velocity and particle uncorrelated energy. Hereafter, the characteristics of the dispersed phase simulated are presented in Section 3.2.1 and the main results obtained by Kaufmann et al. (2006) are summarised in Section 3.2.2.
3.2.1 Dispersed phase properties

Kaufmann et al. (2006) used the fluid decaying HIT test case described in Section 3.2 to characterise the motion of particles in such a flow, depending on the inertia of the particles. Interaction between the carrier phase and the dispersed phase is restricted to Stokes drag force (see Eq. 1.15 in Section 1.2.1). Only one-way coupling is considered, which means that the influence of the particles on the fluid flow is neglected. With these restrictions, the dynamics of particles in a given HIT fluid flow realization depend only on the Stokes number and the initial conditions.

Kaufmann et al. (2006) performed two-phase flow simulations for a wide range of Stokes numbers, from 0.037 to 1.1. Here, the Stokes numbers are based on the fluid integral time scale evaluated when the particles are injected in the gas flow, \( \tau_{f,i}^{+} \left( \tau_{0}^{+} \right) = 4.19 \). In this chapter, focus is made on the most difficult case to simulate with the EE mesoscopic approach, corresponding to the characteristic Stokes number \( St = 1.1 \), and exhibiting very strong particle number density gradients. Table 3.4 summarises the parameters of the dispersed phase for this specific case at time \( t_{0}^{+} = 4.233 \) when the particles are added to the fluid flow. \( t_{0}^{+} = 4.233 \) corresponds to one turnover time of the biggest eddies when the fluid flow is a true HIT field (see Section 3.1.2).

<table>
<thead>
<tr>
<th>( t^{+} \left( - \right) )</th>
<th>( St = \tau_{p}/\tau_{f,i} )</th>
<th>( \rho_{p} \left( kg.m^{-3} \right) )</th>
<th>( d_{p} \left( \mu m \right) )</th>
<th>( \tilde{n}_{p} \left( m^{-3} \right) )</th>
<th>( \tilde{u}_{p,i} \left( m.s^{-1} \right) )</th>
<th>( \delta \tilde{\theta}_{p} \left( m^{2}.s^{-2} \right) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_{0}^{+} )</td>
<td>1.1</td>
<td>1916</td>
<td>17.3</td>
<td>( 10^{13} )</td>
<td>( u_{f,i} )</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 3.4 - Properties of the dispersed phase at time \( t_{0}^{+} = 4.233 \) when the particles are injected into the fluid flow. HIT configuration.

The particle density corresponds to typical fuel density but their diameter is smaller than the mean diameter usually observed in a droplet spray. The particle distribution is initially uniform, leading to a uniform volume fraction: \( \alpha_{p} = 2.7\% \). As the Stokes number of the two-phase flow is rather small, the particle velocity field must be close to the fluid flow. Therefore, it is reasonable to initialise the dispersed phase correlated velocity field with the gas velocity field and consequently, the Random Uncorrelated Energy with a value close to zero. Note that the RUE field cannot be initialised to zero: since all production and dissipation terms in the transport equation for particle RUE are proportional to RUE, it will stay at zero if initialised to zero. An arbitrary small non-zero value is therefore chosen to initialise particle RUE.

3.2.2 Summary of the results obtained by Kaufmann et al. (2006)

The code used by Kaufmann et al. (2006) is a former version of AVBP_TPF (V4.8) where only the Lax-Wendroff scheme was available.
3.2 Two-phase flow simulations: previous work with the EE mesoscopic approach

For small Stokes numbers, the particle velocity field is expected to follow closely the gas one. This induces small preferential concentration effects with a particle Stokes number close to $St = 0.037$. Simulations with the mesoscopic approach show very good agreement with DPS results when focusing on the correlated velocity. As for the number density distribution, little discrepancies may be due to the use of LW, known to smooth the gradients while introducing dispersive errors. This may explain smaller preferential concentration effects compared to DPS results.

When increasing the Stokes number, simulations using the mesoscopic approach fail. At this point, the spatial resolution is questioned. Indeed, the preferential concentration effects increase with the Stokes number, leading to strong variations in the number density field. If the spatial resolution is unsufficient, dispersive errors due to the centred convective scheme induce negative values in the number density field. An increase in the spatial resolution up to $192^3$ cells (which strongly increases the computational cost) did not solve the problem. Therefore, the spatial resolution is not responsible for the simulation failure.

To overcome this numerical difficulty, Kaufmann et al. (2006) introduced a subgrid bulk viscosity, $\xi_{p, sgs}$, in analogy with von Neumann & Richtmeyer (1950) to act directly on the compressible part of the correlated velocity:

$$
\begin{align*}
\frac{\partial}{\partial t} \tilde{n}_p \tilde{u}_{p,i} + \frac{\partial}{\partial x_j} \tilde{n}_p \tilde{u}_{p,i} \tilde{u}_{p,j} &= -\frac{\tilde{n}_p}{\tau_p} (\tilde{u}_{p,i} - u_{f,i}) - \frac{\partial}{\partial x_i} \left( \frac{2}{3} \tilde{n}_p \delta \tilde{\theta}_p \right) \\
&\quad - \frac{\partial}{\partial x_j} \tilde{n}_p \delta \tilde{R}_{p,ij} + \frac{\partial}{\partial x_i} \frac{\xi_{p, sgs}}{\tilde{n}_p} \frac{\partial}{\partial x_k} \tilde{u}_{p,k},
\end{align*}
$$

(3.37)

with $\xi_{p, sgs} = C_{p, sgs} \tilde{n}_p \Delta^2 | \frac{\partial \tilde{u}_{p,k}}{\partial x_k} |$

(3.38)

$C_{p, sgs}$ is the model coefficient that was chosen equal to 50 by Kaufmann et al. (2006). Therefore, the mesoscopic equations were solved for a modified correlated velocity, $\tilde{u}_{p,i}$, and so a modified particle number density, $\tilde{n}_p$. The main effect of the subgrid bulk viscosity is to reduce particle number density gradients. Thus, the dispersive errors introduced by the LW scheme (see Section 2.2.3) have less impact. Moreover, adding the subgrid bulk viscosity in the particle transport equations significantly increased the particle RUE prediction. The model coefficient $C_{p, sgs}$ was chosen so that the particle RUE prediction was in good agreement with the DPS results. Since the particle subgrid viscosity did not affect either the particle mesoscopic energy or the fluid-particle correlation, the total particle kinetic energy predicted by the EE mesoscopic approach was finally in very good agreement with the EL simulations. As a contrast, preferential concentration effects were considerably under-estimated.

87
3.3 Two-phase flow simulations: present work with the EE mesoscopic approach

Strong compressibility effects occur at the Stokes number considered by Kaufmann et al. (2006). They lead to large segregation effects that imply shock-like number density gradients. It is well-known that equations creating such gradients are difficult to handle numerically. The objective here is to show how these numerical difficulties may be overcome, and to validate AVBP_TPF.

The particle-laden decaying HIT flow, with gas and particle characteristics identical to the test case from Kaufmann et al. (2006), is therefore re-investigated. Five cases are computed, accounting first for the subgrid bulk viscosity model or not, changing then the convective scheme, also increasing the grid resolution, and finally decreasing the artificial dissipation for the dispersed phase. The parameters of the five simulations are detailed in Section 3.3.2. Then, the DNS performed by Kaufmann et al. (2006) is re-run to show the impact of the dispersive errors and the subgrid bulk viscosity (see Section 3.2.2) on the results. At this point and till the end of the chapter, the TTGC scheme is preferred without any subgrid bulk viscosity. The influence of the convective scheme, as well as the grid resolution and the particle artificial viscosity, on the results is shown in three steps. First, the results are qualitatively analysed in Section 3.3.3, insisting on the sensitivity of the particle number density field on both the scheme and the resolution. Second, Section 3.3.4 focuses on the temporal evolution of some integral properties such as particle segregation and different particle energies. Finally, spectral properties of the two-phase flow fields are investigated in Section 3.3.5.

### 3.3.1 Test cases

<table>
<thead>
<tr>
<th>Name</th>
<th>Number of cells</th>
<th>Convective Scheme</th>
<th>A.V. Coefficients</th>
<th>RUE flux limitor</th>
<th>SGS bulk viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>EE_64_lw_nosgs</td>
<td>$64^3$</td>
<td>LW</td>
<td>0.055 / 0.03</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>EE_64_lw_sgs</td>
<td>$64^3$</td>
<td>LW</td>
<td>0.055 / 0.03</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>EE_64_ttgc_nosgs</td>
<td>$64^3$</td>
<td>TTGC</td>
<td>0.055 / 0.03</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>EE_128_ttgc_nosgs</td>
<td>$128^3$</td>
<td>TTGC</td>
<td>0.055 / 0.03</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>EE_128_ttgc_nosgs2</td>
<td>$128^3$</td>
<td>TTGC</td>
<td>0.04 / 0.03</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>

Table 3.5 - Test cases and corresponding parameters for the dispersed phase. HIT configuration.
Table 3.5 summarises the parameters of the five calculations investigated hereafter. The two convective schemes as well as the grid resolution are the major varying parameters. The use of artificial viscosity for the dispersed phase is classically required and the two coefficients given in Table 3.5 correspond to the two AV coefficients, $\nu_2^{AV}$ and $\nu_4^{AV}$, defined in Section 2.3.1. As discussed in Section 2.3.2, the particle RUE flux limitor prevents non-physical negative values for particle RUE due to dispersion errors. The SGS bulk viscosity model proposed by Kaufmann et al. (2006) is presented in Section 3.2.2.

The calculation noted $EE_{64}\_lw\_sgs$ is not completely identical to the simulation performed by Kaufmann et al. (2006): the particle Artificial Viscosity model is different. Kaufmann et al. (2006) directly applied the fluid Jameson AV model to the dispersed phase quantities. Here, the Jameson artificial viscosity model developed for the dispersed phase and presented in Section 2.3.1 is preferred because it acts more locally in the regions where strong gradients of particle number density or velocity field appear, which is the main difficulty here. Moreover, the RUE flux limitor is employed to prevent from local negative values in the particle number density field. As a result, the two simulations do not provide exactly the same solutions. Nevertheless, it has been verified that the discrepancies are very small and that the temporal evolution of both the particle segregation and the particle total kinetic energy are quasi-identical (Maximum differences are respectively 2.2% and 1.3%). The use of the subgrid bulk viscosity is the only difference between the cases $EE_{64}\_lw\_nosgs$ and $EE_{64}\_lw\_sgs$.

The case $EE_{64}\_ttgc\_nosgs$ can be directly compared to the case $EE_{64}\_lw\_sgs$ to highlight the benefits of the TTGC scheme. There is however another difference between the two cases since the subgrid bulk viscosity required by LW is no longer needed for TTGC. The same levels of artificial viscosity are imposed and the RUE flux limitor is used in both cases. The influence of the resolution is investigated with the case $EE_{128}\_ttgc\_nosgs$, where only the number of grid points is changed compared to the case $EE_{64}\_ttgc\_nosgs$.

Finally, the only difference between the cases $EE_{128}\_ttgc\_nosgs$ and $EE_{128}\_ttgc\_nosgs2$ is the amount of particle 2nd order Artificial Viscosity. The value $\beta_2^{AV} = 0.04$ corresponds to the minimum level required to prevent simulation failure.

<table>
<thead>
<tr>
<th>Case</th>
<th>$EE_{64}_lw_sgs$</th>
<th>$EE_{64}_ttgc_nosgs$</th>
<th>$EE_{128}_ttgc_nosgs$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU time (s)</td>
<td>1091</td>
<td>2451</td>
<td>39878</td>
</tr>
<tr>
<td>Efficiency / ite / node (\mu s)</td>
<td>7.34</td>
<td>16.55</td>
<td>17.18</td>
</tr>
</tbody>
</table>

Table 3.6 - Code efficiency for the different test cases. The statistics are given for 0.09 ms ($t^+ \approx 30$) computed on 8 processors on a COMPAQ Alpha Server SC45 machine. HIT configuration.

It must be noticed that the computational cost of the three simulations is really different, due
to the different convective scheme and the different grid resolution. Using TTGC instead of LW is about 2.25 times more expensive on the $64^3$ grid, doubling the resolution multiplies the computational cost by 16. Details are available in Table 3.6.

### 3.3.2 Questioning the accuracy of the Lax-Wendroff scheme

In this section, the test cases $EE_{64} lw nosgs$ and $EE_{64} lw sgs$ (see Table 3.5) are analysed to push forward the dispersion error of the LW scheme and to investigate the role of the subgrid bulk viscosity $\xi_{p,sgs}$ defined in Section 3.2.2.

When the subgrid bulk viscosity is not included, the simulation fails at point $B$ where the number density becomes negative (see Fig. 3.7) at an early time $t_4$ that corresponds to 9 iterations. Figure 3.8 shows the fields of particle number density and particle correlated velocity at this time. As expected, point $B$ is located in a region where the particle number density is very low corresponding to a strong correlated velocity gradient.

To show the dispersion error introduced by the LW scheme, both the particle number density and the particle correlated velocity profiles are plotted on the three lines $x = x_B$, $y = y_B$ and $z = z_B$ (see Fig. 3.7). This is done in Fig. 3.9 for four increasing times: $t_1$ corresponds to the initial condition whereas $t_4$ is the time when the simulation fails. With increasing time, the gradients of particle number density become stronger along all lines. This increases the
dispersion error, leading to a negative value for $\nabla n_p$. The evolution of the particle correlated velocity seems smoother, except in the vicinity of the non-physical values of $\nabla n_p$. Besides, the particle RUE is also sensitive to this dispersive phenomenon and becomes locally negative.

Figure 3.8 - Fields of particle number density (a.) and particle correlated velocity (b.) in the cross section ($P_B$) at time $t_4$. HIT configuration.

Figure 3.10 shows the influence of the subgrid bulk viscosity model (see Section 3.2.2) on the results in the $EE_{64}lw_{sgs}$ test case. Direct comparison with Fig. 3.9 can be made since the same quantities are plotted at the same times. It is clear that the bulk viscosity gets around the dispersion problem, as it leads to smoother number density gradients. In this case, the simulation does not fail. However, the particle RUE still remains negative at some points in the domain.

To overcome the critical problem of numerical dispersion, the TTGC scheme presented in Section 2.2.2 has been extended to the dispersed phase in the version V2.0 of AVBP_TPF. As expected, the reduction of the dispersion errors is sufficient to prevent the simulation to fail and the subgrid bulk viscosity is no longer useful. Nevertheless, some local negative values of RUE are still observed, and the RUE flux limitor (see Section 2.3.2) is used to keep it positive. Note that for all the test cases, the use of some artificial dissipation is necessary for both phases and the Jameson model developed for the dispersed phase in Section 2.3.1 is therefore added to the standard mesoscopic equations for the dispersed phase. Hereafter, the results provided by $EE_{64}lw_{sgs}$ test case are compared with the three other cases carried out with TTGC, $EE_{64}tgc_{nosgs}$, $EE_{128}tgc_{nosgs}$ and $EE_{128}tgc_{nosgs2}$.
Figure 3.9 - Particle number density (left side) and correlated velocity (right side) profiles on lines $x = x_B$ (a. & b.), $y = y_B$ (c. & d.) and $z = z_B$ (e. & f.) for increasing times. $t_1$ corresponds to the initial condition whereas $t_4$ is the time when the simulation fails. The subgrid bulk viscosity model was not used here. HIT configuration
3.3 Two-phase flow simulations: present work with the EE mesoscopic approach

Figure 3.10 - Particle number density (left side) and correlated velocity (right side) profiles on lines $x = x_B$ (a. & b.), $y = y_B$ (c. & d.) and $z = z_B$ (e. & f.) for increasing times. The subgrid bulk viscosity model was used in this case. HIT configuration.
3.3.3 Results: local instantaneous properties

Figure 3.11 shows instantaneous fields of particle number density non-dimensionalised by the mean value in the box \( \langle \hat{n}_p \rangle = 10^{13} \) and particle correlated velocity magnitude in the cutting plane \( z = 0 \). The time considered is \( t^+ = 10.8 \) that corresponds to the first occurrence of a peak of segregation. The case \( EE_{128,ttgc,nosgs} \) is not plotted because differences with the case \( EE_{128,ttgc,nosgs2} \) are minor.

Comparing the fields provided by the LW and the TTGC schemes on the coarsest grid shows that both schemes globally capture the large scales of the dispersed phase flow. The particle correlated velocity fields show little differences, not only in the dispersed phase flow structure but also in the levels. The main difference is in the particle number density field with much higher values when using TTGC than when using LW.

Increasing the grid resolution gives access to a wider range of scales as observed on the particle number density field. Again the impact on the particle correlated velocity is very small.

3.3.4 Results: integral properties

Figure 3.12 displays the temporal evolution of the mean particle correlated energy, the mean fluid-particle correlation and the mean particle random uncorrelated energy versus time for the last four cases detailed in Table 3.5. As the first case \( EE_{64,lw,nosgs} \) failed at an early time (see Section 3.2.2), it is not shown here. In addition, the results from the EL simulations obtained by Moreau (2006) are plotted for direct comparison.

The particle correlated energy and the fluid-particle correlation are identical for all the cases, and in particular to the Lagrangian simulations. Only the initial decay of the two integral quantities shows little discrepancy between the EE simulations performed on the \( 64^3 \) grid and the EL ones, but the EE simulations performed on the \( 128^3 \) grid are in very good agreement with the EL ones.

In contrast, the temporal evolution of the particle uncorrelated energy greatly differs for the different cases. The effect of the subgrid bulk viscosity model used in the case \( EE_{64,lw,sgs} \) clearly appears to be too large on this quantity. The bulk viscosity artificially produces particle RUE, with a model coefficient \( C_{p,sgs} \), chosen to match the EL results. Without this term, an important part of particle RUE is missed for low resolution. However, the particle RUE greatly increases with the grid resolution, and even more when the particle AV is decreased to its minimum value. The case \( EE_{128,ttgc,nosgs2} \) finally gives results as good as the case \( EE_{64,lw,sgs} \) without artificially producing particle RUE. This reaches the conclusions of Moreau (2006) who showed that the particle RUE predictions obtained by filtering the EL simulations were largely influenced by the projector filter width. As a conclusion and not
3.3 Two-phase flow simulations: present work with the EE mesoscopic approach

Figure 3.11 - Comparison of the non-dimensional particle number density, $\tilde{n}_p / \langle \tilde{n}_p \rangle$, and the particle correlated velocity field, $\tilde{u}_p$, at time $t^+ = 10.8$ in the cutting plane $z = 0$ for the cases EE$_{64}$lw_sgs (a. & b.), EE$_{64}$ttgc_nosgs (c. & d.) and EE$_{128}$ttgc_nosgs2 (e. & f). HIT configuration.
surprisingly, the predictions for the temporal evolution of particle RUE finally shows very good agreement with the EL simulations when the TTGC scheme is used on the finest grid and artificial dissipation is reduced to the minimum required. For this specific case referenced as $EE_{128\_ttgc\_nosgs2}$, the temporal evolution of the particle correlated energy $\langle \delta q_p^2 \rangle$, the particle RUE $\langle \delta q_p^2 \rangle$, and the fluid-particle correlation $\langle q_{fp} \rangle$, are plotted in Fig. 3.13, as well as the fluid kinetic energy $\langle q_f^2 \rangle$, as well as the total particle kinetic energy $\langle q_p^2 \rangle$. The overall agreement between the EL and the EE simulations is very good. The carrier phase kinetic energy decreases due to viscosity. There is a delay before the total particle kinetic energy follows the fluid kinetic energy decay that corresponds almost to one particle relaxation time. Besides, due to particle inertia, the particle velocities become partially uncorrelated with the fluid velocities, leading to an increase in particle RUE. The peak of particle RUE, that accounts for about 14% of the total particle energy, is well predicted, leading to an accurate prediction of the total particle kinetic energy.

Finally, the temporal evolution of the particle segregation defined as $\langle \hat{n}_p^2 \rangle / \langle \hat{n}_p \rangle^2$, is plotted on Fig. 3.14 for the four EE cases and the EL simulation. An important difference in the maximum value obtained with LW and TTGC is observed. It is mainly due to the subgrid bulk viscosity model introduced by Kaufmann et al. (2006) that artificially produces particle RUE, and decreases preferential concentration effects. When using the TTGC scheme, the production of particle RUE is due exclusively to the physical production terms in the transport equations for particle RUE, and the particle number density field is not affected. As expected, the results obtained with TTGC for particle segregation improve when the grid resolution is increased and the artificial dissipation is decreased. Finally, the case $EE_{128\_ttgc\_nosgs2}$ again provides the best agreement with the EL simulations. The EE mesoscopic approach still underestimates the particle segregation about 20%, which may be due to the ensemble averaging operator, and the numerical scheme still to be improved.

3.3.5 Results: spectral properties

Additional information is provided in Fig. 3.15, comparing the spectra of fluid kinetic energy and particle correlated energy obtained with the Lagrangian and the Eulerian simulations. For the EE results, only the cases $EE_{64\_ttgc\_nosgs}$ and $EE_{128\_ttgc\_nosgs}$ are analysed. This is done for increasing times varying from $t^+ = 2.1$ to $t^+ = 5.7$ with a constant time increment $\Delta t^+ \approx 0.5$.

Fluid spectra are in good agreement between the EL and EE simulations. All the cases show a decrease with time of the spectrum amplitude. Due to the very low Reynolds number, most of the energy is concentrated around the smallest wave numbers and the spectra rapidly decrease in the region of large wave numbers. Note that the agreement between EL an EE calculations is slightly better when using the finest grid.
3.4 Conclusions

Discrepancies between the two approaches (EE and EL) are more significant for the particle spectra. A decrease with time of the spectrum amplitude is still observed on the three plots. The spectrum evolution is well predicted with the EE approach at small wave numbers. In this region, the particle spectrum is very similar to the fluid one due to the strong interaction through drag force. At large wave numbers however, the EE results do not exhibit the change in slope at a transition wave number, noted $k_p^{tr}$, underscored by Moreau (2006) on the Lagrangian fields. For wave numbers larger than $k_p^{tr}$, the Lagrangian spectra exhibit a slope with a constant coefficient: $\tilde{E}_p(k) \simeq k^{-2}$. Moreau (2006) used an analogy with supersonic turbulent flows to justify this specific slope: it appears in HIT supersonic fluid flows (Porter et al., 1992) and is associated with a regime where shocks dominate the flow evolution. Looking back at the mesoscopic transport equations for the dispersed phase, one may observe that the dissipation of particle correlated energy is due to the uncorrelated motion term $\delta \tilde{R}_{p,ij} \partial \tilde{u}_{p,i} / \partial x_j$. This term is shown by Moreau (2006) to be non-zero around the particle clusters, that can be considered as surfaces, or even shocks, due to the strong gradients of particle number density observed. Why the EE simulations do not show any change in the slope is not clear. Either the use of artificial dissipation in the particle transport equations or the RUV viscosity assumption may be at the origin of this behavior.

3.4 Conclusions

The particle-laden HIT flow already calculated by Kaufmann et al. (2006) using the mesoscopic transport equations for the dispersed phase has been re-investigated. The authors showed that the case was difficult to handle numerically because of large compressibility effects in the particle field.

The numerical tools specifically developed for the dispersed phase in this work and detailed in Chapter 2, have been tested on this configuration. The capability of the TTGC scheme coupled with the particle AV model to stabilise the simulations of such two-phase flows has been shown. The main advantage of TTGC in comparison with LW is its low dispersion. A RUE local flux limiter is needed to guarantee positive values of particle RUE but its impact on the results is minor. As a consequence, the subgrid bulk viscosity introduced by Kaufmann et al. (2006) is no longer required and is dropped in the transport equation for particle correlated velocity.

The comparisons with the Lagrangian results obtained by Moreau (2006) show very good agreements when analysing the temporal evolution of particle total kinetic energy and fluid-particle correlation. Even the prediction of particle segregation, that remains the main difficulty of the EE mesoscopic approach, is good although the maximum value is still slightly under-
estimated. The spectral analysis of the results for the dispersed phase reveal that the Eulerian mesoscopic simulations are not able to predict the $k^{-2}$ slope underscored by Moreau (2006) at large wave numbers. Some additionnal work should be done on the numerical aspects that are questioned at this point. Nevertheless, there is sufficient confidence at this point in the numerical tool to consider more complex geometries.
Figure 3.12 - Temporal evolution of the non-dimensional mean particle correlated energy (a.), mean fluid-particle correlation (b.), and mean particle RUE computed with the EL simulation (squares) and the four EE simulations: EE\textsubscript{64} lw\_sgs (dashed line + circles); EE\textsubscript{64} ttgc\_nosgs (dotted-dashed line); EE\textsubscript{128} ttgc\_nosgs (long-dashed line + triangles); EE\textsubscript{128} ttgc\_nosgs2 (solid line)
Figure 3.13 - Comparison of non-dimensional integral properties resulting from the EL simulation (symbols) and the case EE_{128}ttgc_nosgs (lines)

Figure 3.14 - Temporal evolution of the particle segregation. Comparison between the EL simulation (squares) and the four EE simulations: EE_{64}lw_sgs (dashed line + circles); EE_{64}ttgc_nosgs (dotted-dashed line); EE_{128}ttgc_nosgs (long-dashed line + triangles); EE_{128}ttgc_nosgs2 (solid line)
3.4 Conclusions

Figure 3.15 - Comparison of the fluid turbulent kinetic energy spectrum (left side) and the particle correlated energy spectrum (right side) for the EL simulations (Moreau, 2006) (a. & b.), and the EE cases EE_64_ttg_c_nosgs (c. & d.) and EE_128_ttg_c_nosgs2 (e. & f.). The times considered vary from $t^+ = 2.1$ to $t^+ = 5.7$ with a time spacing, $\Delta t^+ = 0.5$. On the right side, the dashed line stands for the $k^{-2}$ slope whereas the dotted-dashed line represents the $k^{-5}$ slope.

101
Chapter 4

Large Eddy Simulation

Large-Eddy Simulation (LES) (Sagaut, 2000; Pope, 2000) is nowadays recognized as an alternative approach to the classical Reynolds Averaged Navier-Stokes (RANS) methodologies. Although conceptually very different, these two approaches aim at providing new systems of governing equations to mimic the characteristics of turbulent flows. The derivation of the governing LES equations is obtained by applying operators to the exact set of transport equations. Unclosed terms arise from these manipulations and models need to be supplied for the problem to be solved. The major differences between RANS and LES come from the operator employed in the derivation.

- In RANS the operation consists of an ensemble average over a set of realizations of the studied flow (Pope, 2000; Chassaing, 2000). The unclosed terms are representative of the physics taking place over the entire range of turbulent scales present in the ensemble of realizations under consideration.

- In LES, the operator is usually a spatially localized time independent filter of given size, \( \Delta \), to be applied to a single realization of the studied flow. Resulting from this spatial filtering is a separation between the large (greater than the filter size) and small (smaller than the filter size) scales. The unclosed terms are in LES representative of the physics associated with the small-scale structures (with high frequencies) present in the flow.

LES has clearly shown its potential in predicting gaseous turbulent flows in complex geometries. Indeed, the filtering approach allows a dynamic representation of the large-scale motions that are crucial to determine the flow in such configurations (Caraeni et al., 2000; Forkel & Janicka, 2000; Selle et al., 2004; Moureau et al., 2005; Martin et al., 2006; Schmitt et al., 2007). Small-scale processes still need to be modeled but they are thought to be more “universal”, making the simulation in principle less sensitive to the models.
Extension of LES to two-phase flows in complex geometries is recent. Deutsch & Simonin (1991) and Wang & Squires (1996) for instance, applied the Euler-Lagrange approach to academic configurations, while Ham et al. (2003) or Riber et al. (2006) worked on more complex geometries. In this approach, LES is performed for the carrier phase and particle trajectories are computed only with the LES-filtered fluid velocity in the drag force model. Some recent work (Armenio et al., 1999; Pozorsky et al., 2004; Fede & Simonin, 2006) addresses the problem of the subgrid fluid turbulence effects on the particle motion. The main issue consists there in determining the subgrid fluid velocity fluctuations along inertial particle trajectories, and to take it into account in the calculation of the particle Lagrangian velocity.

Other approaches for LES of two-phase flows are the Euler-Euler ones, much less developed and used. Shotorban & Balachandar (2006) extended the Equilibrium Eulerian approach in a volume-filtering formulation of the equations (see Section 1.4.3) but their formalism is limited to very small Stokes numbers. Pandya & Mashayek (2002) also developed a LES formalism for a two-fluid approach, introducing a particle density in the space phase that verifies the kinetic equation proposed by Reeks (1992). Subgrid terms classically arise, that are modeled in analogy with Reeks (1992) work. However, no LES using either the Equilibrium Eulerian approach or the two-fluid approach has been published up to now.

The development of a LES formulation for the Euler-Euler mesoscopic approach is the main objective of this work and has been done in close collaboration with Moreau (2006). The aim is to propose a set of LES equations for the dispersed phase. To this purpose, the classical LES-filtering is applied to the mesoscopic transport equations detailed in Section 1.5, and unclosed terms classically arise. An important particularity of the filtered mesoscopic transport equations is in the two different contributions to the unclosed terms, either due to the ensemble averaging or to the spatial filtering. As discussed by Pope (2000), the ideal way to assess the accuracy of subgrid (or turbulent) models is to compare their performances over a broad range of test flows in two steps. The first one consists in a priori testing of a certain number of suitable models on academic configurations, while in the second step, the accuracy of the models is shown a posteriori on different flows. Moreau (2006) computed seven sets of particle Lagrangian simulations of particle-laden decaying HIT flow coupling DNS of the fluid flow and DPS of the dispersed phase. Euler-Euler Mesoscopic fields were then extracted by projecting the Lagrangian fields on the grid. The resulting EE mesoscopic fields were then LES-filtered (using a classical spatial filtering) to obtain LES EE mesoscopic fields. Moreau (2006) tested several models for the different unclosed terms of the LES EE mesoscopic equations. The most accurate models have been implemented in the version V2.0 of AVBP_TP. Then, a posteriori testing was performed on the particle-laden confined jet flow and the confined bluff body gas-solid flow presented respectively in Chapters 5 and 6.

This chapter describes the equations solved for LES of non reactive two-phase flows in AVBP_TP. First, the filtered equations solved for both phases are described in Section 4.1.
Section 4.2 presents the subgrid models, briefly for the gas phase since classical models are used, and more in detail for the dispersed phase since it is the first time they are implemented and tested *a posteriori*. The LES results are validated by comparison with experimental data obtained in statistically stationary flows. Experience showed that great care must be taken when averaging the LES results and comparing numerical and experimental results: this is discussed in Section 4.3.

### 4.1 Filtered transport equations

#### 4.1.1 Filtering procedure

To separate large and small scales, a low-pass (in frequency) filter, $G_\Delta$, is applied to the exact equations (Leonard, 1974). Mathematically, it consists of a convolution product of any quantity $\Phi$, with the filter function $G_\Delta$:

$$\bar{\Phi}(x) = \int_D G_\Delta(x - x') \, \Phi(x') \, dx'$$  \hspace{1cm} (4.1)

The resulting filtered quantity, $\bar{\Phi}$, stands for the large-scale structures of the flow whereas all the structures of size smaller than the filter length, $\Delta$, are contained in the residual field, $\Phi'$:

$$\Phi = \bar{\Phi} + \Phi'$$  \hspace{1cm} (4.2)

When performing LES, the local grid spacing, $\Delta$, determines the filter length: typically, motions smaller than $2\Delta$ are not resolved but modeled. Moreover, the filter length may be increased by dissipation and dispersion of the numerical schemes. Note that the shape of the filter is implicit since it does not appear explicitly in the filtered transport equations.

To apply this filtering procedure to the transport equations described in Chapter 1, the filter $G_\Delta$ must verify some properties that are: conservation of constants, linearity and commutation with temporal and spatial derivatives. The latter is verified only for homogeneous filters (i.e. grid meshes). For the sake of simplicity, this property is assumed hereafter.

For variable density flows, mass weighted filtering (called Favre averaging (Favre, 1969)) is preferred, in order to avoid modeling of additional terms introduced by density fluctuations:

$$\hat{\phi} = \frac{1}{\bar{\rho}} \bar{\rho} \phi$$  \hspace{1cm} (4.3)

In the present case, both phases are compressible and Favre averaging is applied to both sets of equations, considering $\rho_f$ and $\bar{n}_p$ respectively as fluid and particle density.
The resulting LES-filtered gaseous Navier-Stokes equations and particle Euler-Euler mesoscopic equations can be rewritten as standard equations: on the Left-Hand Side (LHS), the convective parts of the equations remain unchanged using the filtered quantities. The residual part of the filtered convective term is regrouped on the Right-Hand Side (RHS) with the diffusive and the source terms that are also modified by the filtering.

### 4.1.2 Filtered Navier-Stokes equations

The gaseous transport equations for LES are obtained by Favre-filtering the instantaneous transport equations (1.1) – (1.3), leading to:

\[
\frac{\partial}{\partial t} \bar{\rho}_f + \frac{\partial}{\partial x_i} \bar{\rho}_f \hat{u}_{f,i} = 0 \tag{4.4}
\]

\[
\frac{\partial}{\partial t} \bar{\rho}_f \hat{u}_{f,i} + \frac{\partial}{\partial x_j} \bar{\rho}_f \hat{u}_{f,i} \hat{u}_{f,j} = -\frac{\partial}{\partial x_j} [\bar{P}_f \delta_{ij} - \bar{T}_{f,ij} + \bar{\rho}_f T_{f,ij}] \tag{4.5}
\]

\[
\frac{\partial}{\partial t} \bar{\rho}_f \hat{E}_f + \frac{\partial}{\partial x_i} \bar{\rho}_f \hat{E}_f \hat{u}_{f,i} = -\frac{\partial}{\partial x_j} [\hat{u}_{f,i}(\bar{P}_f \delta_{ij} - \bar{T}_{f,ij}) + \bar{\tau}_{f,j} + \bar{\rho}_f Q_{f,j}] \tag{4.6}
\]

The resulting subgrid terms noted with block letters, are defined as:

\[
T_{f,ij} = \hat{u}_{f,i} \hat{u}_{f,j} - \hat{u}_{f,i} \hat{u}_{f,j} \tag{4.7}
\]

\[
Q_{f,j} = \hat{u}_{f,i} \hat{E}_f - \hat{u}_{f,i} \hat{E}_f \tag{4.8}
\]

Assumptions and closure models are required for all RHS terms of Eqs. (4.5) and (4.6). They are detailed in Section 4.2.1.

### 4.1.3 Filtered Eulerian mesoscopic equations

- **Transport equations**

Here, the filtering procedure described in Section 4.1.1 is applied to the conservation equations of the dispersed phase (Eqs. (1.53) – (1.55)) as obtained from the ensemble averaging
4.1 Filtered transport equations

procedure:

\[ \frac{\partial}{\partial t} \bar{n}_p + \frac{\partial}{\partial x_i} \bar{n}_p \hat{u}_{p,i} = 0 \] (4.9)

\[ \frac{\partial}{\partial t} \bar{n}_p \hat{u}_{p,i} + \frac{\partial}{\partial x_j} \bar{n}_p \hat{u}_{p,j} = \frac{\bar{n}_p}{\tau_p} (\hat{u}_{f@p,i} - \hat{u}_{p,i}) \]

\[ - \frac{\partial}{\partial x_j} \bar{n}_p \left( \frac{2}{3} \delta \theta_{p} \delta_{ij} + \delta R_{p,ij}^* + T_{p,ij} \right) \] (4.10)

\[ \frac{\partial}{\partial t} \bar{n}_p \delta \theta_{p} + \frac{\partial}{\partial x_j} \bar{n}_p \delta \theta_{p} \hat{u}_{p,j} = -2 \frac{\bar{n}_p}{\tau_p} \delta \theta_{p} - \bar{n}_p \left[ \frac{2}{3} \delta \theta_{p} \delta_{ij} + \delta R_{p,ij}^* \right] \frac{\partial \hat{u}_{p,i}}{\partial x_j} + \bar{n}_p \Pi_p \]

\[ - \frac{\partial}{\partial x_j} \bar{n}_p \left( \frac{1}{2} \delta Q_{p,ij} + Q_{p,j} \right) \] (4.11)

The filtered dispersed phase equations contain three nonlinear unclosed terms detailed in Eqs. (4.12) – (4.14). Section 4.2.1 focuses on their modeling as well as the underlying assumptions in the RHS terms of Eqs. (4.10) and (4.11).

\[ T_{p,ij} = u_{p,j} \hat{u}_{p,j} \hat{u}_{p,j} \] (4.12)

\[ \Pi_p = -[ \delta R_{p,ij} \frac{\partial \hat{u}_{p,i}}{\partial x_j} - \delta R_{p,ij} \frac{\partial \hat{u}_{p,i}}{\partial x_j} ] \] (4.13)

\[ Q_{p,j} = u_{p,j} \delta \theta_{p} - \hat{u}_{p,j} \delta \theta_{p} \] (4.14)

Four terms appear on the RHS of the transport equation for the particle filtered correlated velocity (Eq. (4.10)). The first one stands for the coupling between gas and dispersed phases through the drag force. The filtered Random Uncorrelated Motion (RUM) is the cause of the next two terms that by analogy may be compared to the fluid filtered pressure term and the fluid filtered diffusion term respectively in Eq. (4.5). The last term, defined in Eq. (4.12), is due to the subgrid correlated motion and is analogous to the fluid subgrid term (see Eq. (4.7)).

This distinction between the two contributions (RUM and subgrid) is specific to the two-step methodology used here which consists in the LES-filtering of the equations obtained from ensemble-averaging. Other Eulerian methods using LES-filtering of the equations obtained from volume-averaging (Pandya & Mashayek, 2002) exhibit only one global subgrid term that must therefore account for both subgrid and RUM effects.

- **A priori analysis of the transport equations**

Moreau (2006) provides an interesting description of the mechanisms responsible for the evolution of quantities such as particle filtered correlated energy, particle filtered RUE and particle subgrid correlated energy for instance. The *a priori* analysis is done on the HIT test case presented in Chapter 3. Particle Lagrangian fields are first projected on the grid using a
filter with size $\Delta_p$, and then filtered in the LES sense. The LES filter width varies from twice to eight times the size of the projection filter: $\Delta = 2\Delta_p$, $4\Delta_p$, $6\Delta_p$ and $8\Delta_p$, which allows to determine the dependence on the LES filter.

Figure 4.1 shows the temporal evolution of the ratio $<\bar{n}_p^2> / <\bar{n}_p>^2$ (where $< \cdot >$ is the volume-filtering operator) that can be considered as a measure of the preferential concentration. A homogeneous particle number density field corresponds to $<\bar{n}_p^2> / <\bar{n}_p>^2 = 1$, while the ratio can increase infinitely with segregation. As expected, the bigger is the LES filter $\Delta$, the smaller is the preferential concentration. Thus, a posteriori LES computations are expected to under-estimate preferential concentration, leading to smaller gradients of particle number density and reducing numerical problems such as dispersion. The use of numerical stabilization method such as presented in Section 2.3 (Artificial Viscosity and RUE flux limitor) should therefore be more limited for LES than for DNS.

Figure 4.1 - Temporal evolution of the particle preferential concentration measure: $<\bar{n}_p^2> / <\bar{n}_p>^2$ depending on the filter width. Symbols: unfiltered field – solid line: $\Delta = 2\Delta_p$ – dotted line: $\Delta = 4\Delta_p$ – dashed line: $\Delta = 6\Delta_p$ – dotted-dashed line: $\Delta = 8\Delta_p$. $\Delta_p$ is the projector filter width used by Moreau. Results from the filtered Lagrangian computations (Moreau, 2006). HIT test case (see Chapter 3).

Figures 4.2 a. and b. compare an instantaneous field of filtered particle RUE $\widehat{\delta}\theta_p$, with an instantaneous field of particle subgrid correlated energy $q_{p,sgs}^2$. Iso-lines of the non-dimension particle number density are super-imposed on both fields to localize the particle clusters. Whereas the particle RUE is strongly correlated with high preferential concentration zones, the particle subgrid correlated energy seems located at the interface of the clusters. It would be interesting to confirm such tendencies when performing LES of turbulent jet or bluff body flow. Moreover, tests with increasing LES filter width $\Delta$, confirm that the particle RUE does
not depend on the filter width, while the particle subgrid correlated energy increases with $\Delta$. This result is not surprising since the particle filtered RUE is constructed so as not to depend on the LES filter whereas any subgrid energy increases with the filter size. As a consequence, modeling the filtered uncorrelated terms and the subgrid terms in Eqs. (4.9) – (4.11) should be conceptually different, as shown in Section 4.2.2.

Figure 4.2 - Comparison of instantaneous fields of filtered particle RUE (a.), and particle subgrid energy (b.). Both quantities are non-dimensionalised by their mean value over the box. The lines define isovalues of the non-dimension particle number density: $\bar{n}_p/ \langle \bar{n}_p \rangle = 1$: solid line – $\bar{n}_p/ \langle \bar{n}_p \rangle = 1.5$: dashed line. The cutting plane is defined as $z = 0$. Results from the filtered Lagrangian computations (Moreau, 2006). HIT test case (see Chapter 3).

4.2 Turbulence models

4.2.1 The gas phase

Table 4.1 summarises the models used for the gaseous turbulence terms. The filtered laminar stress tensor $\tau_{f,ij}$, and filtered laminar heat fluxes $q_{f,j}$ models assume that the molecular viscosity does not change across the filtering and can be extracted from the filtering operator. The filtered laminar stress tensor and heat fluxes finally write as the exact expression, introducing the gradients of filtered velocity and temperature respectively.

The effects of the subgrid scales on the filtered energy are represented through a gradient assumption by analogy to the heat fluxes for molecular diffusion. The thermal conductivity due to the residual turbulent motions $\lambda^t_{f,j}$, is defined from the turbulent viscosity $\nu^t_{f,j}$, and
the turbulent Prandtl number $P_{r,f}$, so that $\lambda_f^T/\bar{\rho}_f = v'_f C_p/P_{r,f}$. In AVBP_{TPF}, $P_{r,f}$ is fixed to 0.9.

**Fluid Reynolds stress tensor**

In Eq. (4.5), $T_{f,ij}$ describes the impact of the subgrid scales on large-scale resolved turbulence. A simple way of modeling this term is to use the Boussinesq's assumption (Boussinesq, 1877) : the energy transfer mechanism from the resolved to the subgrid scales is analogous to the molecular mechanisms represented by the diffusion term. The molecular viscosity is then replaced by a fluid turbulent viscosity denoted $v'_f$ and the fluid subgrid model is written:

$$T_{f,ij} - \frac{1}{3} T_{f,ll} \simeq 2 v'_f \left( \hat{S}_{f,ij} - \frac{1}{3} \delta_{ij} \hat{S}_{f,ll} \right) \quad \text{where} \quad \hat{S}_{f,ij} = \frac{1}{2} \left( \frac{\partial \hat{u}_{f,i}}{\partial x_j} + \frac{\partial \hat{u}_{f,j}}{\partial x_i} \right) \quad (4.15)$$

The complementary spherical tensor $\frac{1}{3} T_{f,ll}$, is in fact added to the fluid filtered static pressure term in Eq. (4.5), and does not require modeling. Numerical simulations (Zang et al., 1992) have shown that taking into account this contribution explicitly has very few consequences on the results in a moderately compressible HIT configuration.

Finally, the closure of the fluid unresolved Reynolds stress tensor only consists in determining the fluid turbulent viscosity $v'_f$.

**Fluid Smagorinsky Model**

The simplest model has been proposed by Smagorinsky (1963) and is based on the analogy to the mixing-length hypothesis: the fluid turbulent viscosity is written as the product of the Smagorinsky length scale $l_{S,f}$, and the characteristic filtered rate of strain:

$$v'_f = l_{S,f}^2 \sqrt{2 \hat{S}_{f,ij} \hat{S}_{f,ij}}, \quad (4.16)$$
4.2 Turbulence models

$l_{S,f}$ is taken proportionnal to the filter width $\Delta$ through the Smagorinsky coefficient $C_{S,f}$: $l_{S,f} = C_{S,f} \Delta$. A first drawback of this model is that the constant $C_{S,f}$ depends on the flow configuration. It can vary between 0.1 and 0.18 (Smagorinsky, 1963; Germano et al., 1991; Lilly, 1992; Piomelli, 1999; Meneveau & Katz, 2000) and the value $C_{S,f} = 0.18$ is chosen in AVBP-TPF. In this model, the fluid turbulent viscosity becomes never negative, which prevents from any energy transfer from the subgrid scales to the resolved scales (back-scatter effect). If this closure supplies the right amount of dissipation of kinetic energy in high Reynolds homogeneous isotropic turbulent flows, locality in space and time is lost. Finally, the model does not predict zero turbulent viscosity at a solid boundary and has difficulties to predict transition from laminar to turbulent flows (Vreman, 1995). However, the Smagorinsky model is widely used, not only because it is easy to implement, but also because errors due to the LES modeling are often small compared to the numerical errors due to the low-order schemes and the artificial dissipation.

- Fluid WALE model

To obtain the right scaling for the fluid turbulent viscosity when approaching a solid boundary, the use of the WALE (Wall-Adapting Local Eddy-viscosity) model proposed by Ducros et al. (1998b) is relevant. The filtered strain rate is replaced by a term that does not detect shear, but strong rates of deformation and/or rotation:

$$v'_f = (C_{f,w} \Delta)^2 \frac{(s^d_{f,ij}s^d_{f,ij})^{3/2}}{(\hat{S}_{f,ij}\hat{S}_{f,ij})^{5/2} + (s^d_{f,ij}s^d_{f,ij})^{5/4}} ,$$  \hspace{1cm} (4.17)

$$s^d_{f,ij} = \hat{S}_{f,ik}\hat{S}_{f,kj} + \hat{\Omega}_{f,ik}\hat{\Omega}_{f,kj} - \frac{1}{3} \delta_{ij} \left[ \hat{S}_{f,mm}\hat{S}_{f,mm} + \hat{\Omega}_{f,mm}\hat{\Omega}_{f,mm} \right] ,$$  \hspace{1cm} (4.18)

where $\hat{\Omega}_f$ is the filtered fluid rotation rate tensor and $C_{f,w} = 0.5$ is the model constant. The WALE model recovers the scaling laws of the wall and allows the prediction of transition. However similarly to the Smagorinsky model, locality is lost and only global quantities may be trusted.

4.2.2 The dispersed phase

Modeling the unclosed terms has been done in collaboration with Moreau (2006). Several SGS model have been proposed and a priori tested in the decaying HIT flow presented in Chapter 3 (Moreau, 2006) by LES-filtering the Eulerian mesoscopic fields resulting from the Lagrangian fields. This section aims at presenting Moreau’s main results, and the subgrid models that have been implemented in the code.
Equations (4.9) – (4.11) show five unclosed terms with two different origins: the filtered RUV tensor, \( \delta \tilde{R}_p^* \), and the filtered diffusive tensor, \( \frac{1}{2} \delta \tilde{Q}_p \), are due to the ensemble averaging whereas the SGS tensor in the filtered momentum equation, \( T_p \), the SGS production term, \( \Pi_p \), and the SGS diffusion term, \( Q_p \), in the filtered RUE equation, appear when LES-filtering the Eulerian mesoscopic equations.

The accuracy of the different models is evaluated through the correlation coefficient \( C(A, B) \) that measures the degree to which the exact LES field, \( A \), and the modeled one, \( B \), are linearly dependant. It yields:

\[
C(A, B) = \frac{\langle AB \rangle - \langle A \rangle \langle B \rangle}{\sqrt{(\langle A^2 \rangle - \langle A \rangle^2) (\langle B^2 \rangle - \langle B \rangle^2)}}
\]  

(4.19)

This correlation coefficient takes values from \(-1\) for anti-correlated fields to 1 for totally correlated fields. The fields are totally uncorrelated when the correlation coefficient is zero.

- **Unclosed terms due to ensemble averaging**

The models developed by Kaufmann (2004) for the non-filtered quantities, \( \delta \tilde{R}_p^* \) and \( \delta \tilde{Q}_p \), are adapted to LES by using filtered quantities and introducing SGS terms due to the spatial variations of the RUV viscosity and diffusivity:

\[
\bar{n}_p \delta \tilde{R}_p^*_{ij} = -\bar{n}_p \hat{\nu}_{RUV} \dot{\hat{S}}^*_{p,ij} - \left( \bar{n}_p \nu_{RUV} \dot{\hat{S}}^*_{p,ij} - \bar{n}_p \hat{\nu}_{RUV} \dot{\hat{S}}^*_{p,ij} \right)
\]

(4.20)

\[
\bar{n}_p \frac{1}{2} \delta \tilde{Q}_p_{ii,j} = -\bar{n}_p \hat{\kappa}_{RUV} \frac{\partial}{\partial x_j} \delta \theta_p - \left( \bar{n}_p \kappa_{RUV} \frac{\partial}{\partial x_j} \delta \theta_p - \bar{n}_p \hat{\kappa}_{RUV} \frac{\partial}{\partial x_j} \delta \theta_p \right)
\]

(4.21)

where \( \dot{\hat{S}}^*_{p,ij} = \left( \frac{\partial \hat{u}_p}{\partial x_j} + \frac{\partial \hat{u}_p}{\partial x_i} - \frac{1}{2} \delta_{ij} \frac{\partial \hat{u}_p}{\partial x_l} \right) \), \( \hat{\nu}_{RUV} = \frac{\tau_p}{2} \delta \theta_p \) and \( \hat{\kappa}_{RUV} = \frac{5}{3} \tau_p \delta \theta_p \). Both SGS terms in parenthesis in Eqs. (4.20) and (4.21) are neglected hereafter, mainly because the corresponding non-filtered terms themselves are still under investigation.

Figure 4.3 shows the temporal evolution of the correlation coefficients for different filter sizes and for both models. The model for the filtered RUV tensor provides good results whatever the filter width considered. The filtered diffusion tensor model shows little agreement with the exact quantity, which was already the case for the non-filtered quantity. Therefore, from now on, it is prefered to omit this term in the transport equation for the particle filtered RUE.

- **Unclosed terms due to spatial filtering**
4.2 Turbulence models

Figure 4.3 - Temporal evolution of the correlation coefficient for the filtered RUV tensor, \( \hat{R}_{p,ij} \) (a.), and the filtered diffusive tensor, \( \frac{1}{2} \hat{Q}_{p,ij} \) (b.), depending on the filter width. Solid line: \( \Delta = 2\Delta_p \) – dotted line: \( \Delta = 4\Delta_p \) – dashed line: \( \Delta = 6\Delta_p \) – dotted-dashed line: \( \Delta = 8\Delta_p \). \( \Delta_p \) is the projection filter width used by (Moreau, 2006). The correlation coefficients obtained by the model for the unfiltered terms are plotted with symbols. Results from the filtered Lagrangian computations (Moreau, 2006). HIT test case (see Chapter 3).

LES closures for gaseous subgrid terms have been worked on for several decades. Smagorinsky (1963), Lilly (1967), Germano (1992) and Ghosal et al. (1995) among others proposed numerous models and modifications of them for incompressible gas flow. Extension to compressible gas flow is more recent and mainly due to Vreman et al. (1995) and Lenormand et al. (2000). Subgrid models for the dispersed phase as developed by Moreau (2006) are based on the work achieved on compressible gas flows.

Particle subgrid stress (SGS) tensor

For the particle SGS tensor \( T_{p,ij} \), Moreau (2006) tested three different models. The first one is the classical Smagorinsky model, where the compressible effects are accounted for through a non-zero spherical term by analogy to Yoshizawa’s model (Yoshizawa & Horiuti, 1985). As noticed in Section 4.2.1, no model is used for this term in the gas transport equations because its impact is very limited when dealing with very low-compressible gas flows. However, this is no longer true for the dispersed phase. Indeed, Moreau (2006) not only showed that particle subgrid kinetic energy and particle RUE were not localised in the same regions (see Fig. 4.2), but he also quantified both energies at the same order of magnitude in the studied cases. Therefore, it is essential to model the spherical part of the particle Reynolds tensor. Equation (4.22) gives the form of the Smagorinsky-like model tested for the dispersed phase.
that is referred to as particle eddy viscosity model in the rest of the manuscript:

\[ T_{p,ij} = \frac{2}{3} \left[ C_{p,Y} \frac{\Delta^2}{v_{p,j}} \left| \mathbf{\hat{S}}_p \right|^2 \delta_{ij} - C_{p,S} \frac{\Delta^2}{v_{p,i}} \left| \mathbf{\hat{S}}^*_{p,j} \right| \left| \mathbf{\hat{S}}^*_{p,ij} \right| \right] \quad (4.22) \]

Classically, the values of the coefficients \( C_{p,Y} \) and \( C_{p,S} \) are determined by ensuring that the global SGS dissipation and energy induced by the model corresponds to the exact one in the HIT test case. Moreau fixed: \( C_{p,Y} = 0.051 \) and \( C_{p,S} = 0.16 \).

Obviously, the particle eddy viscosity model has the same disadvantages as the fluid Smagorinsky model: among them, the coefficient values depend on the configuration and no back-scatter effect can be modeled. Therefore, Moreau (2006) tested the Scale-Similarity model (Bardina et al., 1983) that uses a double filtering to predict more accurately the energy transfer between large scales and subgrid scales:

\[ T_{p,ij} = C_{p,B} \left( \mathbf{\hat{u}}_{p,i} \mathbf{\hat{u}}_{p,j} - \mathbf{\hat{u}}_{p,i} \mathbf{\hat{u}}_{p,j} \right) \quad (4.23) \]

Back-scattering effects are correctly accounted for with this model in fluid channel flows (Horiuti, 1989). Nevertheless, the value \( C_{p,B} = 1 \) is required to ensure galilean invariance (Speziale, 1985). Previous numerical simulations (Vreman, 1995) show that, within this restriction, the Scale-Similarity model is not able to predict the global amount of global SGS dissipation and provides numerical instabilities. To account for the advantages of both previous models, the Mixed-Scale model (Erlebacher et al., 1992) can be written using a linear combination of the particle eddy viscosity model and the Scale-Similarity model:

\[ T_{p,ij} = (\mathbf{\hat{u}}_{p,i} \mathbf{\hat{u}}_{p,j} - \mathbf{\hat{u}}_{p,i} \mathbf{\hat{u}}_{p,j}) + \frac{2}{3} C'_{p,Y} \frac{\Delta^2}{v_{p,j}} \left| \mathbf{\hat{S}}_p \right|^2 \delta_{ij} - C'_{p,S} \frac{\Delta^2}{v_{p,i}} \left| \mathbf{\hat{S}}^*_{p,j} \right| \left| \mathbf{\hat{S}}^*_{p,ij} \right| \quad (4.24) \]

The determination of the two coefficients yields: \( C'_{p,Y} = 0.025 \) and \( C'_{p,S} = 0.12 \). The Mixed-Scale model is expected to predict accurately both the energy transfer between resolved and subgrid scales, including back-scatter effects, and the global amount of SGS dissipation.

The three models were tested \textit{a priori} in the HIT configuration and Fig. 4.4 presents the correlation coefficients for the particle subgrid kinetic energy, \( q^2_{p,sgs} = T_{p,ll} \), and the particle deviatoric SGS tensor, \( T^*_{p,ij} \). The agreement between model results and exact quantities is very good for the Scale-Similarity and Mixed models, and slightly worse for the eddy viscosity model. Although the Scale-Similarity model shows the best correlation coefficient, it is un-useful since it underestimates the SGS dissipation. Due to the numerical cost of the Bardina refiltering procedure in the unstructured AVBP TPF code, the Mixed-Scale model has not been implemented either. Finally, because it is easy to implement and predicts accurately the total amount of SGS dissipation, which is the main purpose of a SGS model, and despite its worst performance, the particle eddy viscosity model has been implemented in AVBP TPF and a
4.2 Turbulence models

posteriori tested.

Subgrid Scale diffusion and production of filtered RUE

![Graph](image)

Figure 4.4 - Temporal evolution of the correlation coefficient for the particle subgrid kinetic energy, $q_{P,SGS}^2$ (a.), and the particle deviatoric SGS tensor, $T_{P,ij}^*$ (b.). Solid line: Eddy viscosity model – dotted line: Scale-Similarity model – dashed line: Mixed-Scale model. The fluid Smagorinsky model is super-imposed for the particle deviatoric SGS tensor only (symbols). Results from the filtered Lagrangian computations (Moreau, 2006). HIT test case (see Chapter 3).

The transport equation for particle non-filtered RUE still requires a lot of work, especially because the assumptions made to model the unclosed terms due to ensemble averaging are very restrictive, and therefore rarely true in complex geometries. Simulations carried out in the turbulent confined jet (see Chapter 5) transporting the particle RUE show some difficulties handling this transport equation. As a result, a posteriori analysis of the influence of the SGS diffusion and production terms of filtered RUE is very limited in the present work. The models tested by Moreau are only briefly described hereafter.

By analogy to the gaseous SGS heat flux model proposed by Moin et al. (1991), a particle turbulent Prandtl number is introduced to model the SGS diffusion of filtered RUE:

$$Q_{P,j} = -\nu_{d,P} \frac{\partial \delta \theta_p}{\partial x_j},$$  \hspace{1cm} (4.25)

where $\nu_{d,P}$ is given by Eq. (4.22) and the particle Prandtl number is evaluated: $P_{r,P}^* \approx 0.7$. After introducing this model, Moreau (2006) uses the same methodology as summarised above for
the particle SGS tensor, testing not only the SGS diffusion model described by Eq. (4.25), but also the Scale-Similarity model, and the Mixed-Scale model that combined the SGS diffusion model and the Scale-Similarity model. Figure 4.5 compares the correlation coefficients of the three models. The same conclusion as for the particle SGS tensor can be made: the Mixed-Scale model provides better accuracy than the Scale-Similarity and the SGS diffusion models. Once again, although the SGS diffusion model shows the worst correlation coefficients, it has been implemented in AVBP_TPF because it is easier to implement than the Mixed-Scale model and because the Scale-Similarity does not predict the right amount of SGS dissipation, which is unacceptable for a subgrid model.

Figure 4.5 - Temporal evolution of the correlation coefficient for the SGS diffusion term, $Q_{p,j}$, in the transport equation for filtered RUE. Solid line: Eddy viscosity model – dotted line: Scale-Similarity model – dashed line: Mixed-Scale model. Results from the filtered Lagrangian computations (Moreau, 2006). HIT test case (see Chapter 3).

For the SGS production of filtered RUE $\Pi_p$, three models are proposed by Moreau (2006). The first one is the Scale-Similarity model, by analogy to the model written by Martin et al. (2000) for the SGS viscous dissipation of total energy in a compressible gas flow. Based on dimensional analysis of the SGS production term, a Ghosal-type model (Ghosal et al., 1995) may be written:

$$\Pi_p = C_{p,G} \left( \frac{q_{p,sgs}^2}{\Delta} \right)$$

Originally, such a model was developed for the SGS production term of gaseous subgrid kinetic energy. The third model tested by Moreau (2006) requires an equilibrium assumption on the
4.2 Turbulence models

Particle filtered correlated subgrid energy. Neglecting also the diffusion terms, it yields:

$$- \frac{\bar{n}_p}{\tau_p} \left( \frac{T_{p,kk}}{\bar{n}_p} - q_{f.p, sgs} \right) + \Pi_p - T_{p,ij} \frac{\partial \hat{u}_{p,i}}{\partial x_j} = 0,$$

(4.27)

where the subgrid covariance is $q_{f.p, sgs} = u_{p,k} u_{p,k} - \hat{u}_{p,k} \hat{u}_{p,k}$. In a first approximation, the drag force can be neglected and $\Pi_p$ can be modeled by:

$$\Pi_p = T_{p,ij} \frac{\partial \hat{u}_{p,i}}{\partial x_j},$$

(4.28)

with the particle SGS tensor given by Eq. (4.22). This model ensures that the filtered correlated energy dissipated by subgrid effects is fully transferred into filtered RUE. No constant adjustment is needed. Of course, the subgrid energy equilibrium assumption is known to be often uncertain in gas flows, and remains questionable.

The *a priori* tests carried out by Moreau (2006) do not show good correlation coefficients, whatever the model is considered. However, it is important to notice that the exact quantity $\Pi_p$ is itself difficult to measure, and that it is hazardous to conclude about the accuracy of these models without any *a posteriori* testing.

Table 4.2 summarises the models that have implemented in AVB*TPF* and *a posteriori* tested in the two geometries of Chapters 5 & 6.

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Exact term</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filtered RUV Tensor</td>
<td>$\Bar{n}<em>p \delta R</em>{p,ij}$</td>
<td>$- \frac{\bar{n}<em>p}{\tau_p} \delta R</em>{p,ij}$</td>
<td>$- \frac{\bar{n}<em>p}{\tau_p} \delta R</em>{p,ij}$</td>
</tr>
<tr>
<td>Filtered diffusion Tensor</td>
<td>$\frac{\partial}{\partial x_j} \bar{n}<em>p \frac{1}{2} \delta Q</em>{p,ij}$</td>
<td>$- \frac{\bar{n}<em>p}{\tau_p} \delta Q</em>{p,ij}$</td>
<td>0</td>
</tr>
<tr>
<td>Subgrid Scale Tensor</td>
<td>$T_{p,ij}$</td>
<td>$u_{p,i} u_{p,j} - \hat{u}<em>{p,i} \hat{u}</em>{p,j}$</td>
<td>$v_{p,i} \delta \hat{u}<em>{p,j} - v</em>{p,j} \delta \hat{u}_{p,i}$</td>
</tr>
<tr>
<td>SGS diffusion of filtered RUE</td>
<td>$Q_{p,j}$</td>
<td>$u_{p,j} \delta \theta_p - \hat{u}_{p,j} \delta \theta_p$</td>
<td>$- \frac{\bar{n}_p}{\tau_p} \delta \theta_p$</td>
</tr>
<tr>
<td>SGS Production of filtered RUE</td>
<td>$\Pi_p$</td>
<td>$- [\delta R_{p,ij} \frac{\partial u_{p,i}}{\partial x_j} - \delta R_{p,ij} \frac{\partial \hat{u}_{p,i}}{\partial x_j}]$</td>
<td>$T_{p,ij} \frac{\partial \hat{u}_{p,i}}{\partial x_j}$</td>
</tr>
</tbody>
</table>

Table 4.2 - *Closure models implemented in AVB*TPF for the dispersed phase LES terms.*
4.3 Analysis and validation of LES results

LES provides unsteady filtered fields that may be validated by comparison with DNS or experimental data. In addition to images of instantaneous fields, post-processing has to be carried out to access statistical data, such as mean and fluctuating fields. This is usually done during the simulation after reaching a quasi-steady state. This latter strongly depends on the geometry and the flow. To ensure that the comparisons are relevant, both the total time of the simulation and the recording time must be carefully defined. Moreover, the definition of the quantities that are compared must be compatible, or at least, one should be aware of the discrepancies.

4.3.1 Average quantities

In this work, LES results are validated by comparison with experimental data. The measurements have been obtained in statistically stationnary flows. An averaging procedure of LES results is introduced hereafter.

The Reynolds mean field (denoted by \{\cdot\}) of a variable \(\phi\) at a certain location \(x\) is written as:

\[
\{\phi\} = \frac{1}{T_{av}} \int_{0}^{T_{av}} \phi(t) \, dt \tag{4.29}
\]

The so-called fluctuating part (denoted by a prime) is the residual part of the decomposition. By definition, the mean of the fluctuating part is zero:

\[
\{\phi'\} = 0 \tag{4.30}
\]

The variance is the mean square of the fluctuating part and reads:

\[
\{\phi'^2\} = \{\phi^2\} - \{\phi\}^2 = \Phi_{rms}^2 \tag{4.31}
\]

The Root Mean Square (RMS) of the variance is the standard deviation of \(\phi\) and denoted by the subscript \(\text{rms}\). This quantity is usually directly compared to the fluctuating quantities given by the experiments.

For variable density flows, mass weighted averages are used. Such time-averaged quantities are more coherent with the Favre-averaging procedure introduced in Section 4.1.1. Mass weighted quantities are denoted by the superscript \((F)\) and defined as:

\[
\{\phi\}^{(F)} = \frac{1}{\{\rho\}T_{av}} \int_{0}^{T_{av}} \rho(t)\phi(t) \, dt \tag{4.32}
\]

\[
\Phi_{rms}^{(F)} = \{\phi^2\}^{(F)} - \{\phi\}^{(F)}^2, \tag{4.33}
\]
4.3 Analysis and validation of LES results

where $\rho$ stands either for the fluid density, $\rho_f$, or the particle number density, $n_p$.

Some recent work has been achieved on the differences between the Reynolds and Favre time-averaged quantities by Veynante & Knikker (2006). For the gas flows calculated in this work, the differences remain small due to the low compressibility of the air at ambient conditions. Consequently, it seems relevant to compare the Reynolds time-averaged mean and RMS fields with the experimental data. Concerning the variances however, the comparison is not direct and depends on the quality of the LES performed, which is discussed in Section 4.3.3. As far as the dispersed phase is considered, compressibility effects are much more important and only Favre time-averaged quantities are analysed in the manuscript. No specific study has been carried out to compare the two time-averaged quantities and this is obviously to be done.

For the sake of simplicity, the symbol $\{\} \ldots$ is omitted in the following since almost all quantities plotted and analysed are time-averaged. The use of instantaneous quantities will be mentioned explicitly. For the same reason, the superscript $(F)$ concerning the dispersed phase is also omitted.

### 4.3.2 Characteristic time scales

The total time span of the simulation $T_{av}$, and the recording frequency $\Delta t_r$, are determined according to several time-scales, that depend on the flow and the geometry.

Before collecting statistics, a transient time is required that typically corresponds to a convective time $\tau_{f,\text{conv}}$. It is defined by the time needed by a hydrodynamic perturbation to travel from one end to the other of the domain. Using the length $L_D$, of the domain, and the bulk velocity $U_f,\text{bulk}$, the convective time yields:

$$\tau_{f,\text{conv}} = \frac{L_D}{U_f,\text{bulk}}$$  \hspace{1cm} (4.34)

The minimum total time of the simulation theoretically depends on the type of statistics to compute. Indeed, convergence is faster for lower order moments. Considering the mean fields, it is common practice to link them to the phenomenon with the lowest frequency. Denoting its size $L_{f,l}$, and its velocity $U_{f,l}$, the largest time scale to represent is defined by:

$$\tau_{f,l} = \frac{L_{f,l}}{U_{f,l}}$$  \hspace{1cm} (4.35)

The total recording time $T_{av}$, should include about 5 cycles of the lowest frequency phenomenon to obtain a meaningful mean field. Naturally, a much longer total time span is necessary for the variances.
Finally, to determine the interval between data samples $\Delta t$, the phenomena with the highest frequency contributing to the statistics must be considered. The turnover time of the biggest eddies is a reasonable choice. Accounting for their length $l_{f,t}$, and their characteristic velocity $u'_{f,t}$, (see Section 3.1.1) yields:

$$\tau_{f,t} = \frac{l_{f,t}}{u'_{f,t}}$$

(4.36)

The recording frequency is then linked to the characteristic time of the biggest eddies: $\Delta t \approx \tau_{f,t}$.

### 4.3.3 Quality criteria for LES

The LES methodology depends to some extent on the type of flow considered and on the numerical method used. Indeed, LES can be performed for a Homogeneous Isotropic Turbulence on a structured grid as well as for a flow in a complex geometry on an unstructured grid. In Table 4.3, Pope (2000) distinguishes three variants of LES, depending on the resolution of the flow remote from walls and the resolution of the wall-bounded flow itself. Considering

<table>
<thead>
<tr>
<th>Model</th>
<th>Acronym</th>
<th>Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES with Near-Wall Resolution</td>
<td>LES-NWR</td>
<td>The filter and the grid are sufficiently fine to resolve 80% of the energy everywhere.</td>
</tr>
<tr>
<td>LES with Near-Wall Modeling</td>
<td>LES-NWM</td>
<td>The filter and the grid are sufficiently fine to resolve 80% of the energy remote from the wall, but not in the near-wall region.</td>
</tr>
<tr>
<td>Very Large-Eddy Simulation</td>
<td>VLES</td>
<td>The filter and the grid are too coarse to resolve 80% of the energy.</td>
</tr>
</tbody>
</table>

Table 4.3 - Resolution in LES as defined by Pope (2000)

first the flow remote from walls, the difference between LES and Very Large-Eddy Simulation (VLES) comes from the amount of turbulent kinetic energy resolved in the flow field. In VLES, the grid and the filter are too large and more than 20% of the kinetic energy reside in the subgrid motions. This makes VLES less expensive than LES, but strongly dependent on the modeling of the subgrid motions. A second distinction is made for wall-bounded flows. The same criterion is applied for the treatment of the near wall motions. If the filter and the grid are chosen so that 80% of the energy contained in these motions is resolved, the result is a LES with Near-Wall Resolution (LES-NWR). Obviously, this kind of simulation requires a very fine
grid in the near-wall region, which increases the computational cost. Therefore, it is never used in a complex geometry where the influence of the walls is modeled, resulting in a LES with Near-Wall Modelling (LES-NWM).

Following Pope’s classification, it is interesting to evaluate the quality of the LES carried out with AVBP-TPF by quantifying the ratio of the turbulent kinetic energy resolved $\hat{q}^2$, and the turbulent kinetic energy modeled $q_{sgs}^2$, for both phases.

$$Q^{LES} = \frac{\hat{q}^2}{\hat{q}^2 + q_{sgs}^2}$$ (4.37)

The access to the subgrid kinetic energy is not direct and different for both phases, due to the different turbulent closures.

- **LES criterion for the gas phase**

When using the Smagorinsky-type models described in Section 4.2.1, the diagonal part of the fluid turbulent tensor is hidden in the modified pressure (see Section 4.2.1), and the subgrid viscosity is evaluated using global quantities related to the resolved scales (the LES-filtered fluid Boussinesq tensor $\hat{S}_{f,ij}$ in the present case). The determination of subgrid scales at a given point in space and time requires therefore the introduction of assumptions. Among them, the local equilibrium hypothesis assumes that there is no accumulation of energy at any frequency. Other subgrid viscosity models exist, that are based on the subgrid scales (Sagaut, 2000) and do not require the local equilibrium hypothesis. For instance, the resolution of an evolution equation for the subgrid energy has been used by Kim & Menon (1999); Schumann (1975); Yoshizawa & Horiuti (1985). These models provide a better description of the subgrid scales, but are more expensive in CPU time than the Smagorinsky model. In this case, the subgrid viscosity $\nu_{f,sgs}$, simply reads:

$$\nu_{f,sgs} = C_m A \sqrt{q_{f,sgs}^2}$$ (4.38)

where $C_m$ is defined as $C_m = \sqrt{2/3A/(\pi K_0^3/2)}$. The coefficient $K_0 = 1.4$ corresponds to an infinite inertial spectrum for an Homogeneous Isotropic Turbulence in the framework of Kolmogorov’s hypothesis. The constant $A$ is evaluated as $A = 0.44$ in the Eddy-Damped Quasi-Normal Markovian (EDQNM) theory (Aupoix & Cousteix, 1982).

Equation (4.38) is used to evaluate the fluid subgrid turbulent kinetic energy $q_{f,sgs}^2$. As for the filtered kinetic energy $\hat{q}_{f}^2$, it is calculated as:

$$\hat{q}_{f}^2 = \frac{1}{2} \left( \hat{u}_{f,i} \hat{u}_{f,i} - \hat{u}_{f,i} \hat{u}_{f,i} \right)$$ (4.39)
so that the LES criterion for the gas phase becomes:

\[ Q_f^{LES} = \frac{\hat{q}_f^2}{\hat{q}_f^2 + \hat{q}_{f,sgs}^2} \]  

(4.40)

• LES criterion for the dispersed phase

For the dispersed phase, the evaluation of the resolved particle correlated kinetic energy is done the same way as for the gas phase. Here however, the access to the particle subgrid turbulent mesoscopic kinetic energy is direct since it is contained in the Yoshizawa’s part of the particle turbulent tensor \( \tau_{p,ij}^l \):

\[ q_{p,sgs}^2 = \frac{1}{\bar{n}_p} \tau_{p,ii}^l = C_p \gamma \Delta^2 |\hat{S}_p|^2 \]  

(4.41)

Then, the quantification of the particle LES criterion, \( Q_p^{LES} \), is straightforward:

\[ Q_p^{LES} = \frac{\hat{q}_p^2}{\hat{q}_p^2 + \hat{q}_{p,sgs}^2} , \]  

(4.42)

with \( \hat{q}_p^2 = \frac{1}{2} \left( \bar{u}_{f,i} \bar{u}_{f,i} - \hat{u}_{f,i} \hat{u}_{f,i} \right) \).

Calculations of the turbulent gas-particle confined jet (Chapter 5) and the particle-laden bluff-body flow (Chapter 6) are a posteriori test cases to measure the accuracy of the methods developed and used in this work. Their accuracy is assessed by comparison of the calculated statistics (typically mean and fluctuating velocity) with experimental data. However, special care has to be taken in the comparison because the calculated and measured quantities are not directly equivalent. Their difference decreases with the filter width, but as it is not possible yet to perform DNS for these configurations, some discrepancies will remain. As a consequence, before comparing numerical and experimental data, the LES criterion is evaluated for both phases to guarantee that there is sufficiently little subgrid energy, and to ensure that the comparisons are relevant.
Chapter 5

LES of particle-laden turbulent confined jet flow

The LES-filtered transport equations derived for two-phase flows in Chapter 4 are now validated with *a posteriori* testing. Since the LES Euler-Euler mesoscopic model proposed do not yet account for all physical phenomena present in two-phase reacting flows, the configurations have been chosen where these phenomena are not dominant. Two main criteria have been retained:

- First, the particle-wall interactions should be negligible because they are not modeled in the present approach. Much work has been devoted to particle motion in wall-bounded flows using the EL approach ([Wang & Squires, 1996; Vance et al., 2006; Picciotto et al., 2005b; Marchioli et al., 2006]). However, modeling the particle-wall interaction with the EE approach is still a challenge ([Sakiz, 1999; Konan et al., 2006; Alipchenkov & Zaichik, 2006]). Considering a combustion chamber where liquid fuel is used, the fuel droplets evaporate rapidly due to the hot temperatures in the device. As a consequence, the interaction between particles and solid walls is not the main mechanism to account for when predicting the dispersion of droplets in a combustion chamber.

- Second, valuable experimental data should be available for the comparison with LES. Yet, statistics of multiphase flows are difficult to measure since both velocity and particle size measurements are required to completely characterise the two-phase flow. [Tsuji et al. (1984), Hishida et al. (1987), Hishida & Maeda (1990), Kulick et al. (1994), Borée et al. (2001) and Caraman et al. (2003)] are the main studies where such data is provided.

As a consequence, the vertical particle-laden turbulent confined jet flow from [Hishida et al. (1987)] where particle-wall interaction can be neglected, has been preferred. This test-case is often used in the two-phase flow community for model validation purposes. Thus, the
mechanisms responsible for the two-phase flow topology in this geometry are well-known. In particular, it was one of the test cases chosen for the “5th workshop on Two-Phase Flow Predictions” organised in Erlangen, Germany, in 1990.

The main advantage of this configuration is that the geometry is very simple. Besides, the particle mass loading is small enough to assume one-way coupling between the gas and the particles. Therefore, after accurately predicting the gas phase, work on the dispersed phase itself can be achieved. RANS calculations have already been performed by Simonin (1991) and later by Février & Simonin (2000) with reasonable agreements with the measurements. Performing LES of this configuration will give access to the unsteady motion of the particles in the jet in terms of both velocity and mass flux. Accurate predictions of both quantities require the use of particle subgrid models as well as representative inlet boundary conditions. Special care has then been devoted to inlet boundary conditions, that will be also useful when characterising the motion of fuel droplets in a combustion chamber.

Hereafter, the experimental test-rig is detailed in Section 5.1 whereas Section 5.2 describes the simulation in terms of computational domain, grid characteristics and boundary conditions. Due to one way-coupling, the results of the gas flow are independent of the particulate phase and are presented separately in Section 5.3. Finally, Section 5.4 illustrates the role of the particle subgrid models detailed in Section 4.2 to achieve LES of two-phase flows as well as the importance of inlet boundary conditions to accurately predict the particle mass flow.
5.1 Description of the experimental setup

In this section, the experimental setup is described and the characteristics of the two phases are detailed. The specific measurement technique used to access velocity components for both phases, and particle size is emphasised.

5.1.1 Concept and main purpose

The confined jet flow involving glass particles was experimentally examined by Hishida et al. (1987) twenty years ago. At that time, the measurement techniques to characterise the topology of turbulent two-phase flows were still under investigation (see Section 5.1.2). Meanwhile, first attempts to numerically predict two-phase flows were emerging, based either on a continuum approach (Danon et al., 1977; Elghobashi et al., 1984) or on a stochastic approach (Shuen et al., 1983; Desjonqueres et al., 1988). Some difficulties concerning turbulence closures as well as turbulence modification by particles arised (and they are still open questions nowadays) and experimental data were necessary to increase modeling accuracy. Consequently, a series of experiments were carried out in round jets by Hishida et al. (1985) and Fleckhaus et al. (1987), while Hishida et al. (1987) considered a vertical jet (see Fig. 5.1).

Figure 5.1 - Sketch of the configuration from Hishida et al. (1987). The diameters of the inner and outer tubes are respectively: $D_1 = 13$ mm, $D_2 = 60$ mm. Their length is $L_T = 1$ m whereas the length of the experimental chamber is $L_D = 0.3$ m.
A central jet of air confined in an annular tube is laden with solid particles. Three conditions of air flow profiles were examined, varying the primary and secondary flow air velocities. The influence of the particle mass loading was also investigated. The aim was to provide a detailed description of the particle motion as well as a better understanding of the turbulence modifications induced by particles (Hishida & Maeda, 1990).

### 5.1.2 Two-phase flow measurement techniques

- **Laser Doppler Anemometry (LDA) with Particle Size Discrimination**

LDA is a single point optical measuring technique commonly used to measure velocities in single-phase flows. Particles are seeded in the fluid flow and their velocity are measured in a non-intrusive manner. The seeded particles are big enough to scatter sufficient light for signal detection but small enough to follow the flow faithfully. The area of interest within the flow field is sampled by a crossed-beam in a point by point manner. By analysing the Doppler-equivalent frequency of the laser light scattered by the seeded particles within the flow, the local velocity of the fluid can be determined. Consequently, using high quality optical windows along the test section is required. More information about this technique can be found in Durst et al. (1976) for instance.

When dealing with two-phase flows, it is necessary to choose different material for particles, so that they can either be a measure of the fluid flow or a measure of the dispersed phase itself. Another difficulty when characterising the dispersed phase is the measurement of particle diameter and particle mass flux.

- **Phase Doppler Anemometry (PDA)**

PDA is an extension of LDA that allows measurements of particle diameter and particle mass flux using a temporal counting method. Some improvements of the technique give access to polydisperse aspects through refraction index measurement or particle shapes for instance. Bachalo & Houser (1984) is one of the main developer of PDA.

To characterise both the gas phase and the dispersed phase in the considered configuration, Hishida et al. (1987) used respectively alumnia powder and glass beads. Special care has to be taken when seeding the flow with particles. First, it must be verified that the glass beads remain spherical and do not break so that the particle size measurement is reliable. Then, the alumnia particles must be small enough to be perfect tracers of the fluid flow. Considering their low diameter, \( d_{p,al} \approx 2 \, \mu m \), and their density, \( \rho_{p,al} = 2700 \, kg.m^{-3} \), their particle relaxation time is about \( \tau_{p,al} \approx 34 \, \mu s \). This corresponds to a Stokes number based on the most energetic eddies \( St \approx 0.02 \) (see Section 5.1.3), which is small enough to guarantee that alumnia powder...
is a good tracer of the fluid flow. Finally, it must be ensured that the tracers do not affect the motion of glass beads, by carrying out two-phase flow experiments with and without alumina powder and comparing the statistics of the glass beads. All these verifications were done by Hishida et al. (1987).

5.1.3 Characteristics of both phases

Hereafter, the characteristics of both phases for the test case investigated in this work are presented, as well as the main characteristic time-scales involved. Hishida & Maeda (1990) also examined the influence of the air velocity magnitude as well as the particle mass loading. A brief summary of the main observations is proposed below.

• The gas phase

The experiments are conducted at ambient conditions: \( P_f = 1.013 \times 10^5 \ Pa \) and \( T_f = 293 \ K \). The length of the tubes is \( L_T = 1 \ m \) whereas the chamber exhibits a length, \( L_D = 0.3 \ m \). The primary jet diameter is \( D_1 = 13 \ mm \) and the air emerges from the tube with a maximum velocity, \( U_{f,1}^{\text{max}} = 29.7 \ m.s^{-1} \). This leads to a bulk velocity, \( \bar{U}_{f,1} = 24.7 \ m.s^{-1} \). The resulting Reynolds number is \( Re_1 = D_1 \bar{U}_{f,1} / \nu_f \approx 22000 \), which is rather low. The ratio \( U_{f,1}^{\text{max}} / \bar{U}_{f,1} \approx 1.21 \) at the outer of the inner tube is however consistent with a fully developed turbulent pipe flow. The central jet is confined with an annular tube with diameter, \( D_2 = 60 \ mm \). The coflow air velocity at the inlet of the chamber is \( U_{f,2} = 15.6 \ m.s^{-1} \) and no fluctuations are experimentally observed. Neither swirl nor recirculation has been detected in the fluid flow. The characteristics of the two air jet flows are summarised in Table 5.1.

<table>
<thead>
<tr>
<th>Gas phase</th>
<th>Length (mm)</th>
<th>Radius (mm)</th>
<th>Mean velocity (m.s(^{-1}))</th>
<th>Max. velocity (m.s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central tube</td>
<td>1000</td>
<td>13</td>
<td>24.7</td>
<td>30</td>
</tr>
<tr>
<td>Annular tube</td>
<td>1000</td>
<td>60</td>
<td>15.6</td>
<td>15.6</td>
</tr>
</tbody>
</table>

Table 5.1 - Characteristics of the gas phase at the outlet of the inner and annular tubes. Configuration of Hishida et al. (1987).

• The dispersed phase

Polydisperse spherical light hollow glass particles are loaded in the inner jet with a mass loading of \( M_{p,1} = 3.3\% \). Their material density is \( \rho_p = 280 \ kg.m^{-3} \). As shown in Fig. 5.2, particle diameters cover a wide range of sizes from \( d_p = 50 \ \mu m \) to \( d_p = 120 \ \mu m \). The resulting
mean diameter in mass and in number is respectively $d_{p,M} = 91.1 \, \mu m$ and $d_{p,N} = 85.1 \, \mu m$. Note that both results over-estimate the mean diameter proposed by Hishida et al. (1987): $d_p = 80.1 \, \mu m$. Looking at their velocity, the particles emerge from the inner tube slightly more slowly than the gas. Their maximum velocity on the centerline is: $U_{p,max}^{\max} = 28.1 \, m.s^{-1}$.

![Mass distribution](image1.png) ![Number distribution](image2.png)

Figure 5.2 - Initial mass (a.), and number (b.) distribution of the particle size. Configuration of Hishida et al. (1987).

- **Characteristic Stokes number**

The Stokes number indicates whether the inertia of the particles play an important role in the two phase flow topology. To evaluate it, a characteristic time scale of the fluid most energetic eddies, noted $\tau_{f,t}$, is used. It is estimated by assuming that the length of the most energetic eddies is a third of the central tube diameter and their velocity is the maximum fluctuating velocity in the tube:

$$St = \frac{\tau_p}{\tau_{f,t}} \quad \text{where} \quad \tau_{f,t} = \frac{D}{3} \frac{u_{f,\text{max}}}{u_{f,\text{max}}} \approx 1.5 \, ms$$

Table 5.2 presents the characteristic Stokes number of the two-phase flow depending on the particle diameter. Whatever the diameter considered, the particle response time is larger than the characteristic time-scale of the most energetic eddies. As a result, the inertia of the particles is expected to play an essential role. This is shown for instance on the gas and particle mean axial velocity profiles at the outlet of the central tube.

- **Experimental results**

In Sections 5.3, 5.5 and 5.6, LES results are validated by comparisons with experiments for both phases. The experimental results are plotted using symbols. The cylindrical coordinate system $(z, r, \theta)$ is used to indicate axial (downward), radial and azimuthal directions. No mean
5.2 Numerical parameters

<table>
<thead>
<tr>
<th>$d_p , (\mu m)$</th>
<th>50</th>
<th>60</th>
<th>70</th>
<th>80</th>
<th>90</th>
<th>100</th>
<th>110</th>
<th>120</th>
</tr>
</thead>
<tbody>
<tr>
<td>$St , (-)$</td>
<td>1.5</td>
<td>2.2</td>
<td>2.9</td>
<td>3.8</td>
<td>4.8</td>
<td>6.0</td>
<td>7.2</td>
<td>8.6</td>
</tr>
</tbody>
</table>

Table 5.2 - Stokes number depending on the particle diameter. Configuration of Hishida et al. (1987).

swirling or rotating motion was detected. As a result, only the axial and radial velocity components are provided. The mean components in $(z, r)$ directions resulting from LES-averaging are respectively noted $W$ and $V$ whereas the RMS components are $w_{rms}$ and $v_{rms}$. The symbols $\cdot_f$ and $\cdot_p$ denote the fluid and the particles.

5.2 Numerical parameters

All simulations were performed with AVBP_TPF. The following section presents the computational domain, the boundary conditions and the grid. Finally, the main characteristic time scales of the gas flow are used to determine the total simulation time as well as the recording frequency required to analyse the results.

5.2.1 Computational domain

![Sketch of the computational domain and boundary conditions](image)

Figure 5.3 - Sketch of the computational domain and boundary conditions. Configuration of Hishida et al. (1987).

Figure 5.3 shows the computational domain used for the calculations. The dimensions of the
chamber itself, in terms of diameter and length, are identical to the experimental setup, but the central and annular tubes have been dropped. There are several reasons for this choice. First, considering the gas phase, the resolution in the central tube should be fine enough to obtain the characteristic mean and fluctuating velocity profiles of a fully-developed pipe at the outlet of the duct. Considering the low Reynolds number of the central jet, the supplying pipes should also be long compared to the chamber length. That would considerably increase the computational cost of the simulation. Moreover, the first experimental data available for comparison are located five inner diameters downward of the chamber inlet. This length is long enough to consider an inlet fluctuating velocity forcing method for the gas phase (Prière et al., 2005) without altering accuracy on the mean and fluctuating fluid velocity profiles at the position $z = 5 D_1$. Moreover, as already mentioned, particle-wall interactions are difficult to model using the EE approach. In the pipe and despite the low mass rate, collisions with walls and between particles should be accounted for, which is not the main purpose of the present work. Consequently, the two supplying pipes are replaced by specific boundary conditions at the inlet of the chamber capable to reproduce the experimental fluctuating velocity profiles. The fluid inlet BC treatment is detailed in Section 5.2.2 whereas the influence of the inlet BC for the particles is discussed in Section 5.4.

### 5.2.2 Boundary conditions

A schematic representation of the boundary conditions is shown in Fig. 5.3. Details of the conditions used in the LES are given in Tables 5.3 and 5.4 for the gas phase and the dispersed phase respectively.

- **The gas phase**

The NSCBC method (Poinsot & Lele, 1992) is employed for both the inlets and the outlet in order to reduce acoustic disturbances. On Patch 2, the mean axial velocity is imposed in agreement with the coflow experimental measurements. As discussed in Section 5.3, the BC treatment on Patch 1 is more complex. The mean axial velocity profile is imposed in agreement with the experiments. However, this information is not sufficient to make the gas flow destabilise downward of the inlet. Therefore, the Random Flow Generation (RFG) algorithm (Celik et al., 1999; Smirnov et al., 2001) is used to make the fluid velocity vary in time and space at the main inlet. This method reproduces the effect of an incoming turbulent field as observed in the experiment. The incoming field consists of a superposition of harmonic functions (50 modes projected in the three directions) with characteristic length-scales prescribed by the user. The imposed fluctuating velocity profile is also adjusted to the experiments. Forcing the flow in such a way considerably accelerates the establishment of fully developed turbulence. It also ensures the presence of coherent perturbations, which is not warranted when a pure white noise is used.
5.2 Numerical parameters

As for the walls, it was verified that using law-of-the-wall modeling for the chamber did not bring any improvement. Therefore, no wall modeling was finally used.

<table>
<thead>
<tr>
<th>Patch number</th>
<th>Boundary Condition</th>
<th>Imposed quantities</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Injection inlet</td>
<td>Mean and RMS velocity, temperature</td>
</tr>
<tr>
<td>2</td>
<td>Coflow inlet</td>
<td>Mean velocity, temperature</td>
</tr>
<tr>
<td>3</td>
<td>Outlet</td>
<td>Pressure</td>
</tr>
<tr>
<td>4</td>
<td>Isothermal wall</td>
<td>Velocity, temperature</td>
</tr>
</tbody>
</table>

Table 5.3 - *LES set of boundary conditions for the gas phase. Configuration of Hishida et al. (1987).*

- The dispersed phase

Dirichlet-like boundary conditions are used for the dispersed phase. To ensure that the particle mass flux imposed on Patch 1 is in agreement with the experiments, both the mean axial particle correlated velocity and the particle number density are given with respect to the measurements. Nevertheless, predictions of the particle dispersion are closely linked to the inlet treatment on Patch 1, in particular to the particle fluctuating velocity that is therefore required. This is investigated in Section 5.4.

Experimentally, no glass beads emerge from the coflow. However when using the EE approach, imposing zero particle number density is not consistent with the set of equations for the dispersed phase. Thus, a small but not zero value for particle number density (typically a thousand times smaller than the maximum particle number density on Patch 1: $\bar{n}_p \approx 10^6$) is imposed on Patch 2, sufficiently small to ensure that there is no influence on the particles injected on Patch 1.

Slip wall conditions are used for the dispersed phase but the wall treatment has no influence on the results since particles do not interact with the walls.

<table>
<thead>
<tr>
<th>Patch number</th>
<th>Boundary Condition</th>
<th>Imposed quantities</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Injection inlet</td>
<td>Mean and RMS velocity, number density</td>
</tr>
<tr>
<td>2</td>
<td>Coflow inlet</td>
<td>Mean velocity, number density</td>
</tr>
<tr>
<td>3</td>
<td>Outlet</td>
<td>–</td>
</tr>
<tr>
<td>4</td>
<td>Slipping wall</td>
<td>Wall-normal velocity component</td>
</tr>
</tbody>
</table>

Table 5.4 - *LES set of boundary conditions for the particles. Configuration of Hishida et al. (1987).*
5.2.3 Grid characteristics

Different types of grid (structured or unstructured) and different resolutions have been tested to determine the best mesh. The whole analysis is not provided hereafter, as the influence on the results stays limited. The dependency of the results on the grid is discussed in more detail in Chapter 6 for the case of the bluff body flow.

<table>
<thead>
<tr>
<th>Name</th>
<th>hishida_meshnst</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid type</td>
<td>Tetrahedra</td>
</tr>
<tr>
<td>Number of nodes</td>
<td>341285</td>
</tr>
<tr>
<td>Number of cells</td>
<td>1946749</td>
</tr>
<tr>
<td>Smallest cell volume</td>
<td>$1.6 \times 10^{-12} m^{-3}$</td>
</tr>
<tr>
<td>Time step ($\mu s$)</td>
<td>0.99</td>
</tr>
</tbody>
</table>

Table 5.5 - Main characteristics of the unstructured mesh used. Configuration of Hishida et al. (1987).

Using a structured grid may be tricky since it is known to artificially create preferential directions in the flow. In the present case, the fluid jet spreading, and to some extent the particle motion, could be affected. This has been verified and led to the conclusion that the accurate prediction of the fluid jet spreading along all the axis would require too many grid points in the radial direction. Using an unstructured grid is easier because mesh refinement in specific regions is affordable without artificially directing the flow. Grid convergence has been verified and the tetrahedral mesh characterised in Table 5.5 provided a reasonable compromise between accuracy of the predictions and computational cost.

All the results analysed in this chapter use the unstructured grid of Table 5.5 named hishida_meshnst. Figure 5.4 shows a longitudinal view of the mesh, as well as two transversal views of the radial resolution in the inlet and outlet sections. The main difficulty is to adapt the mesh refinement to the two-phase flow scales keeping a good control of the number of grid points. First, the central jet must be sufficiently resolved to capture the proper range of length scales introduced by the RFG method, and to reproduce accurately the fluid fluctuating motion at the inlet. Then, to prevent from any artificial direction in the flow, the grid is refined in the radial direction over an extended length. Nevertheless, looking at the experimental profiles in the second-half of the domain, both radial and axial resolutions can be decreased as all gradients are smoother. Finally, due to the injection of particles at the central inlet only, the gradient of particle number density at the coflow frontier is difficult to handle numerically. Therefore, the gradient zone close to the inlet must be meshed with special care. The computational cost of a typical two-phase flow simulation using the grid hishida_meshnst
5.2 Numerical parameters

Figure 5.4 - Overview of the unstructured grid used for the computations. Longitudinal \((x = 0)\) (a.), and transversal (inlet (b.), and outlet (c.)) cutting planes. Configuration of Hishida et al. (1987).

is available in Table 5.6. The time span considered is the typical total simulation time used to provide the LES statistics of the flow, as discussed in Section 5.2.4.

<table>
<thead>
<tr>
<th></th>
<th>hishida_meshnst</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total CPU time ((s))</strong></td>
<td>227166</td>
</tr>
<tr>
<td><strong>Efficiency / iteration / node ((\mu s))</strong></td>
<td>6.13</td>
</tr>
<tr>
<td><strong>Efficiency / iteration / cell ((\mu s))</strong></td>
<td>1.08</td>
</tr>
</tbody>
</table>

Table 5.6 - Code efficiency for a two-phase flow simulation. Statistics given for 0.146 \(s\) (physical time) computed with TTGC on 128 processors on the SGI ORIGIN 3800 machine from CINES. Configuration of Hishida et al. (1987).
5.2.4 Time scales

As discussed in Section 4.3.2, the analysis of the averaged quantities resulting from the LES requires a total simulation time long enough to ensure convergence, and a sampling time small enough to ensure that the smallest structures contribute to the averaged solution.

In this two-phase flow jet configuration, the largest time scale is the convective time of the gas flow. Considering the length of the domain, \( L_D = 0.3 \, \text{m} \), and the fluid bulk velocity, \( \bar{U}_{f,1} = 24.7 \, \text{m.s}^{-1} \), the convective time reads \( \tau_{f,\text{conv}} = L_D/\bar{U}_{f,1} \approx 12.1 \, \text{ms} \) (see Eq. (4.34) in Section 4.3.2). The most energetic eddies at the inlet of the chamber constitute a reasonable choice to determine the highest frequencies to be represented. Considering their size, \( l_{f,t} \approx D_1/3 \approx 4.3 \, \text{ms} \), and their velocity, \( u'_{f,t} \approx 3 \, \text{m.s}^{-1} \), the order of magnitude of the associated time-scale is \( \tau_{f,t} \approx 1.4 \, \text{ms} \) (see Eq. (4.36) in Section 4.3.2).

All the simulations discussed in Sections 5.3, 5.5 and 5.6 have been run for \( T_{av} \approx 0.15 \, \text{s} \) and the time between two samples is \( \Delta t_r \approx 0.124 \, \text{ms} \). Consequently, the statistics of the mean fields are well converged. This is not always the case for the RMS quantities but the overall tendency gives sufficient information for the purposes of this work.

5.3 Results for the gas-phase

Due to small particle mass loading, one-way coupling between the gas and the particles is assumed. Thus, the gas flow can be analysed independently of the particle motion. This is done hereafter, where predictions of the LES for the fluid flow are compared with the existing measurements. A brief summary of the simulations performed for the gas flow is given in Section 5.3.1. Only the most accurate predictions are discussed afterwards. First, the fluid flow topology obtained with LES is presented in Section 5.3.2. Second, Section 5.3.3 provides a quantitative analysis through the use of statistical diagnostics. These include the gas LES criterion and the mean and RMS profiles of axial and radial fluid velocities.

5.3.1 Test cases

In addition to grid type and resolution, many numerical parameters must be investigated to predict accurately the fluid flow. Table 5.7 summarises the tests carried out for the confined jet configuration.

Without imposing a turbulent velocity field on Patch 1, the gas flow remains laminar, due to the low Reynolds number. The RFG method presented in Section 5.2.2 solves the problem by making the inlet velocity vary in time and space at the main inlet. Changing the numerical...
5.3 Results for the gas-phase

<table>
<thead>
<tr>
<th>Name</th>
<th>Scheme</th>
<th>Turb. model</th>
<th>Wall model</th>
<th>Inlet BC for patch 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>LW_smago_lwm_norfg</td>
<td>LW</td>
<td>Smagorinsky</td>
<td>Law-of-the-Wall</td>
<td>No RFG method</td>
</tr>
<tr>
<td>LW_smago_lwm_rfg</td>
<td>LW</td>
<td>Smagorinsky</td>
<td>Law-of-the-Wall</td>
<td>RFG method</td>
</tr>
<tr>
<td>TTGC_smago_lwm_rfg</td>
<td>TTGC</td>
<td>Smagorinsky</td>
<td>Law-of-the-Wall</td>
<td>RFG method</td>
</tr>
<tr>
<td>TTGC_wale_wnm_rfg</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>RFG method</td>
</tr>
</tbody>
</table>

Table 5.7 - Test cases carried out on the grid hishida.meshnst and corresponding parameters tested. The RFG method for turbulence injection is described in Section 5.2.2. Configuration of Hishida et al. (1987).

The LW方案（cases LW_smago_lwm_norfg and TTGC_smago_lwm_rfg）确认了LW方案的更耗散行为：喷射扩展太宽，湍流速度被低估。虽然近壁区域对内层喷射预测的影响较小，但子网格WALE模型优于子网格Smagorinsky模型，因为它在近壁区域的更准确行为。

所有不同的情况给出了非常接近的结果，只讨论了表5.7中TTGC_wale_wnm_rfg的结果。

5.3.2 流拓扑

图5.5显示了在切片面上的气体速度的瞬时场。大量的涡旋可以观察到在中央喷射中，其在室中增长，尽管它被共流所限制。由于RFG方法，这些结构在入口处立即被观察到。逐渐地，它们的尺寸增加，但振幅减小。

![Instantaneous gas velocity](image)

Figure 5.5 - Topology of the gas flow. Instantaneous field of gas velocity modulus in the cutting plane $y = 0$. Configuration of Hishida et al. (1987).

如图5.5所示，一种基于Q准则的等值面图被显示在图5.6。Q准则基于...
the second invariant of the deformation tensor, and is used to visualise the coherent structures (Hussain & Jeong, 1995; Dubief & Delcayre, 2000). It compares the magnitude of the rotation and shear rates. Positive values of the Q-criterion mean that the rotation rate is larger than the shear rate, indicating the presence of a vortex. The Q-criterion is often preferred to the vorticity because it has the advantage to ignore the strong velocity gradients in the near-wall regions. In Fig. 5.6, azimuthal coherent structures arise close to the injection and progressively disappear.

Figure 5.6 - Iso-surface of Q-criterion colored by instantaneous fluid velocity. Configuration of Hishida et al. (1987).

Comparing Figs. 5.5 and 5.7 highlights the differences between the instantaneous and mean fields resulting from LES. The mean and RMS axial velocity fields in the cutting plane \( y = 0 \) are almost symmetrical, showing sufficient convergence of the statistics. In Fig. 5.7 a., the decay of the mean velocity from the inlet is small on the first third of the domain, and is larger afterwards. The same comment can be made for the jet spreading. In the first third of the chamber, RMS axial and radial velocities displayed in Figs. 5.7 b. and c. respectively, are much more significant in the shear layer than in the inner jet itself. The fluctuations are almost homogeneous, except close to the inlet where the radial velocity fluctuations are smaller. Further downstream in the central jet, the fluctuations are much more homogeneous across the jet.
5.3 Results for the gas-phase

5.3.3 Statistical analysis

In this section, the predictions of the LES are compared with the experiments for the gas phase. As discussed in Section 4.3.3, mean fields can be directly compared whereas the comparison for RMS quantities depends on the importance of the gas subgrid model. Therefore, the quality of the LES for the gas phase is first evaluated by plotting the gas LES criterion (see the definition in Section 4.3.3). This is done in Fig. 5.8 in the cutting plane $y = 0$. As suggested by the iso-contour line $Q_f^{LES} = 0.8$, the subgrid motion represents less than 20% of the total energy in the central zone, where the main turbulent structures are observed. Lower values are observed in the coflow, but no turbulent motion is present in this zone. Thus, the resolved fluctuating velocities resulting from the simulations may be directly compared to the measurements without accounting for the subgrid contribution.

Figure 5.9 compares the mean and RMS profiles of axial and radial fluid velocities with the
measurements. At the inlet, the mean and RMS velocities imposed by the BC fit well the experimental data. This shows that the RFG method works as expected: it creates turbulent fluctuations that match the imposed fluctuating velocity profiles. In the chamber, the overall agreement between LES and experiments is good. Considering the mean axial velocity, the jet spreading is slightly over-estimated, leading to a lower axial velocity on the axis at the station $z = 10 D_1$. This is confirmed by looking at the axial and radial fluctuations. Nevertheless, the quasi-isotropy and the amplitude of the fluid fluctuations are well predicted.
5.3 Results for the gas-phase

Figure 5.9 - Radial profiles of mean axial gas velocity (a.), mean radial gas velocity (b.), RMS axial gas velocity (c.), and RMS radial gas velocity (d.) at 4 stations along z axis. Symbols; experiment – Solid line: AVBP_JPF.
5.4 Inlet boundary conditions for the dispersed phase

In the simulations, the jet of particles is assumed monodisperse, with a particle diameter equal to the mean diameter given by Hishida et al. (1987), $d_p = 80.1 \mu m$, and the particle eddy viscosity model proposed by Moreau (2006) is used. Due to the vertical jet configuration, not only the drag force but also gravity act on the particles. As discussed in Section 5.1.3, the comparison between the characteristic time-scale of the particles with diameter $d_p$, and a characteristic time-scale of the most energetic turbulent eddies suggests that particle inertia plays an important role in the dispersed phase flow.

Hereafter in Section 5.4.1, length-scales evaluation as well as experimental data considerations show that the treatment of the inlet boundary condition for the particles is crucial for the prediction of particle dispersion, which is of main interest in the prospect of two-phase flow combustion. Therefore, four different boundary conditions are proposed in Section 5.4.2 for the particles in the inner tube, corresponding to different particle total velocity fluctuations imposed at the inlet of the chamber.

5.4.1 Observations

The impact of the inlet boundary condition on the particle motion can be foreseen by evaluating the length, $L_{p,H}$, over which the particles are still sensitive to their initial condition. Considering both the particle maximum velocity at the outlet of the inner pipe, $U_{p,1}^{\text{max}}$, and their response time $\bar{\tau}_p = 55 \, \text{ms}$, $L_{p,H}$ reads:

$$L_{p,H} = U_{p,1}^{\text{max}} \ast \bar{\tau}_p \approx 0.15 \, \text{m}$$

(5.2)

Since $L_{p,H}$ is about a half of the chamber length, the chamber can be divided into two zones. In the first half of the domain, the particle motion strongly depends on the two-phase flow features at the inlet of the chamber. The second half of the domain corresponds to a region where the fluid turbulence prevails on the particle motion. It is therefore essential to propose an adequate modeling of the particle inlet boundary condition to predict accurately the particle velocity field and dispersion in this geometry.

To model the particle inlet BC, the experimental setup must be considered again. Indeed, in the experiments, the hollow glass beads dispersing in the chamber emerge from a supplying pipe. In this tube, several mechanisms are responsible for the particle motion: the interactions with the fluid flow through drag force, the interactions with the pipe walls and finally, the particle-particle interactions. Comparing both the mean axial velocity profile, and the axial and radial fluctuations provided by Hishida et al. (1987) for both phases at the inlet of the chamber confirms that the particle motion in the tube is only partially correlated to the gas flow. First,
the fluid mean axial fluid velocity profile is close to the $1/7^{th}$ power law turbulent velocity profile characteristic of fully developped pipes whereas the particles show a slower velocity on the axis. Second, the fluid agitation at the outlet of the supplying pipe is almost isotropic (see Figs. 5.9 a. and b.) whereas the particle velocity fluctuations are about three times larger in the axial direction than in the radial direction. The influence of this significant anisotropy on the particle motion must be evaluated.

### 5.4.2 Particle inlet boundary condition

#### Decomposition of the particle total fluctuating velocity

The main idea for treating the particle inlet BC is to assume that the particle correlated fluctuations at the inlet can be divided into three contributions. The first step of decomposition follows the idea proposed by Février et al. (2005) when introducing the mesoscopic formalism. This decomposition is used here for the particle total velocity fluctuation:

$$u'_p = \bar{u}'_p + \delta u_p$$ (5.3)

In the second step, the particle correlated velocity fluctuation is assumed to be partially correlated to the fluid velocity one. It is therefore decomposed into two contributions. The first one is colinear with the fluctuating gas velocity. The second one, noted $w'$, is completely decorrelated from $u'_f$:

$$\bar{u}'_p = A u'_f + w'$$ (5.4)

where $A$ is assumed to be a scalar.

#### Determination of coefficient $A$

To determine the coefficient $A$ and the intensity of the synthetic field $w'$, two relations deriving from Eq. (5.4) are written, using the total decorrelation of the turbulent fields $u'_f$ and $w'$:

$$\langle \bar{u}'_{p,a} \bar{u}'_{p,a} \rangle = A^2 \langle u'_{f,a} u'_{f,a} \rangle + \langle w'_a w'_a \rangle$$ (5.5)

$$\langle \bar{u}'_{p,a} u'_{f,a} \rangle = A \langle u'_{f,a} u'_{f,a} \rangle$$ (5.6)

where $a$ stands for the direction (without summation on this index) and $\langle . \rangle$ denotes an average.
The coefficient $A$ is determined by assuming local equilibrium for the radial ($\alpha = 2$) velocity fluctuations at the inlet. Such an assumption is valid in dilute flows when the influence of collisions is negligible:

$$\left< u_{p,2}'u_{f,2}' \right> = \left< u_{p,2}'u_{p,2}' \right>$$

Using together Eqs. (5.6) and (5.7) yields:

$$A = \frac{\left< u_{p,2}'u_{p,2}' \right>}{\left< u_{f,2}'u_{f,2}' \right>}$$

where $\left< u_{p,2}'u_{p,2}' \right>$ and $\left< u_{f,2}'u_{f,2}' \right>$ are measured data.

- **Determination of the synthetic field $w'$ intensity**

Finally, to determine the amplitude of the synthetic field $w'$, Eq. (5.5) can be written as:

$$\left< w'_\alpha w'_\alpha \right> = \left< u'_{p,\alpha}u'_{p,\alpha} \right> - A^2 \left< u'_{f,\alpha}u'_{f,\alpha} \right>$$

The decomposition of the particle total velocity fluctuation into two contributions from Eq. (5.3) leads to:

$$\left< w'_\alpha w'_\alpha \right> = \left< u'_{p,\alpha}u'_{p,\alpha} \right> - \left< \delta u_{p,\alpha}\delta u_{p,\alpha} \right> - A^2 \left< u'_{f,\alpha}u'_{f,\alpha} \right>$$

where the Random Uncorrelated Motion contribution $\left< \delta u_{p,\alpha}\delta u_{p,\alpha} \right>$, needs to be modeled.

- **Description of the four inlet BCs tested for the dispersed phase**

With the above decomposition, four types of inlet boundary conditions with increasing complexity are proposed for the dispersed phase. For all cases, both the mean axial particle velocity profile and the mean particle number density profile remain unchanged, and in agreement with the measurements. Only the particle fluctuations imposed at the main inlet differ.

- **BC:nofl**: no particle fluctuations are imposed at the inlet of the chamber.

- **BC:corrisofl**: the particle fluctuations at the inlet are due to the correlated motion of particles only. Besides, the particle correlated (in the mesoscopic approach sense) velocity is completely correlated to the fluid fluctuations, and isotropic.
5.4 Inlet boundary conditions for the dispersed phase

- **BC\_corrasisofl**: the particle fluctuations at the inlet are due to the correlated motion of particles only. The particle fluctuations are assumed anisotropic.

- **BC\_totalfl**: both the correlated motion and the RUM of the particles are accounted for at the inlet of the chamber. The RUM contribution $\langle \delta u_{p,\alpha} \delta u_{p,\alpha} \rangle$ in Eq. (5.10), is assumed to be fully isotropic and the associated fluctuations are deduced from the experimental data following the relation of Février et al. (2005) and Vance et al. (2006) (see Section 1.5.2 for more details). Thus, the three terms of the decomposition are non-zero.

Note that the two turbulent fields $u'_f$ and $w'$ are generated the same way using the RFG method (see Section 5.2.2), and with the same characteristic length-scales. Table 5.8 summarises the four BCs tested, and details the three contributions for each of them:

<table>
<thead>
<tr>
<th>BC Name</th>
<th>$A$</th>
<th>$\langle w'<em>\alpha w'</em>\alpha \rangle$</th>
<th>$\langle \delta u_{p,\alpha} \delta u_{p,\alpha} \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC_nofl</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>BC_corrasisofl</td>
<td>$\frac{\langle u'_p u'_p \rangle}{\langle u'_f u'_f \rangle}$ (=$A_1$)</td>
<td>$A_1 \langle u'_f u'_f \rangle - A_1 \langle \underline{u}'_f \underline{u}'_f \rangle$</td>
<td>0</td>
</tr>
<tr>
<td>BC_corranisofl</td>
<td>$A_1$</td>
<td>$A_1 \langle u'_f u'_f \rangle \left( \frac{\langle u'_p u'_p \rangle}{\langle u'_f u'_f \rangle} - A_1 \right)$</td>
<td>$A_1 \frac{\langle u'_p u'_p \rangle}{\langle u'_f u'_f \rangle} \frac{\langle u'_f u'_f \rangle}{\langle u'_p u'_p \rangle}$</td>
</tr>
<tr>
<td>BC_totalfl</td>
<td>$A_1$</td>
<td>$A_1 \langle u'_f u'_f \rangle \left( \frac{\langle u'_p u'_p \rangle}{\langle u'_f u'_f \rangle} - A_1 \right)$</td>
<td>$A_1 \frac{\langle u'_p u'_p \rangle}{\langle u'_f u'_f \rangle} \frac{\langle u'_f u'_f \rangle}{\langle u'_p u'_p \rangle}$</td>
</tr>
</tbody>
</table>

Table 5.8 - Description of the four BCs tested for the particles. Configuration of Hishida et al. (1987).

**Description of the four LES performed**

Four different LES have been performed for the four types of BC. The carrier phase remains the same for all the simulations, corresponding to the case TTGC\_wale\_wnm\_rfg analysed in Section 5.3. As far as the dispersed phase is concerned, the use of TTGC is combined with some, but little, particle Artificial Viscosity (see Section 2.3.1). In addition, the particle subgrid eddy viscosity model presented in Section 4.2.2 is always used.

The four calculations can be divided into two main categories, depending on the explicit resolution of the particle RUM or not. Indeed, for the boundary conditions BC\_nofl, BC\_corrasisofl and BC\_corranisofl, no particle RUE is imposed at the inlet of the chamber. As the particle RUE field is initially zero in the whole domain, the quantity remains zero during the simulation, due to the specificities of the source or sink terms in the transport equation for particle RUE. Therefore, for these three cases, the transport equations for particle number density and particle
correlated velocity omitting the RUM terms are the only equations solved for the dispersed phase. The RUM contribution is \textit{a posteriori} evaluated using the correlation proposed by Février \textit{et al.} (2005) and Vance \textit{et al.} (2006). The fourth case with $BC_{total}$ is conceptually very different since it imposes a particle RUE profile at the inlet of the domain and requires the explicit resolution of the transport equation for particle RUE.

Subsequently, Section 5.5 focuses on the three first LES performed without accounting for the RUM motion whereas the fourth simulation directly using the transport equation for RUE is dealt with in Section 5.6.

### 5.5 LES for the dispersed phase without accounting for the RUM

The particle-laden jet flow is the first configuration where LES using the Euler-Euler mesoscopic approach is performed. In this section however, neither the dissipation term due to the RUM that is part of the transport equation for particle mesoscopic equation nor the transport equation for particle RUE are accounted for. In Section 5.5.1, the role of the particle subgrid model is first investigated. Second, Section 5.5.2 summarises the numerical characteristics (see Chapter 2) for the dispersed phase. Then, the influence of the particle BC treatment on the particle motion is qualitatively shown in Section 5.5.3. The quantification of the particle inlet BC impact is dealt with in Section 5.5.4.

#### 5.5.1 Role of the particle eddy viscosity model

In LES of two-phase flow, the particle subgrid model is at least as essential as it is for the gas phase. Preliminary calculations carried out without activating the particle eddy viscosity model showed that handling numerically both the gradients of particle number density in the shear layer and the clusters of particles in the central jet was impossible.

To show the role of the particle eddy viscosity model, instantaneous fields of particle deviatoric and spherical subgrid viscosities (respectively noted $v_{\rho,d}$ and $v_{\rho,s}$ in Section 4.2.2) are displayed in Fig. 5.10, as well as instantaneous fields of particle correlated velocity and particle number density. The simulation $BC_{corranisofl}$ is considered here but the observations are similar for the two other calculations. First, the large difference in magnitude between the spherical and the deviatoric subgrid viscosities must be noticed. Contrary to the gas phase where the spherical part is omitted, the particle spherical subgrid viscosity is about three orders of magnitude higher than the particle deviatoric viscosity, and so cannot be neglected. Then,
the two subgrid viscosity fields are closely linked to the particle number density field: they are maximum where there are clusters of particles. Note that it is in contradiction with the \emph{a priori} analysis of Moreau (2006) when investigating HIT flows, where extrema of particle subgrid energy were located at the interface between clusters of particles. This may be due to the absence of RUM, that would move the location of the activation of the particle subgrid model.

One last comment to make is that the particle spherical subgrid viscosity is more localised (or less diffused) than the particle deviatoric contribution.

Figure 5.10 - Instantaneous fields of particle correlated velocity magnitude (a.), particle number density (b.), particle deviatoric subgrid viscosity (c.) and particle spherical subgrid viscosity (d.) in the cutting plane $y = 0$. \emph{BCcorrainisof}. Configuration of Hishida et al. (1987).
5.5.2 Numerical method for the dispersed phase

A brief summary of the numerical models, detailed in Chapter 2, and used for the dispersed phase in this geometry is proposed in Table 5.9. Since the TTGC scheme has shown a better accuracy than LW for the gas phase, all the two-phase flow simulations are performed with TTGC. This convective scheme is centered and some artificial dissipation is therefore required for the dispersed phase, as for the gas phase, to stabilise the calculations. Thus, the Jameson artificial viscosity model detailed in Section 2.3.1 for the dispersed phase is used in all the two-phase flow simulations presented below. As shown in Section 5.5.1, the use of particle eddy-viscosity model is also required and is used in all the LES investigated hereafter. Finally, as the transport equation for particle RUE is not computed in this section, there is no RUE flux limitor.

<table>
<thead>
<tr>
<th>Convective scheme</th>
<th>AV model</th>
<th>Subgrid model</th>
<th>RUE flux limitor</th>
</tr>
</thead>
<tbody>
<tr>
<td>TTGC</td>
<td>Jameson</td>
<td>eddy viscosity</td>
<td>No</td>
</tr>
</tbody>
</table>

Table 5.9 - Numerical method for the dispersed phase when the RUM is not explicitly accounted for. Configuration of Hishida et al. (1987).

5.5.3 Qualitative influence of the particle inlet BC on the flow topology

In this section, the impact of the three first boundary conditions noted $BC_{\text{nofl}}$, $BC_{\text{corrisofl}}$ and $BC_{\text{corranisofl}}$ in Table 5.8 is shown by qualitatively analysing instantaneous and time-averaged LES fields of particle correlated velocity and particle number density.

Figures 5.11 and 5.12 respectively compare instantaneous fields of particle correlated velocity and particle number density in the cutting plane $y = 0$ for the three boundary conditions. The impact on the dispersed phase flow topology is easily visible for both quantities. The particle jet spreading is more important when velocity fluctuations are imposed at the inlet, and even more if the fluctuations are anisotropic. As a consequence, the decrease in particle correlated velocity is much slower along the axis when no fluctuations are applied. The topology of the particle number density field also greatly differs with the BC modeling. Clusters of particles are created much closer to the inlet when particle fluctuations are imposed. Moreover, the differences due to isotropic or anisotropic particle velocity fluctuations are also non-negligible: anisotropy makes particles more numerous close to the inlet and enhances diffusion in the second half of the domain.

Time-averaged LES fields are less different, although the impact of the inlet BC is not
negligible and is quantified in Section 5.5.4. In Fig. 5.13, the mean fields of particle axial correlated velocity and particle mass flux as well as the RMS fields of particle axial and radial correlated velocity fluctuations are displayed only for the case $BC_{corranisoft}$. First, similarly to the gas phase, instantaneous and mean fields resulting from LES show very different topologies. Then, the perfect symmetry of the mean and RMS fields indicates good convergence of the simulations. The main information here is the considerable anisotropy of the particle fluctuations. The topology of both components is very similar but the axial fluctuations are three times bigger than the radial ones. This makes a great difference with the gas flow where the fluctuations stay almost isotropic.

Figure 5.11 - Topology of the dispersed phase. Comparison of instantaneous fields of particle number density in the cutting plane $y = 0$ for $BC_{nofl}$ (a.), $BC_{corrisoft}$ (b.), and $BC_{corranisoft}$ (c.). Configuration of Hishida et al. (1987).
5.5.4 Quantitative comparison of the particle motion depending on the particle inlet treatment

To quantify the above observations, results of the calculations are compared with measurements. Profiles of mean axial and radial particle correlated velocity, and mean particle mass flux are plotted in the four measured stations along $z$. RMS fields of axial and radial particle correlated velocity are also compared to the experimental data. This implies that the subgrid contributions can be neglected, as is done below with the particle LES quality criterion.

- Particle LES quality criterion

Figure 5.14 displays the particle LES quality criterion introduced in Section 4.3.3 in the
5.5 LES for the dispersed phase without accounting for the RUM

Figure 5.13 - Configuration of Hishida et al. (1987). Topology of the dispersed phase. Mean field of axial particle velocity (a.), RMS fields of axial (b.) and radial (c.) particle velocity, and mean particle mass flux field (d.) in the cutting plane \( y = 0 \). Only BC_corranisoft is considered here.

The iso-contour line \( \Omega_p^{LES} \) indicates that the LES for the dispersed phase is sufficiently resolved in the region of interest. Thus, the particle velocity fluctuations can be compared to the measurements without accounting for the subgrid contributions. It must be noticed that the injection zone, and especially the shear gradient region close to the inlet is more difficult to capture accurately.
• Particle mean fields

Figure 5.14 - Mean field of LES criterion for the dispersed phase in the cutting plane \( y = 0 \). The black line represents the iso-contour line \( Q_p^{LES} = 0.8 \). Only \( BC_{corranisofl} \) is shown here. Configuration of Hishida et al. (1987).

The first step of validation consists in comparing the mean axial and radial particle correlated velocity profiles as well as the mean particle mass flux profiles with the measurements. Figures 5.15 – 5.17 display this information for the three boundary conditions, respectively \( BC_{nofl} \), \( BC_{corrisofl} \) and \( BC_{corranisofl} \). Overall agreement on velocity profiles is good for the three calculations, all showing very similar results in terms of mean axial and radial velocities. Yet, as already mentioned, the particle jet spreading is wider when anisotropic particle velocity fluctuations are imposed at the inlet. Predictions of the mean particle mass flux are more dependent on the inlet treatment. When no fluctuations are imposed at the inlet of the chamber, the particle mass flux is greatly overestimated at every stations downward of the inlet. Predictions of the particle dispersion is much better when isotropic particle velocity fluctuations are imposed. The best result is obtained when accounting for the anisotropic distribution of particle fluctuations at the inlet as shown in Fig. 5.17 c. This is coherent with the measurements, where fluctuation anisotropy is present not only at inlet but also in the chamber.

To sum up, the inlet treatment has a minor influence on the mean particle velocity field, but a strong impact on the particle dispersion. It is then essential to impose particle velocity fluctuations at the inlet of the chamber, and to account for their anisotropy, in order to predict accurately the particle dispersion.

• Particle RMS fields

The second step of validation deals with particle agitation. Again, no transport equation for particle RUE is solved in the LES discussed up to this point. Nevertheless, as explained in Section 1.5, the RUM contribution may be quantified by using the correlation proposed by
Février et al. (2005) or Vance et al. (2006). All the quantities required for this correlation, that is to say the fluid and the particle velocity fluctuations, and the fluid-particle correlation, may be post-processed from LES. Results are shown in Figs. 5.18 – 5.20 for the three boundary conditions tested, where contributions of the correlated motion and uncorrelated motion to the total particle fluctuations are plotted. Besides, the sum of both contributions that represent the total particle velocity fluctuation, can directly be compared with the measurements. Considering the differences in the three inlet boundary conditions and the resulting particle velocity fluctuations, large differences in the RMS axial and particle velocities could be expected. This is however not confirmed by the simulations. Indeed, whatever the fluctuations imposed at the inlet, whether they are zero, isotropic, or anisotropic, the profiles at the second measurement station $z = 5 D_1$ are similar and quasi-independent of the inlet treatment. Both the amplitude and the anistropy of the correlated velocity fluctuations are similarly predicted downward of the inlet. Another conclusion is that accounting only for the correlated motion does not allow accurate predictions of the level of velocity fluctuations that is under-estimated. Nevertheless, when estimating the total particle fluctuations as the sum of the calculated mesoscopic fluctuations and the $a$ posteriori evaluated uncorrelated fluctuations, the agreement with the measurements is good.
Figure 5.15 - Radial profiles of mean axial particle correlated velocity (a.), mean radial particle correlated velocity (b.), and mean particle mass flux (c.) at 4 stations along z axis. Symbols: experiment – Solid line: AVBP_TPF_BC_nofl case.
Figure 5.16 - Radial profiles of mean axial particle correlated velocity (a.), mean radial particle correlated velocity (b.), and mean particle mass flux (c.) at 4 stations along z axis. Symbols: experiment – Solid line: AVBP_TPF. BC_corrisofl case.
Figure 5.17 - Radial profiles of mean axial particle correlated velocity (a.), mean radial particle correlated velocity (b.), and mean particle mass flux (c.) at 4 stations along z axis. Symbols: experiment – Solid line: AVBP_TPF. BC_corranisofl case.
Figure 5.18 - Radial profiles of RMS axial (a.) and radial (b.) particle velocity at 4 stations along z axis. Correlated contribution (solid line) resulting from the simulation, uncorrelated contribution (dotted-dashed line) a posteriori calculated, resulting total RMS particle velocity (dashed line), and measurements (symbols). BC_nofl case.
Figure 5.19 - Radial profiles of RMS axial (a.) and radial (b.) particle velocity at 4 stations along z axis. Correlated contribution (solid line) resulting from the simulation, uncorrelated contribution (dotted-dashed line) a posteriori calculated, resulting total RMS particle velocity (dashed line), and measurements (symbols). BC corrisoft case.
Figure 5.20 - Radial profiles of RMS axial (a.) and radial (b.) particle velocity at 4 stations along z axis. Correlated contribution (solid line) resulting from the simulation, uncorrelated contribution (dotted-dashed line) a posteriori calculated, resulting total RMS particle velocity (dashed line), and measurements (symbols). BC : corranisofl case.
5.6 LES for the dispersed phase with explicit account for the RUM

The analysis of the simulations performed with the simplified LES Euler-Euler mesoscopic model approach shows that neglecting the RUM contributions mainly affects the predictions of the particle agitation. The next step consists in explicitly accounting for the uncorrelated motion of the particles, which is the main purpose of the case noted BC_total/I and described in Table 5.8. In this case, a particle RUE profile is imposed at the inlet of the domain to mimic the inter-particle collisions as well as the wall-particle interactions that occur in the pipe.

The numerical model used in this case is very close to the one used in Section 5.5. As shown in Table 5.10, the only difference is the use of the RUE flux limitor. It must be noticed that the preferential concentration phenomenon is less critical than in the particle-laden HIT flow focused on in Chapter 3. Consequently, the RUE flux limitor is rarely active in this case.

<table>
<thead>
<tr>
<th>Convective scheme</th>
<th>AV model</th>
<th>Subgrid model</th>
<th>RUE flux limitor</th>
</tr>
</thead>
<tbody>
<tr>
<td>TTGC</td>
<td>Jameson</td>
<td>eddy viscosity</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Table 5.10 - Numerical method for the dispersed phase when the RUM is explicitly accounted for. Configuration of Hishida et al. (1987).

Although the numerical method developed in this work is still stable and robust in this case, no analysis of the simulations can be proposed hereafter. Indeed, there is a huge difference between the LES and the experiments, due to a relaminarisation of the dispersed phase flow. Actually, only the RUM contributes to the particle agitation, leading to a consequent underestimation of the total agitation. To investigate the problem, many tests have been carried out that lead to the following remarks:

- In the transport equation for particle RUE, the RUM viscosity term dominates.
- The regions where this term shows the highest values correspond to significant mean particle velocity gradient zones.
- Arbitrary decreasing the RUM viscosity model by a factor 5 or even 10 notably improves the results.

These preliminary tests suggest that the viscosity assumption used to model the particle second order velocity correlations must be questioned. One idea would be to write a viscosity model.
without accounting for the particle mean velocity gradients, which corresponds more or less to the filtered Smagorinsky model (Ducros et al., 1998a) used to for the gaseous subgrid term in the momentum equation (see Chapter 4). This model was developed for the gas phase in order to allow a better representation of local phenomena typical of complex turbulent flows. Such a change in the particle viscosity model may significantly decrease the RUM viscosity term contribution in the regions of large particle velocity gradients and prevent from relaminarisation of the particular flow.

5.7 Conclusions

To our knowledge, the calculations of the vertical particle-laden turbulent confined jet flow presented in this chapter are the first tentatives to apply LES with an Eulerian description of the dispersed phase to a real turbulent two-phase flow.

The code AVBP_TPF is dedicated to the simulation of two-phase flows in complex geometries such as aeronautical combustion chambers. It uses therefore unstructured grids, on which high-order schemes are however very delicate to develop. As shown by the numerous tests investigating the influence of the grid type, the number of cells, the numerical scheme and the subgrid model, it is delicate to obtain very accurate results even for the gas phase in the confined jet configuration considered. However both the mean and fluctuating gas velocity profiles show good agreements with the measurements. The analysis of the results for the two-phase flow provides a lot of information while raising new questions:

- The subgrid models proposed by Moreau (2006) and implemented in AVBP_TPF are essential for the LES since the calculations fail when they are not activated. Moreover, the spherical part of the particle SGS tensor is much bigger than the deviatoric part, suggesting that the deviatoric part can not be omitted as for the gas phase. Testing other subgrid models that give a priori better results but that are more difficult to implement would be interesting to show the impact of the SGS modeling on the results.

- Since it is still difficult to calculate the particle motion in a pipe where the wall-particle interactions can not be neglected and must therefore be modeled, it is essential to develop inlet boundary conditions for the dispersed phase to reproduce their velocity distribution at the pipe outlet. The use of the modified inlet boundary condition confirms that it is crucial to impose particle velocity fluctuations while accounting for their large anisotropy (contrary to the gas phase that shows almost isotropic fluctuations) to predict accurately particle dispersion. Furthermore, the topology of the dispersed phase is strongly affected by the changes in the inlet boundary condition.
• Using the LES Eulerian mesoscopic approach without the terms linked to the uncorrelated motion of the particles still leads to mean velocity and mass flux predictions in very good agreement with the experiments. As may be expected in that case the agitation of the particles is under-estimated since part of it is due to the uncorrelated motion. Restoring this contribution by an a posteriori evaluation using the correlation proposed by Février et al. (2005) and later by Vance et al. (2006) finally gives results in good agreement with the measured particle agitation.

• Accounting explicitly for the uncorrelated motion by resolving the transport equation for particle RUE and including the dissipation term due to RUM in the transport equation for particle correlated velocity, makes the results notably worsen. The resolved fluctuations are considerably damped and only the RUM contributes to the particle agitation. This questions the viscosity assumption used to model the uncorrelated velocity correlations and preliminary tests show that not only it is over-estimated, but even the shape of the model itself may not be correct.
Chapter 6

LES of confined bluff body gas-solid flow

The conclusions of the particle-laden turbulent confined jet presented in Chapter 5 are limited to simple geometries. However, in the context of combustion, such a configuration is often prohibited because the resulting jet flame is too long in comparison with the length of the combustion chamber, and is difficult to stabilise. Thus, most combustion devices are designed so as to anchor the flame at a specific location. The use of a flame holder is tricky due to the very high temperatures that may damage the device itself. Another possibility is to stabilise the flame behind a sudden expansion like a backward-facing step, like in gas ovens for instance. The flow is strongly decelerated and forms a corner recirculation zone (CRZ). The recirculating hot gases provoke the ignition of the incoming fresh gases. As far as aeronautical combustion chambers are concerned, highly swirling flows that pass through a sudden expansion are preferred since they provide a much more compact stabilised flame. A central toroidal recirculation zone (CTRZ) is created, acting as a flame holder in the center of the flow, close to the injector tip. The combustion chamber of the Mercato test-rig, experimentally and numerically investigated respectively at ONERA and CERFACS, exhibits the two types of recirculation zones, as shown in Fig. 6.1. In such devices, the recirculation zones induce high turbulence levels and high mixing rates, which greatly stabilises the flame and also reduces pollutant emissions. Before computing reactive two-phase flows in such devices, which requires evaporation and combustion modeling, a validation of the turbulent dispersion of the particles is needed. Indeed, the accurate description of the fuel droplet motion is crucial to determine the resulting fuel vapor distribution. To this purpose, a particle-laden confined bluff body experimentally investigated by Borée et al. (2001) in a flow-loop of EDF-GDF is focused on hereafter. A large amount of detailed data is available in this geometry where a jet of air and solid particles emerges without any swirl in a coflow of air. RANS simulations using the EE approach have already been performed by Vit et al. (1999). The same kind of experiment, but including a swirling air flow, has been conducted by Sommerfeld & Qiu (1991), and has been simulated by Apte et al. (2003b) with the EL approach, and by Boileau et al. (2007) with the EE mesoscopic approach.
with the objective of evaluating the model performances.

Although there is no swirling flow, the bluff body flow from Borée et al. (2001) is interesting for aeronautical applications. First, combustion chambers like the Mercato one exhibit the same flow structures with corner recirculation zones and stagnation points. Their accurate prediction is closely linked to the capture of the large structures and the intermittency of the fluid flow (see for instance Chin & Tankin (1992); Schefer et al. (1994); Namazian et al. (1992)), and requires accurate turbulence modeling. Second, the dispersed phase itself is also important in such devices (Hardalupas et al., 1994; Boileau et al., 2007). Depending on their inertia and their mass loading, the particles remain more or less in the recirculation zones, modifying the burner efficiency as well as the pollutant emissions. With this in prospect, the data provided by Borée et al. (2001) allow to test in detail not only the gas LES models, but also the dispersed phase modeling. The objective in this chapter is to study in detail the models behavior and the underlying mechanisms.

Part of this work has been done in collaboration with Marta Garcia and Vincent Moureau during the Summer Program organised by the Center for Turbulence Research (CTR) of Stanford University in July 2006. Such a collaborative work has allowed three different validations, as shown in Fig. 6.2. First, the gas LES solver from AVBP_TPF was confronted to the gas LES solver from CDP\(^1\). Since the two codes gave very similar results and captured most of fluid

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\(^1\)The LES solver CDP developed at Stanford University solves implicitly the incompressible Navier-Stokes equations. The time integration of CDP is based on the fractional-step method (Kim & Moin, 1985) and the space integration relies on a second-order central scheme that conserves the kinetic energy (Mahesh et al., 2004; Ham & Iaccarino, 2004). The dynamic Smagorinsky model (Germano et al., 1991) is used to model the subgrid stress tensor. The dispersed phase is treated using the EL approach described in Section 1.2. More details can be found in Apte et al. (2003b).
flow structures, the EE and EL formulations were then evaluated. This was done in two steps. First, the EL solver from AVBP_TPF developed by García et al. (2005)\(^2\) was also confronted to the EL solver from CDP. Then, the EL and EE mesoscopic approaches were compared using the same gas LES solver from AVBP_TPF. Note that the EE mesoscopic approach used in this configuration corresponds to the simplified model tested in Section 5.5 where the RUM contributions are neglected.

Section 6.1 briefly presents the experimental setup, the measurement methods and the available data. In Section 6.2, the gas phase results are compared and analysed. The sensitivity of the results to the convective scheme, the grid, the LES model, the wall treatment, and the inlet boundary conditions is investigated. Finally, Section 6.3 deals with the two-phase flow simulation for the lowest mass loading of the central jet and monodisperse particle distribution. The main purpose is to compare the two approaches (EL and EE). For the sake of clarity, only the results obtained with AVBP_TPF using either the EE or the EL approach are shown, the CDP results being available in Riber et al. (2006).

\(^2\) In AVBP_TPF, both the EE mesoscopic approach and the EL approach are available. The gas LES solver is identical and only the formulation for the dispersed phase is different.
6.1 Description of the configuration

This section describes the bluff body configuration from Borée et al. (2001), explains the underlying concept and details the experimental setup.

6.1.1 Concept and main purpose

Borée et al. (2001) created a vertical axisymmetrical particle-laden confined bluff body flow (see Fig. 6.3) on the flow loop Hercule of EDF-DER-LNH. Both air and particles are injected in the inner jet whereas air blowers are used to generate the coflow. The measurement zone is located downstream of the inner and annular ducts ($z > 0$), where large recirculation zones are created between the central jet and the coflow due to the geometry. The resulting flow is similar to the flows obtained in industrial combustion devices, where fuel droplets are injected together with air.

![Schematic of the configuration of Borée et al. (2001).](image)

Figure 6.3 - Schematic of the configuration of Borée et al. (2001). The dimensions are: $R_j = 10$ mm, $R_1 = 75$ mm, $R_2 = 150$ mm. The length of the experimental chamber is 1.5 m.

The topology of the gas flow mainly depends on the ratio between the velocity in the inner pipe and the velocity in the coflow. With a low velocity in the annular flow, Borée et al. (2001) managed to obtain two stagnation points on the axis. Such a single phase flow has been shown to be very interesting when adding particles. Indeed, particle inertia as well as fluid-particle interactions are the main mechanisms in such two-phase flows (Simonin, 1991).

The volume and the accuracy of the data make this configuration a very good test case to study turbulent closure models. The data include radial profiles of the following quantities at seven stations along the axis ($z = 3, 80, 160, 200, 240, 320$ and $400$ mm) in the measurement zone:
- Mean axial and radial velocity components for the carrier and the dispersed phases,
- RMS axial and radial velocity components for both phases,
- Particle number density and particle mass flux.

Furthermore, axial profiles of mean and RMS axial velocities are provided on the centerline.

### 6.1.2 Characteristics of the flow for both phases

#### The gas phase

The experiments are conducted at ambient temperature, \( T_f = 293 \, K \), and standard pressure, \( P_f = 1.013 \times 10^5 \, Pa \).

The inner pipe is 1.5 m long and the radius is \( R_j = 10 \, mm \). The air volume flux of the inner jet is \( Q_{f,j} = 3.4 \, m^3.h^{-1} \), which corresponds to a mean velocity, \( \bar{U}_{f,j} = 3.4 \, m.s^{-1} \), whereas the maximum velocity in the inner duct reaches \( U_{f,j}^{\text{max}} = 4 \, m.s^{-1} \). As a result, the Reynolds number is \( Re_j = 2R_j\bar{U}_{f,j}/v_f \approx 4500 \), which is rather low. The ratio \( U_{f,j}^{\text{max}}/\bar{U}_{f,j} = 1.18 \) at the outlet of the inner pipe is however consistent with fully developed turbulent pipe flow.

The dimensions of the annular outer region are: \( L_e = 2 \, m, R_1 = 75 \, mm, R_2 = 150 \, mm \). The air volume flux in the co-flow is \( Q_{f,e} = 780 \, m^3.h^{-1} \), which corresponds to mean and maximum velocities equal to: \( \bar{U}_{f,e} = 4.1 \, m.s^{-1} \) and \( U_{f,e}^{\text{max}} = 6 \, m.s^{-1} \). The associated Reynolds number of the annular jet is \( Re_e = 2(R_2 - R_1)\bar{U}_{f,e}/v_f \approx 40000 \).

Table 6.1 summarises this information.

<table>
<thead>
<tr>
<th>Gas phase</th>
<th>Length (mm)</th>
<th>Radius (mm)</th>
<th>Volume flux ( m^3.h^{-1} )</th>
<th>Mean velocity ( m.s^{-1} )</th>
<th>Max. velocity ( m.s^{-1} )</th>
<th>Reynolds number (–)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner pipe</td>
<td>1500</td>
<td>10</td>
<td>3.4</td>
<td>3.4</td>
<td>4.4</td>
<td>4500</td>
</tr>
<tr>
<td>Annular pipe</td>
<td>2000</td>
<td>75</td>
<td>780</td>
<td>4.1</td>
<td>6.0</td>
<td>40000</td>
</tr>
</tbody>
</table>

Table 6.1 - Characteristics of the gas phase at the outlet of the inner and annular pipes. Configuration of Borée et al. (2001).

Schefer et al. (1994) show that the topology of a turbulent bluff body flow strongly depends on the ratio \( \bar{U}_{f,j}/\bar{U}_{f,e} \). The three possible configurations are illustrated in Fig. 6.4, where sketches of mean gas velocity vectors are drawn for three decreasing ratios: \( \bar{U}_{f,j}/\bar{U}_{f,e} = 2.8, 1.4 \) and 0.84. Moreover, seeding the gas flow with small particles gives access to photographs of the particle distribution, and so on the flow topology. This is done in Fig. 6.5 by Schefer et al.
LES OF CONFINED BLUFF BODY GAS-SOLID FLOW

(1994) for the three ratios given above. At the highest ratio \( \bar{U}_{f,j}/\bar{U}_{f,e} = 2.8 \), the flow along the axis is similar to a free-jet flow. The air flows coming from the inner and annular pipes converge far from the outlet of the inner duct. Two counter-rotative eddies separate the two flows before they converge. There is no stagnation point on the axis, but one is visible on both sides of the central jet. In the vicinity of \( \bar{U}_{f,j}/\bar{U}_{f,e} = 1 \), a single stagnation point is formed along the centerline and the flow looks like a non-penetrating jet. When decreasing the ratio down to one, a second stagnation point appears on the axis. The location of the stagnation point closest to the inner pipe is linked to the inner air mass flux. The location of the second one mainly depends on the bluff body geometry, and does not move when \( \bar{U}_{f,j}/\bar{U}_{f,e} < 1 \). The two counter-rotative eddies move away from each other with decreasing ratio.

In Borée et al. (2001), the ratio in the gaseous flow is: \( \bar{U}_{f,j}/\bar{U}_{f,e} = 0.83 < 1 \). Similarly to Schefer et al. (1994), two stagnation points are observed along the centerline. Choosing a ratio lower than one creates an interesting gas flow behaviour when modeling particle dispersion, as the particles, depending on their inertia, are more or less kept in the recirculation zone delimited by the two stagnation points.

Figure 6.4 - Plots of the measured mean velocity vectors in a bluff body stabilised methane jet for \( \bar{U}_{f,j}/\bar{U}_{f,e} = 2.8 \) (a.), \( \bar{U}_{f,j}/\bar{U}_{f,e} = 1.4 \) (b.), and \( \bar{U}_{f,j}/\bar{U}_{f,e} = 0.84 \) (c.). Black dots show the location of the stagnation points and round arrays give the direction of rotation of the shear layer vortices. From Schefer et al. (1994).
6.1 Description of the configuration

Figure 6.5 - Mie scattering measurements of the instantaneous particle distribution in a bluff body stabilised methane jet for $\bar{U}_{f,j}/\bar{U}_{f,e} = 2.8$ (a.), $\bar{U}_{f,j}/\bar{U}_{f,e} = 1.4$ (b.), and $\bar{U}_{f,j}/\bar{U}_{f,e} = 0.84$ (c.). From Schefer et al. (1994).

- The dispersed phase

Polydisperse glass particles with material density, $\rho_p = 2470 \text{ kg.m}^{-3}$, are injected through a particle feeder in the inner jet only. The particle feeder is located two meters upstream of the inner pipe outlet. Two mass flux of glass beads, $Q^1_{p,j} = 1 \text{ kg.h}^{-1}$ and $Q^2_{p,j} = 5 \text{ kg.h}^{-1}$, have been experienced to study the influence of particle inertia on the two-phase flow, and also the role of particle-particle collisions. The corresponding mass loading in the inner duct then varies from $M^1_{p,j} = 22\%$ to $M^2_{p,j} = 110\%$.

The particle diameter covers a wide range of size classes from $d_p = 20 \mu m$ to $d_p = 110 \mu m$. Figure 6.6 shows the particle distribution, in mass and in number. The resulting mean diameter is respectively $d_{p,M} = 63 \mu m$ and $d_{p,N} = 50 \mu m$. Special care has been taken to analyse the particle distribution. It was important to ensure that the glass beads remained spherical and that the particle-particle collisions did not induce any particle break-up. This was confirmed by repeating the measurements and observing the particles with a microscope.

- Characteristic time scales

Table 6.2 gives the relaxation time of the particles $\tau_p$, depending on the particle diameter $d_p$. To give an order of magnitude of the characteristic time scale of the particles, a Stokes flow around the particles is assumed (see Eq. (1.15) in Section 1.2.1).

The comparison of the particle relaxation time $\tau_p$, with a characteristic time scale of the fluid most energetic eddies $\tau_{f,t}$, gives the Stokes number. Similarly to the particle-laden confined jet flow (see Section 5.1.3), $\tau_{f,t}$ is estimated assuming that the length of the most energetic eddies
corresponds to one third of the duct diameter and their velocity is the maximum fluctuating velocity in the pipe:

$$St = \frac{\tau_p}{\tau_{f,t}} \quad \text{where} \quad \tau_{f,t} = \frac{2R_j}{u_{f,max}} \approx 7 \text{ ms}$$  \hspace{1cm} (6.1)

The influence of particle inertia on the two-phase flow topology increases with the Stokes number. Table 6.3 presents the characteristic Stokes number of the two-phase flow depending on the particle diameter. It comes that the motion of the smallest particles with diameter $d_p = 20 \mu m$ is expected to be very different from the biggest ones, with diameter $d_p = 110 \mu m$: while the smallest particles almost follow the gas flow, the inertia of the biggest ones make them much more independent of the fluid flow.

<table>
<thead>
<tr>
<th>$d_p , (\mu m)$</th>
<th>20</th>
<th>30</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>70</th>
<th>80</th>
<th>90</th>
<th>100</th>
<th>110</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_p , (ms)$</td>
<td>3.1</td>
<td>6.9</td>
<td>12.3</td>
<td>19.2</td>
<td>27.6</td>
<td>37.6</td>
<td>49.1</td>
<td>62.2</td>
<td>76.7</td>
<td>92.9</td>
</tr>
</tbody>
</table>

Table 6.2 - Relaxation time of the particles injected depending on their diameter. Configuration of Borée et al. (2001).

<table>
<thead>
<tr>
<th>$d_p , (\mu m)$</th>
<th>20</th>
<th>30</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>70</th>
<th>80</th>
<th>90</th>
<th>100</th>
<th>110</th>
</tr>
</thead>
<tbody>
<tr>
<td>$St$ (--)</td>
<td>0.4</td>
<td>1.0</td>
<td>1.8</td>
<td>2.7</td>
<td>3.9</td>
<td>5.4</td>
<td>7.0</td>
<td>8.9</td>
<td>11.0</td>
<td>13.3</td>
</tr>
</tbody>
</table>

Table 6.3 - Stokes number depending on the particle diameter. Configuration of Borée et al. (2001).

Contrary to the configuration of Hishida et al. (1987), calculating the supplying pipes is here mandatory since they are at the origin of the large recirculation zones in the chamber itself. In
the inner duct, both air and particles are injected. To determine whether a specific treatment of the particle inlet boundary condition is required (see Section 5.4), it must be quantified if particles have enough time to adapt to the changes in gas mean velocity within the inner duct. To do so, the relaxation time of the particles is compared to their transit time in the pipe.

The transit time of the particles in the inner pipe, $T_{pT}$, is determined using the length of the duct (the starting point is the particle feeder) and the inner maximum gas velocity:

$$T_{pT} = \frac{L_j}{U_{max}} = 250 \text{ ms} \quad (6.2)$$

It comes that the particle relaxation time is largely smaller than their transit time in the inner pipe, whatever the diameter considered. Thus, the particles have time to adapt to fluid turbulence before they reach the outlet of the inner pipe and no specific treatment on particle agitation is required at the inlet of the central pipe.

### 6.1.3 Experimental setup

The mean and RMS velocities, for the gas phase and for each class of particles, are obtained by the Particle Doppler Anemometry (PDA) measuring technique presented in Section 5.1.2.

When dealing with two-phase flows, it is necessary to choose different material for the particles, so that they can be either a measure of the fluid flow or a measure of the dispersed phase itself. Borée et al. (2001) used three types of particles: glass beads for the dispersed phase, smoke for the inner jet fluid flow and water droplets for the annular gas flow.

Seeding the flow with so many different particles is a delicate task and specific care has to be taken. As far as the gas flow is concerned, sufficient volume flux of the seeded particles is required. Considering the high annular volume flux, water droplets were a cheap and safe solution. They were injected using four water injectors and they were checked not to collide with each other close to the injector tip. For the inner pipe, smoke particles were more adapted because they did not collide with glass beads. They were added to the central jet using a smoke machine. Both the smoke and water droplets proved to be good tracers. Their diameter was respectively 2 $\mu$m and 5 $\mu$m, corresponding to particle relaxation times at least 100 times lower than the characteristic time scale of the fluid most energetic eddies. In addition, it was verified that both tracers did not have any effect on the particulate phase measurements, comparing the dispersed phase flow measurements with and without fluid tracers. Finally, all parts of the set-up were grounded and the air flow was humid enough to avoid static electricity influence.
For the dispersed phase, the glass beads did not show any breaking, so that the curvature and the geometric radius remained the same. Their refraction index was \( n = 1.51 \) and because they were hollow, they were well suited for PDA measurements.

Hereafter, the experimental results are plotted using symbols for comparison with numerical results. The cylindrical coordinate system \((z, r, \theta)\) is used to indicate axial (downward), radial and azimuthal directions. As no mean swirling motion was detected, only the axial and radial velocity components are provided. The mean components resulting from LES-averaging are respectively noted \( W \) and \( V \) whereas the RMS components are \( w_{rms} \) and \( v_{rms} \). The symbols \( \cdot_f \) and \( \cdot_p \) denote the fluid and the particles. Section 6.2 deals with the simulations of the single-phase flow whereas results of two-phase flow simulations are analysed in Section 6.3.

### 6.2 Single-phase flow simulations

#### 6.2.1 Computational domain

The total volume of the configuration is large, due to the length of both the ducts (2 m) and the chamber itself (1.5 m). In comparison, the combustion chamber of the Mercato test-rig schematised in Fig. 6.1 is 28 cm long and 13 cm wide. As a consequence, calculating the whole geometry would be computationally expensive.

Since the location of the second stagnation point is known to mainly depend on the geometry global diameter, the diameters of the inner and annular pipes have been kept: \( R_j = 10 \text{ mm} \); \( R_1 = 75 \text{ mm} \); \( R_2 = 150 \text{ mm} \), but the length of the pipes has been shortened to 0.2 m or 0.1 m depending on the mesh considered (see Section 6.2.3), and the length of the chamber itself has been decreased from 1.5 m to 0.8 m. There are two main arguments for this: first, considering the low Reynolds number and the grid resolution in the inner pipe as well as the accuracy of the numerical scheme, it is impossible to wait for natural destabilisation of the gas flow. A specific inlet boundary condition is therefore used to help the flow destabilisation (see Section 6.2.2). Besides, the accurate prediction of particle motion in a pipe (or a channel) is still difficult to obtain, especially because of particle-wall interactions (Wang & Squires, 1996). The modified pipe length stays compatible with the particle relaxation and transit times presented in Section 6.1.2 has been accounted for. The second reason why shortening the length of the chamber is the location of the furthest stagnation point in the vicinity of \( z = 400 \text{ mm} \), that is to say far from the chamber outlet.

Finally, the volume of the computational domain has been divided by two, which drastically decreases the computational cost of LES.
6.2 Single-phase flow simulations

6.2.2 Boundary conditions

Figure 6.7 shows the computational domain and the boundary conditions. The characteristic boundary conditions developed by Poinsot & Lele (1992a) are used for these simulations.

![Computational domain. Configuration of Borée et al. (2001).](image)

The experimental profiles of mean and fluctuating fluid velocities are unknown at the inlet of the pipes, but they are available at the inlet of the test section: \( z = 3 \, \text{mm} \). Consequently, typical mean axial velocity profiles of fully-developed pipes are imposed at the inlet of the inner and annular pipes, corresponding to the experimental mass flux. This method leads to a good agreement between experimental and numerical mean velocity profiles at \( z = 3 \, \text{mm} \).

As already said, due to the low Reynolds numbers in the ducts, no destabilisation of the gas flow can be obtained without flow forcing. At the inlet of both pipes, the fluid velocity varies in time and space to reproduce the effect of an incoming turbulent field as observed in the experiment. The method in constructing the incoming turbulent signal is based on the Random Flow Generation (RFG) algorithm introduced in Section 5.2.2. Forcing the flow in such a way considerably accelerates the establishment of fully developed turbulent flows. It also ensures the presence of coherent perturbations not warranted with a pure white noise. Typical fluctuating profiles of fully-developed pipes are imposed at the inlet of the pipes and again, agreement between experimental and numerical fluctuating profiles are good at \( z = 3 \, \text{mm} \). The influence of this forcing is presented in Section 6.2.8.

The outlet is nearly non-reflective at atmospheric pressure, \( P_f = 1.013 \times 10^5 \, \text{Pa} \).

Wall numerical treatment depends on the grid resolution near the wall. When it is low, only wall modeling is accurate and the law-of-the-wall developed by Schmitt et al. (2007) is employed. Increase in resolution in the near-wall region allows the direct use of non-slipping walls. In all cases, the walls are isothermal at ambient temperature, \( T_f = 293 \, \text{K} \).
6.2.3 Characteristics of the grids

The impact of the grid type is investigated in Section 6.2.7. Table 6.4 details the characteristics of the three meshes tested, with names $bb_{\text{meshst1}}$, $bb_{\text{meshst2}}$ and $bb_{\text{meshst}}$. Figures 6.8 and 6.9 display respectively longitudinal and front views of the three grid resolutions.

<table>
<thead>
<tr>
<th>Name</th>
<th>$bb_{\text{meshst1}}$</th>
<th>$bb_{\text{meshst2}}$</th>
<th>$bb_{\text{meshst}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid type</td>
<td>Tetrahedra</td>
<td>Tetrahedra</td>
<td>Hexahedra</td>
</tr>
<tr>
<td>Number of nodes (−)</td>
<td>367313</td>
<td>549369</td>
<td>3255085</td>
</tr>
<tr>
<td>Number of cells (−)</td>
<td>2058883</td>
<td>3115898</td>
<td>3207960</td>
</tr>
<tr>
<td>Smallest cell volume (10^{−10} m^{−3})</td>
<td>1.72</td>
<td>2.0</td>
<td>4.94</td>
</tr>
<tr>
<td>Length of the pipes (m)</td>
<td>0.2</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Length of the chamber (m)</td>
<td>1.5</td>
<td>1.5</td>
<td>0.8</td>
</tr>
<tr>
<td>$y^+$ in the inner pipe (−)</td>
<td>15</td>
<td>15</td>
<td>7.5</td>
</tr>
<tr>
<td>$y^+$ in the coflow (−)</td>
<td>64</td>
<td>64</td>
<td>15</td>
</tr>
<tr>
<td>Time step (µs)</td>
<td>3.2</td>
<td>3.49</td>
<td>4.22</td>
</tr>
</tbody>
</table>

Table 6.4 - Characteristics of the three meshes tested. Configuration of Borée et al. (2001).

In the unstructured grids, special care has been taken to generate small cells in the recirculation zone and in the near-wall region. The non-dimensional wall distance $y^+$, varies from 15 in the inner jet from 64 in the annular jet. The main difference between the two unstructured grids is the resolution in the region $250 < z < 750$ mm, which considerably increases the number of nodes and cells. Besides, the length of the ducts have been shortened for $bb_{\text{meshst2}}$, thanks to the use of the inlet forcing method mentionned in Section 6.2.2. Still, the resolution in the pipes is almost the same for both unstructured grids.

The main motivation for testing a structured grid on this configuration is the comparison with CDP that uses hexahedral cells. To make exact comparisons with both codes, the length of the test section was decreased down to 0.8 m. Although the number of cells is equivalent for $bb_{\text{meshst2}}$ and $bb_{\text{meshst}}$, it is important to remind that the total volume of both grids is really different. Furthermore, the differences in $y^+$ must be mentionned: the non-dimensional wall distance in the structured grid is twice smaller in the inner pipe and four times smaller in the coflow than in the two unstructured grids. Focusing on the resolution in the pipes, there are much more cells in the inner one as well as in the wall-region of the coflow. As expected, the smallest cell volume is all the same larger in the structured case, which increases the timestep.
6.2 Single-phase flow simulations

Figure 6.8 - Longitudinal cutting plane ($x = 0$) of the three meshes tested: $bb_{meshst1}$ (a.), $bb_{meshst2}$ (b.), and $bb_{meshst}$ (c.). Configuration of Borée et al. (2001).
Figure 6.9 - Global front view (left) and detail of the inner inlet (right) for the three meshes tested: $bb_{meshnt1}$ (a. & b.), $bb_{meshnt2}$ (c. & d.), and $bb_{meshst}$ (e. & f). Configuration of Borée et al. (2001).
6.2 Single-phase flow simulations

6.2.4 Test Cases

A series of test cases have been run, to investigate the following parameters:

- **the numerical scheme** (see Section 3.2): the TTGC scheme, 3rd order accurate in space and time, is known to provide better results than the LW scheme, especially in recirculating flows.

- **the grid**: structured grids are rarely used to calculate swirled flows since they are said to generate preferential directions (Section 6.2.3). Their influence on recirculating but not swirling flows is tested here, as well as the grid resolution.

- **the subgrid-scale model**: the WALE model detailed in Section 4.2.1 is more suited to bounded flows than the Smagorinsky model. The resulting change in fluid turbulent viscosity profile in the near-wall region is analysed to show the influence on the global statistics.

- **the wall treatment**: it is linked to the subgrid-scale model. A law-of-the-wall model (Schmitt et al., 2007) is used with the Smagorinsky subgrid model whereas the WALE model does not require any wall modeling.

- **the inlet boundary condition**: the RFG method detailed in Section 5.2.2 helps the flow destabilise in the pipes and ensures turbulent velocity profiles along the ducts.

Table 6.5 summarises the different cases performed for the gas flow.

<table>
<thead>
<tr>
<th>Name</th>
<th>Mesh</th>
<th>Scheme</th>
<th>Turb. model</th>
<th>Wall model</th>
<th>Inlet BC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nst1_w_smago_lwm_norf</td>
<td>bb_meshnst1</td>
<td>LW</td>
<td>Smagorinsky</td>
<td>Law-of-the-Wall</td>
<td>No RFG</td>
</tr>
<tr>
<td>Nst1_ttgc_smago_lwm_norf</td>
<td>bb_meshnst1</td>
<td>TTGC</td>
<td>Smagorinsky</td>
<td>Law-of-the-Wall</td>
<td>No RFG</td>
</tr>
<tr>
<td>Nst1_ttgc_wale_wnm_norf</td>
<td>bb_meshnst1</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>No RFG</td>
</tr>
<tr>
<td>Nst1_ttgc_wale_wnm_rfgint</td>
<td>bb_meshnst1</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>RFG Int.</td>
</tr>
<tr>
<td>Nst2_ttgc_wale_wnm_rfgint</td>
<td>bb_meshnst2</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>RFG Int.</td>
</tr>
<tr>
<td>Nst2_ttgc_wale_wnm_rfgall</td>
<td>bb_meshnst2</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>RFG All</td>
</tr>
<tr>
<td>S1_ttgc_wale_wnm_rfgall</td>
<td>bb_meshst</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>RFG All</td>
</tr>
</tbody>
</table>

Table 6.5 - Test cases and corresponding parameters. Configuration of Borée et al. (2001).

Results related to the various cases are presented hereafter. The gas LES solver of AVBP_TPF
is validated in Section 6.2.6 by direct comparison with CDP using the same structured grid, and experimental data. Then, in Section 6.2.7, the influence of the convective scheme and the grid are highlighted. These two elements are shown to be the most important parameters. Note that they are also the most CPU-time consumers. Finally, Section 6.2.8 focuses on the influence of the subgrid model coupled with the wall treatment, and the inlet boundary condition. Although these parameters make the calculations closer to the experimental flow, their effects on the flow statistics are less significant than the grid and the convective scheme.

As discussed in Section 4.3.2, the analysis of the averaged quantities resulting from LES requires a simulation time long enough to ensure convergence, and a sampling time small enough to ensure that the smallest structures can contribute to the averaged solution. In the present configuration, the lowest frequency to be represented is associated to the two counter-rotating structures on each side of the axis. Considering their size, \( l_{f,t} \approx 0.08 \text{ m} \), and their mean rotating velocity, \( U_{f,t} \approx 1 \text{ m.s}^{-1} \), the order of magnitude of the associated time is \( \tau_{f,t} \approx 0.08 \text{ s} \). The most energetic eddies in the inner pipe constitute a reasonable choice to determine the highest frequencies. Considering their size, \( l_{f,t} \approx 7 \text{ mm} \), and their velocity, \( u'_{f,t} \approx 1.5 \text{ m.s}^{-1} \), the order of magnitude of the associated time-scale is \( \tau_{f,t} \approx 4.6 \text{ ms} \). All the cases presented in Table 6.5 have been run for \( T_{av} \approx 0.5 \text{ s} \) and the time between two samples is \( \Delta t \approx 1.2 \text{ ms} \). The statistics of the mean fields are then well converged. This is not always the case for the RMS quantities but the overall tendency gives sufficient information to compare the models.

### 6.2.5 Gas flow analysis

Figure 6.10 shows an instantaneous field of the gas velocity modulus in the cutting plane \( y = 0 \) for the case \( St_{ttgc\_wale\_wnm\_rfqgall} \). A large amount of structures of different sizes are visible. The largest ones are linked to the diameter of the coflow, intermediate ones appear in the shear layers and structures coming out of the inner jet are also clearly identified.

![Figure 6.10 - Topology of the gas flow. Instantaneous field of gas velocity modulus obtained with AVBP_TPF in the cutting plane y = 0. St_{ttgc\_wale\_wnm\_rfqgall} case. Configuration of Boré et al. (2001).](image)

176
6.2 Single-phase flow simulations

The time-averaged field considerably differs from the instantaneous flow structure. Figures 6.11 a. – c. respectively present the mean field of gas axial velocity, and the RMS fields of gas axial and radial velocities in the cutting plane \( y = 0 \). The iso-contour line of zero mean axial velocity \( W_f = 0 \), is added on the three pictures. All fields are rather symmetric, which indicates good convergence of the simulations. As expected, there are two points with zero velocity along the axis, corresponding to distinct inner jet and coflow stagnation points. The peak of axial fluctuations is at the inner jet stagnation point whereas the radial fluctuations are maximum in the vicinity of the furthest stagnation point. Both axial and radial fluctuations show secondary peaks, respectively in the external shear layer and close to the first stagnation point. At these locations, turbulence is highly anisotropic.
Figure 6.11 - Topology of the gas flow. Mean field of gas axial velocity (a.), RMS fields of gas axial velocity (b.), and gas radial velocity (c.) obtained with AVBP_TPF in the cutting plane $y = 0$. The black line corresponds to the iso-contour line $<W_f> = 0$. St_tige_wale_wnm_rfgall case. Configuration of Borée et al. (2001).
6.2 Single-phase flow simulations

6.2.6 Validation of the gas LES solver from AVBP_TPF

The accuracy of the LES solver from AVBP_TPF for the gas phase is evaluated by computing the single-phase flow and comparing it to the data provided by Borée et al. (2001) and to the results of CDP. In this section, the case Stテストwaleテストnrmテストrgテストall is analysed, not only because it provides the most accurate results but also because it is the best candidate for direct comparisons with CDP. Indeed, both codes use here the same structured grid. There are however some differences in the two codes, summarised in Table 6.6.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CDP</th>
<th>AVBP_TPF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step ((\mu s) / CFL) (-)</td>
<td>147 / 50</td>
<td>4.2 / 0.7</td>
</tr>
<tr>
<td>Averaging time ((s) / iterations) (-)</td>
<td>2.65 / 18000</td>
<td>0.52 / 120000</td>
</tr>
<tr>
<td>Convective scheme</td>
<td>2\textsuperscript{nd} order that conserves kinetic energy (Ham &amp; Iaccarino, 2004)</td>
<td>TTGC</td>
</tr>
<tr>
<td>LES model / Wall model</td>
<td>Dynamic Smagorinsky/None</td>
<td>WALE/None</td>
</tr>
<tr>
<td>Inner jet / Coflow Inlet BC</td>
<td>Forcing / No forcing</td>
<td>Forcing / Forcing</td>
</tr>
</tbody>
</table>

Table 6.6 - Comparison of the parameters and models used for the single-phase flow LES performed with CDP and AVBP_TPF on the structured grid bb_meshst. Configuration of Borée et al. (2001).

As already mentioned, CDP resolves implicitly the incompressible Navier-Stokes equations whereas AVBP_TPF resolves explicitly the compressible Navier-Stokes equations. The main consequence is that the time step is 35 times larger for CDP, leading to consequent differences in the computational cost of such a calculation. As a result, the total averaging time is smaller for AVBP_TPF, but the convergence has been ensured to be good enough. Another noticeable difference comes from the treatment of the inlet boundary condition in the coflow. No turbulence has been injected on the gas flow in the outer duct in the case of CDP whereas the RFG method described in Section 6.2.2 has been used for both injection ducts with AVBP_TPF.

Before analysing the statistics in terms of mean and RMS velocities, it is useful to evaluate the LES criterion defined in Section 4.3.3. This is done in Fig. 6.12. The location of the iso-contour line \(Q_{LES}^{f} = 0.8\) shows that the LES is rather well-resolved in the domain, especially close to the centerline and in the coflow shear layers. The quality is poorer in the coflow outer region and in the central jet. However, the increase in resolution in this region would decrease the time-step.
Figure 6.12 - Mean field of LES criterion given by Eq. (4.40) for the gas phase in the cutting plane $y = 0$. The black line stands for the iso-contour line $Q^L_E = 0.8$. **Configuration of Borée et al. (2001).**

Figure 6.13 displays mean and RMS gas axial velocities along the axis, and Figs 6.14 – 6.17 present the radial profiles for the two codes along with the experimental measurements. The global agreement between the two codes and experiments is very good and most of the flow physics is captured by the two LES solvers. The width and the length of the recirculation zone are well predicted (Fig. 6.14). Differences between both codes in predicting the location of the two stagnation points (Fig. 6.13 a.) are minor. This point is known to be the main difficulty when calculating bluff body flows and the sensitivity to the parameters is shown in the following sections. The two LES solvers capture the mean radial component correctly, except at the end of the recirculation zone. The mean radial velocity level remains small (less than $1 \text{ m.s}^{-1}$ in Fig. 6.15) compared to the mean axial velocity level. Focusing on the RMS velocities (Fig. 6.16 and 6.17), the agreement with measurements is also good. The location and the amplitude of the peaks are well predicted, except in the coflow where CDP underpredicts both the radial and axial RMS velocities. The origin of the discrepancy is the treatment of the coflow inlet boundary condition, with no turbulence injected with CDP in the outer duct. Section 6.2.8 underlies the influence of this inlet boundary condition.

The overall result is that both codes provide very similar results, also close to the measurements, even though they use different methods. This indicates that the accuracy of the gas LES solver of AVBP-TPF is sufficiently good to test the dispersed phase with reasonable confidence on this configuration. Nevertheless, it must be underlined that the results are greatly sensitive to the numerical parameters and the grid used. This is developed in Sections 6.2.7 and 6.2.8.

For the sake of clarity, only the most informative graphs are discussed hereafter, but all the radial and axial profiles are available, and provided in Appendix A.
6.2 Single-phase flow simulations


6.2.7 Influence of the numerical scheme and the grid

The numerical scheme is critical when performing LES as well as the grid quality. Whether results are more accurate with a low-order scheme used on a refined grid or with a high-order scheme coupled with a coarser grid is still an open question (Sengissen et al., 2005). While Colin & Rudgyard (2000) and Vreman (1995) for example aim at developing high-order schemes on coarse grids, other authors use little dissipative 2nd order schemes on more
Figure 6.15 - Code influence. Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: CDP – Solid line: AVBP TPF/St ttgc wale wnm rfgall.

Figure 6.16 - Code influence. Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: CDP – Solid line: AVBP TPF/St ttgc wale wnm rfgall.
refined grids (Jimenez & Moin, 1991; Mahesh et al., 2004). Naturally, the computational cost of the simulation is a key point for the final choice.

In the following, the results obtained with the LW and TTGC schemes are compared and differences in the flow topology as well as in the mean and RMS profiles are highlighted. For this first test, the coarsest unstructured grid \textit{bb\_meshnst1} is used. In a second step, only the TTGC scheme is kept to study the influence of both the grid resolution and the grid type on the prediction of the stagnation point location.

- **Influence of the convective scheme**

To evaluate the influence of the numerical schemes on the single-phase flow results, the cases \textit{Nst1\_lw\_smago\_lwm\_norfg} and \textit{Nst1\_ttgc\_smago\_lwm\_norfg} (see Table 6.5) are compared. Both computations carried out with the coarsest grid \textit{bb\_meshnst1}, use the subgrid Smagorinsky model associated with the law-of-the-wall model. Moreover, the RFG method is not used at the inlet of the ducts so that the only difference between the two cases is the numerical scheme.

The qualitative impact of the scheme order of accuracy on the small structures is clear on Fig. 6.18 where instantaneous iso-surfaces of Q-criterion introduced in Section 5.3.2 are displayed for both schemes. Both fields exhibit two kinds of coherent structures: some longitu-
dinal vortices come from the inner pipe whereas other are created in the external shear zone and are rather azimuthal. However, the structures created with the TTGC scheme are more detailed and more numerous.

The axial profiles of mean and RMS axial velocities plotted in Fig. 6.19 quantify this observation. When using LW, the zero mean axial velocity iso-contour line that delimits the recirculation zone is located too far downstream of the ducts. Besides, as shown in Fig. 6.20, the LW scheme under-estimates the axial fluctuating velocities at the outlet of the jets. This is also the case for the radial fluctuations.

This leads to the conclusion that two-phase flows must be computed with the TTGC scheme. Indeed, the particle distribution as well as the flame shape in bluff body flows is known to be mainly linked to the first stagnation point. It is however important to keep in mind that the computational cost of a simulation using TTGC is 2.5 bigger than using LW.
6.2 Single-phase flow simulations

Figure 6.19 - Convective scheme influence. Axial profiles of mean (a.), and RMS (b.), axial gas velocity. Symbols: experiment – Dashed line: Nst1\_lw\_smagolwm\_norfg – Solid line: Nst1\_ttgc\_smagolwm\_norfg.

Figure 6.20 - Convective scheme influence. Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1\_lw\_smagolwm\_norfg – Solid line: Nst1\_ttgc\_smagolwm\_norfg.
• **Influence of the Grid**

The simulations are all performed here with the TTGC scheme, the WALE subgrid model associated with no-wall modeling, and the RFG method. The influence of the grid is investigated in two steps.

First, the cases `Nst1_ttgc_wale_wnm_rfgint` and `Nst2_ttgc_wale_wnm_rfgint` (see Table 6.5) are compared to show the impact of the grid resolution. The unstructured grids `bb_meshnst1` and `bb_meshnst2` are respectively used (see Table 6.4).

Second, the cases `Nst2_ttgc_wale_wnm_rfgall` and `St_ttgc_wale_wnm_rfgall` are focused on to show the impact of the grid type. The unstructured grid `bb_meshnst2` and the structured one `bb_meshst` are respectively used.

![Figure 6.21 - Grid influence. Instantaneous iso-surfaces of Q-criterion for the cases Nst1_ttgc_wale_wnm_rfgint (a.), Nst2_ttgc_wale_wnm_rfgint (b.), and St_ttgc_wale_wnm_rfgall (c.). The iso-surfaces are colored by instantaneous velocity. Configuration of Borée et al. (2001).](image)
6.2 Single-phase flow simulations

The visualisation of the instantaneous iso-surfaces of the Q-criterion for the three cases \textit{Nst1\_ttgc\_wale\_wnm\_rfgint}, \textit{Nst2\_ttgc\_wale\_wnm\_rfgint} and \textit{St\_ttgc\_wale\_wnm\_rfgall} is shown in Fig. 6.21. Note that because the RFG method is not used in the coflow for the case \textit{Nst1\_ttgc\_wale\_wnm\_rfgint} only, no coherent structures are visible in the coflow in Fig. 6.21 a. Apart from this, the main difference in flow structure between the two unstructured grids is the location of the vortices, more extended in the case \textit{Nst2\_ttgc\_wale\_wnm\_rfgall}. This is obviously due to the mesh refinement operated in the second quarter of the chamber in \textit{meshnst2}. The finest unstructured grid and the structured grid can be directly compared in Figs. 6.21 b. and c. The major difference is the size of the most visible coherent structures that are much smaller on the structured grid. In other words, both grids resolve large vortices in the same way but the structured grid allows the resolution of smaller vortices.

![Figure 6.22 - Grid influence. Axial profiles of mean (a.), and RMS (b.), axial gas velocity. Symbols: experiment – Dashed line: \textit{Nst1\_ttgc\_wale\_wnm\_rfgint} – Solid line: \textit{Nst2\_ttgc\_wale\_wnm\_rfgint.}](image1)

![Figure 6.23 - Grid influence. Axial profiles of mean (a.), and RMS (b.), axial gas velocity. Symbols: experiment – Dashed line: \textit{Nst2\_ttgc\_wale\_wnm\_rfgall} – Solid line: \textit{St\_ttgc\_wale\_wnm\_rfgall.}](image2)
Figure 6.24 - Grid influence. Radial profiles of mean axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst2 tgc wale wnm fgall – Solid line: St tgc wale wnm fgall.

Figure 6.25 - Grid influence. Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst2 tgc wale wnm fgall – Solid line: St tgc wale wnm fgall.
These observable differences do not appear so clearly on the axial mean and RMS axial velocity profiles, plotted in Fig. 6.22. This also holds for the radial profiles presented in Appendix A. Figure 6.23 compares the same quantities for the finest unstructured grid and the structured one. The location of the peak of RMS axial velocity is well predicted with the two grids but its amplitude is closer to the measurements using the structured grid. The impact of the structured grid on the mean axial velocity is even clearer: the inner jet flow penetrates a little bit farther in the chamber, which improves the prediction of the location of the two stagnation points. When looking at the radial profiles of mean and RMS axial velocities in Figs. 6.24 and 6.25, the most significant change is at the station \(z = 80\, \text{mm}\). At this point, the mean and RMS axial velocities are respectively under and over-estimated with the unstructured grid.

Accounting for the cost efficiency slightly modifies the previous conclusions. Table 6.7 compares the computational cost of the three different meshes when simulating 0.1 s physical time with otherwise the same parameters. Using the coarsest unstructured grid `bb_meshnst1` is about five times cheaper than performing the simulations on the structured grid `bb_meshst`. This figure is to be related to the gain in quality of the predictions choosing the final configuration and grid.

<table>
<thead>
<tr>
<th>Name</th>
<th><code>bb_meshnst1</code></th>
<th><code>bb_meshnst2</code></th>
<th><code>bb_meshst</code></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total CPU time (s)</td>
<td>44604</td>
<td>68460</td>
<td>235823</td>
</tr>
<tr>
<td>Efficiency / iteration / node ((\mu s))</td>
<td>3.88</td>
<td>4.35</td>
<td>3.06</td>
</tr>
<tr>
<td>Efficiency / iteration / cell ((\mu s))</td>
<td>0.69</td>
<td>0.77</td>
<td>3.10</td>
</tr>
</tbody>
</table>

Table 6.7 - **Grid influence.** Code efficiency for single-phase flow calculations depending on the mesh. Statistics given for 0.1 s (physical time) computed with TTGC on 16 processors on a CRAY XD1 machine. Configuration of Borée et al. (2001).
6.2.8 Influence of wall treatment, LES model and inlet boundary conditions

In addition to the numerical scheme and the grid that mainly influence the results, predictions can be improved using appropriate subgrid models (depending on the resolution in the near-wall region) and more realistic boundary conditions. Hereafter, the WALE subgrid model associated with no-wall modeling is compared to the Smagorinsky subgrid model associated with the law-of-the-wall model (Schmitt et al., 2007). The use of turbulent forcing at the inlet of the ducts is also tested. Note that in contrary to the impact of the convective scheme or the on the cost efficiency, these minor modifications do not increase the CPU.

- Influence of the gaseous LES model and the wall treatment

In turbulent bounded flows, all turbulent fluctuations are damped near the walls, so that the fluid turbulent viscosity $\nu_{f,t}$ (see Chapter 2), should go to zero at the wall. This is not the case when using the subgrid Smagorinsky model that gives a non-zero value of $\nu_{f,t}$ where velocity gradients exist. This is the main reason why Ducros et al. (1998b) developed the WALE subgrid model that naturally predicts a zero value of fluid turbulent viscosity at the wall, whatever the geometry considered. As a consequence, the mean velocity profile is expected to be in better agreement with the measurements. In AVBP_TPF, both models are available and adequate wall treatments are then required depending on the resolution:

- When the resolution in the near-wall region is low, the use of the law-of-the-wall model (Schmitt et al., 2007) associated with the Smagorinsky subgrid model is recommended. In this case, the recommended distance to the wall is $y^+ \in [50 \leq 500]$. On the other hand, when the grid in refined at the walls ($y^+ < 8$), no specific wall treatment is required and the WALE model is then more suited. For the sake of simplicity, hereafter, the denomination of the Smagorinsky subgrid model associated with the law-of-the-wall treatment is shortened to the Smagorinsky model. Similarly the WALE model refers to the WALE subgrid model without wall modeling.

- The characteristics of the coarsest unstructured grid, $bb\text{meshnst1}$ (see Table 6.4) allow to test the influence of the two combinations. The corresponding cases are $Nst1_{ttgc_smago_lwm_norfg}$ and $Nst1_{ttgc_wale_wnm_norfg}$ detailed in Table 6.5. In these simulations, the TTGC scheme is used and no turbulent forcing is imposed at the inlet of the pipes.

Figure 6.26 displays the mean fields of non-dimensional fluid turbulent viscosity in the cutting plane $y = 0$ for the two cases. As expected, results differ most in the vicinity of the walls where the fluid turbulent viscosity goes to zero only with the WALE model. The behavior of the two
6.2 Single-phase flow simulations

Figure 6.26 - **LES and wall modeling influence.** *Mean field of non-dimension turbulent viscosity for Nst1_ttgc_smagor (a.), and Nst1_ttgc_wale (b.) in the cutting plane y = 0. The white and black lines respectively stand for ν_l/ν_t = 5 and ν_l/ν_t = 10. Configuration of Borée et al. (2001).*

models in the rest of the chamber is very similar. The impact on the velocity field is restricted to the near-wall region, as shown in Figs. 6.27 and 6.28. The mean axial velocity decreases to zero at the wall of the coflow and a slight increase in the RMS axial velocity is visible in the same zone when the WALE model is employed.

Figure 6.29 focuses on the radial profiles of turbulent viscosity and RMS axial velocities in the ducts themselves. The conclusion slightly differs. Both quantities are compared at four stations in the ducts: \( z = -200 \, mm \); \( z = -150 \, mm \); \( z = -100 \, mm \) and \( z = -50 \, mm \), where the first one corresponds to the inlet of the inner and coflow pipes. There, the axial velocity fluctuations naturally develop in the duct when using the WALE model, which is not the case with the Smagorinsky model. As a consequence, the turbulent viscosity field generated by the Smagorinsky model (see Fig. 6.29 a.) is lower than with the WALE model (see Fig. 6.29 b.), except at the wall where the behaviour is non-physical. As a result, the WALE subgrid model without specific treatment at the wall should be preferred to the Smagorinsky model associated with the law-of-the-wall in our case.
When only a typical mean axial velocity profile of fully-developed pipe is imposed at the inlet of both the inner and the coflow pipes, relaminarisation of the mean velocity profile is expected. This is mainly due to the insufficient grid resolution, the insufficient length of the ducts and the dissipation of the numerical scheme. The impact of the RFG method (see Section 6.2.2) on the mean and RMS velocity profiles is investigated hereafter.

- **Inner pipe turbulent forcing**

The influence of the inlet turbulent forcing method is investigated by comparing the cases Nst1_ttgc_wale_wnm_norfg and Nst1_ttgc_wale_wnm_rfgint described in Table 6.5. The axial profiles of mean and RMS axial velocities displayed in Fig. 6.30 show clearly the influence of the inlet boundary condition treatment. Focusing on the velocity fluctuations, they are shown to decrease in the central pipe due to a lack of resolution. Yet, the numerical value of $w_{f,rms}$ at the outlet of the duct is in good agreement with the experimental value. The consequence of this fluid agitation in the duct itself is a flat mean axial velocity profile in the pipe. Thus, the maximum of mean axial velocity is in better agreement with the experiments at the outlet of the duct ($z = 3 \text{ mm}$). Note that in Fig. 6.30 a., the accurate prediction of the location of the
6.2 Single-phase flow simulations

Figure 6.28 - **LES and wall modeling influence.** Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_ttgc_smago_lwm_norfg – Solid line: Nst1_ttgc_wale_vwm_norfg.

Figure 6.29 - **LES and wall modeling influence.** Radial profiles of mean non-dimension turbulent viscosity (a.), and RMS axial gas velocity (b.) at 4 stations in the pipes along z axis. Dashed line: Nst1_ttgc_smago_lwm_norfg – Solid line: Nst1_ttgc_wale_vwm_norfg.
recirculation zone for the case \( Nst1_{ttgc\_wale\_wnm\_norfg} \) is only due to exact compensation of errors that is completely fortuitous.

Figure 6.30 - **Inner pipe turbulent forcing influence.** Axial profiles of mean (a.), and RMS (b.), axial gas velocity. Symbols: experiment – Dashed line: \( Nst1_{ttgc\_wale\_wnm\_norfg} \) – Solid line: \( Nst1_{ttgc\_wale\_wnm\_rfgint} \).

**– Coflow turbulent forcing**

The influence of the outer inlet boundary condition is less crucial in terms of jet penetration and recirculation zone, and so, for the prediction of particle dispersion. Its impact was checked by comparing the cases \( Nst2_{ttgc\_wale\_wnm\_rfgint} \) and \( Nst2_{ttgc\_wale\_wnm\_rfgall} \). The finest unstructured grid is used, associated with TTGC, the WALE model and no wall modeling. Inlet forcing is used in the central duct for both cases. Injecting turbulence in the coflow still slightly modifies the mean axial velocity profile in the near wall region (see Fig. 6.31) and provides better agreement for the velocity fluctuations, as shown in Fig. 6.32.

**6.2.9 Conclusion for the single-phase flow simulations**

The results provided by the gas LES solver from AVBP_TPF show very good agreement with the measurements. The accuracy is as good as the results from CDP for radial and axial profiles of mean and fluctuating velocities. Nevertheless, the challenge has been difficult to take up and the investigation of many parameters has been necessary: the convective scheme and both the resolution and the type of grid used constitute the two key points of such simulations. Choosing the most accurate subgrid model, wall treatment and inlet boundary condition increases the level of accuracy of the predictions.
6.2 Single-phase flow simulations

Figure 6.31 - **Coflow turbulent forcing influence.** Radial profiles of mean axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst2_ttge_wale_wnm_rfgint – Solid line: Nst2_ttge_wale_wnm_rfgall.

Figure 6.32 - **Coflow turbulent forcing influence.** Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst2_ttge_wale_wnm_rfgint – Solid line: Nst2_ttge_wale_wnm_rfgall.
6.3 Two-phase flow simulations

Although the distribution of particles introduced experimentally in the inner pipe is multidisperse, a monodisperse distribution of particles is calculated and analysed hereafter. There are two main reasons. First, no work has been devoted to the multidisperse description of the dispersed phase using the EE mesoscopic approach during this PhD. Then, this topic has been studied separately by V. Moureau at CTR using the CDP Lagrangian solver to compare the results obtained with a multidisperse jet and a monodisperse distribution. In the monodisperse case, the particle diameter was equal to the mean diameter: $\bar{d}_p = 60 \mu m$. He showed that considering a monodisperse distribution is sufficient to capture both the mean flow effects on the gas (through two-way coupling) and the dynamics of the 60 microns particle class in this case.

The validation of the particle dynamics in this recirculating gas flow is done in two steps using three different codes: CDP and AVBP_TPF-EL that both calculate the particle motion with a Lagrangian approach, and AVBP_TPF-EE that uses the Eulerian mesoscopic approach. First, since the gas LES solvers from AVBP_TPF and CDP give very similar results, the two Lagrangian solvers can be compared and validated by comparisons with the measurements. Second, the two approaches (EL and EE mesoscopic) are compared using AVBP_TPF-EL and AVBP_TPF-EE. As the gas solver and the grid are exactly the same, a direct comparison of the two methods is proposed. Hereafter, for the sake of clearness, the comparison between the two Lagrangian codes is not presented. The main results are however reported in Riber et al. (2006).

In this section, focus is made on comparing the EL and EE mesoscopic approaches using the same gas LES solver of AVBP_TPF and two different solvers for the dispersed phase. According to the results obtained for the particle-laden confined jet in Chapter 5, the simplified EE mesoscopic model, that consists in neglecting the RUM contributions in the particulate transport equations, is preferred for this bluff body configuration. Hereafter, Section 6.3.1 summarises the grid, and the numerical parameters for the gas and the dispersed phase. Then, a qualitative analysis of the particle motion is proposed in Section 6.3.2. Finally, a quantitative comparison of both approaches is provided in Section 6.3.3.

### 6.3.1 Numerical parameters

- **The grid**

  In Section 6.2.7, the predictions of the gas phase have been shown to mainly depend on the grid resolution and type: the structured grid called *bb_meshst* provides the most accurate results mainly because it contains much more cells than the two unstructured grids tested. How-
ever, increasing the number of cells is computationally expensive. As shown in Table 6.7, using the unstructured grid \textit{bb\_meshst1} is about five times cheaper than using the structured grid \textit{bb\_meshst}. Considering the increase in CPU time due to the resolution of the dispersed phase, it has been decided to compare the EL and EE mesoscopic approaches on the unstructured grid \textit{bb\_meshst1}. Note that the quality of the results obtained for the gas phase (see Section 6.2.7) is sufficient to conclude about the accuracy of the method used for the dispersed phase.

- **The gas phase**

  In these two-phase flow simulations, the two codes AVBP\_TPF-EL and AVBP\_TPF-EE use strictly the same parameters for the gas, corresponding to the case \textit{Nst1\_ttgc\_wale\_wnm\_rfgint} detailed in Section 6.2.4. Hereafter, Table 6.8 reminds the parameters for the gas phase.

<table>
<thead>
<tr>
<th>Name</th>
<th>Mesh</th>
<th>Scheme</th>
<th>Turb. model</th>
<th>Wall model</th>
<th>Inlet BC</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textit{Nst1_ttgc_wale_wnm_rfgint}</td>
<td>\textit{bb_meshst1}</td>
<td>TTGC</td>
<td>WALE</td>
<td>None</td>
<td>RFG Int.</td>
</tr>
</tbody>
</table>

  Table 6.8 - Description of the gaseous parameters. Configuration of Borée et al. (2001).

- **The dispersed phase**

  In contrast, the conditions for the dispersed phase are not strictly identical for both approaches. The physical properties of the particles are set in agreement with the experiments: their density is \( \rho_p = 2470 \text{ kg.m}^{-3} \) and their diameter is chosen constant and equal to the mean one, \( d_p = \bar{d}_p = 60 \mu\text{m} \). The treatment of the inlet boundary condition is the main difference. In the Eulerian simulations, the particles are injected at the inlet of the inner pipe (corresponding to \( z = -200 \text{ mm} \)) and their mean velocity and mass flux is imposed in agreement with the measurements. In the Lagrangian simulations, the particles are injected on the centerline of the inner pipe, but at \( z = -1 \text{ mm} \), just before entering the chamber. The main reason for this choice is that modeling of the wall BC for the particles is not available in AVBP\_TPF-EL yet. Moreover, a fluctuating particle velocity corresponding to 10\% of the mean particle velocity is added.

  In terms of numerical parameters, the EE mesoscopic approach uses the same methodology as in the confined jet configuration, as shown in Table 6.9. The TTGC scheme is used with the particle AV model and the particle subgrid eddy-viscosity model is activated to account for the unresolved scales.
6.3.2 Two-phase flow topology

In this section, the motion of particles is qualitatively analysed by showing instantaneous and time-averaged LES fields of particle velocity. The role of the particle subgrid model is briefly presented. Then, the EL and EE mesoscopic approaches are compared showing instantaneous fields of respectively reconstructed particle number density and particle number density.

Figure 6.33 compares instantaneous fields of gas and particle velocity in the cutting plane $y = 0$. Three main comments can be made. First, the gaseous smallest structures are much smaller than the particulate smallest structures. Second, there is a strong correlation between the two velocity fields: the shape and the intensity of the recirculation zones are comparable. Finally, the main difference between the two phases is the penetration of the jet. Indeed, the particles are stopped in the jet further than the gaseous stagnation point. This is confirmed by Fig. 6.33 c. where an instantaneous field of particle number density is plotted. Small clusters of particles form between the chamber inlet and the particle stagnation point. There, lots of particles are stopped before they are ejected from the centerline by the gaseous recirculation zones where they are kept.

The time-averaged LES fields look very different from the instantaneous fields and are displayed in Fig. 6.34 for the dispersed phase only. Focus is made on the particle mean axial velocity, and RMS axial and radial velocities. All the fields are rather symmetrical, suggesting a good level of convergence. When comparing these particulate time-averaged LES fields with the gaseous ones presented in Fig. 6.11, the comments are not very different from the particle-laden confined jet configuration. The mean fields for the two phases are similar whereas the RMS fields show at least two differences. First, the particle RMS quantities are smaller than the gas ones. Second, the particle RMS axial velocity component is larger than the radial component, revealing again an anisotropy of the particle RMS field that is not observed for the gas phase.

In Fig. 6.35, the role of the particle subgrid eddy-viscosity model is shown, making the difference between the deviatoric and the spherical subgrid contributions of the subgrid viscosity. Again, the results are very similar to the confined jet configuration. The two fields show the same topology, suggesting that the subgrid eddy-viscosity model mainly acts in the regions where concentration of particles occurs. Moreover, the spherical part that is negligible for the

<table>
<thead>
<tr>
<th>Convective scheme</th>
<th>AV model</th>
<th>Subgrid model</th>
<th>RUE flux limitor</th>
</tr>
</thead>
<tbody>
<tr>
<td>TTGC</td>
<td>Jameson</td>
<td>eddy viscosity</td>
<td>No</td>
</tr>
</tbody>
</table>

Table 6.9 - Numerical method for the dispersed phase computed with the EE mesoscopic approach. Configuration of Borée et al. (2001).
6.3 Two-phase flow simulations

Figure 6.33 - Topology of the two-phase flow. Instantaneous fields of gas velocity modulus (a.), particle velocity modulus (b.), and particle volume fraction (c.) obtained with AVBP-TPF-EE in the cutting plane \( y = 0 \). The black line corresponds to the iso-contour line \( \langle W_p \rangle = 0 \). Configuration of Borée et al. (2001).

gas phase cannot be omitted for the dispersed phase as it is about three orders of magnitude larger than the deviatoric part.

Finally, as the purpose here is to evaluate the accuracy of the EL and EE mesoscopic approaches in this bluff body configuration, a comparison of instantaneous fields of particle number density for the two methods is provided in Fig. 6.36. Nevertheless, in the Lagrangian approach, real particles are tracked whereas a particle number density is transported in the Eulerian approach. To compare both methods, it is therefore necessary to reconstruct a particle number density
from the Lagrangian simulations using a volumic projection method. Then, the two fields seem very similar although more particles are visible in the recirculation zone close to the walls with the Lagrangian approach. This first comparison between the two approaches is consequently very promising for the EE mesoscopic approach that is often said to be too diffusive for the particle number density.
6.3 Two-phase flow simulations

Figure 6.35 - Instantaneous fields of particle deviatoric (a.) and spherical (b.) subgrid viscosity defined in Eq. (4.22) and obtained with \( AVBP_{TPF-EE} \) in the cutting plane \( y = 0 \). Configuration of Borée et al. (2001).

Figure 6.36 - Instantaneous fields of reconstructed particle number density obtained with \( AVBP_{TPF-EL} \) (a.) and particle number density obtained with \( AVBP_{TPF-EE} \) (b.) in the cutting plane \( y = 0 \). Configuration of Borée et al. (2001).

6.3.3 Comparison of the EL and EE mesoscopic approaches

In this section, radial profiles of mean and RMS velocities for both phases are displayed and direct comparisons between the \( AVBP_{TPF-EL} \) and the \( AVBP_{TPF-EE} \) results (respectively dotted-dashed and solid lines) are proposed. The symbols stand for the experiments.
The results for the gas phase are presented in Figs. 6.37 – 6.40. There are at least three main points to comment. First, the two approaches give very similar results for all the quantities considered. Second, these results are in good agreements with the measurements, although there are some discrepancies when considering the mean axial velocity on the centerline of the chamber and the RMS velocities in the coflow. The same observations were made in Section 6.2, due to the gaseous parameters that are not optimum in this simulation: the resolution for grid $bb_{meshnt1}$ has been shown to be unsufficient and the RFG method must be used in the coflow to improve the results in this region. Therefore, these discrepancies should not be due to the particle solver. Finally, the influence of the two-way coupling can be evaluated comparing Figs. 6.37 – 6.40 with Figs. A.4 – A.7 displayed in Appendix A. For this low mass loading case, the impact of the two-way coupling seems very little, both when comparing the experiments and the simulations. Consequently, extending the EE mesoscopic approach to two-way coupling without theoretically proving its validity (see Section 1.5) is not crucial in our case. The same conclusion may not be straightforward when calculating the high mass loading case.

![Figure 6.37 - Radial profiles of mean axial gas velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.](image-url)
6.3 Two-phase flow simulations

Figure 6.38 - Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.

Figure 6.39 - Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.
Figure 6.40 - Radial profiles of RMS radial gas velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.
The results for the dispersed phase are displayed in Figs. 6.41 – 6.44. The overall agreement of both methods with the experiments is good. When comparing the mean axial and radial velocities, the EL and EE mesoscopic approaches give almost the same results. The particle jet spreading is well predicted while the location of the stagnation point is slightly under-estimated. This may be due to the discrepancies observed on the gas mean axial velocity in Fig. 6.37. The conclusion is slightly different when focusing on the RMS quantities. On the one hand, the two methods have some difficulties predicting the particle agitation at the locations $z = 80$ $m$ and $z = 160$ $mm$, that is to say upstream from the stagnation point. This may be linked to the discrepancies observed at the same locations for the gas phase (see Fig. 6.39 for instance). Note that the over-predictions of RMS velocities in the coflow with the EL approach are due to the averaging process that would require more particles in this region. On the other hand, the EE mesoscopic approach under-predicts the particle agitation. This is not surprising since the RUM contributions are neglected here as it was the case in the confined jet configuration.

Figure 6.41 - Radial profiles of mean axial particle velocity at 7 stations along $z$ axis. Symbols: experiment – Dotted-dashed line: AVBP\_TPF-EL – Solid line: AVBP\_TPF-EE.
Figure 6.42 - Radial profiles of mean radial particle velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.

Figure 6.43 - Radial profiles of RMS axial particle velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.
Figure 6.44 - Radial profiles of RMS radial particle velocity at 7 stations along z axis. Symbols: experiment – Dotted-dashed line: AVBP_TPF-EL – Solid line: AVBP_TPF-EE.
6.4 Conclusion

There are two main reasons why the particle-laden bluff body configuration has been calculated using LES:

- The context of this work is the simulations of reactive turbulent two-phase flows in aeronautical combustion chambers. After the promising results obtained in the particle-laden confined jet (see Chapter 5), it was necessary to test the new LES EE mesoscopic model in a more realistic geometry showing recirculation zones for instance.

- The validations of the method must be precise and numerous. This is the case for the bluff body configuration: detailed measurements are provided in Borée et al. (2001) and direct comparisons between the EL and EE mesoscopic approaches have been made during the CTR Summer program.

In this configuration where particles are inertial, but still much dependent on the gas flow, the predictions of the particle motion strongly depend on the results for the gas phase. Nevertheless, accurate predictions of the gas phase have been delicate to obtain. Therefore a detailed study has been required to investigate the influence of numerous parameters on the gas flow. The grid and the convective scheme are the major parameters to account for. Concerning the grid, numerous points are required in the whole domain, and especially in the inner pipe and close to the walls. In our case, a structured grid has given the most accurate results. As for the numerical scheme, TTGC is once again the best candidate for the grid resolution affordable today. Then, some other parameters show minor influence on the predictions: the Random Flow Generation method used at the inlet of the pipes prevents relaminarisation of the gas flow in the pipes themselves. Combining no wall treatment with the WALE subgrid model also improves the results. Thus, this detailed study has shown the capability of the gas LES solver from AVBP_TPF to very precisely predict the fluid flow in such a configuration. The results the code provide are in very good agreement with the experiments, and with the results provided by the gas LES solver from CDP.

The accuracy of the Eulerian mesoscopic approach has then been shown by comparison with the experiments and the Lagrangian approach. Because the two approaches can be used in AVBP_TPF, the comparison is direct as both the grid and the gas solver are identical. The results for the dispersed phase are in good agreement with the measurements for both approaches. Concerning the mean quantities, the predictions are very close for both methods. Only the agitation of the particles is slightly under-estimated with the EE mesoscopic approach, suggesting again than the RUM contribution cannot be neglected.

There is still lots of points to be investigated in this bluff body configuration. First, accounting for the RUM modeling is undoubtedly required to better predict the particle agitation, provided the RUM viscosity model is improved (see Section 5.6). Then, the impact of the two-way
coupling on the gas phase should be analysed in details. As it seems more important for the larger mass loading \((\text{Borée et al., 2001})\), this second case should also be investigated, which requires to model the inter-particle collisions and to account for polydispersion.
Conclusion

Une nouvelle méthode de Simulation aux Grandes Echelles pour les écoulements diphasiques à phase dispersée, turbulents et non-réactifs est proposée. Elle repose sur le formalisme Eulérien mésoscopique introduit par Février et al. (2005) qui suggère une décomposition de la vitesse de chaque particule en une vitesse spatialement corrélée, et une vitesse décortélée. La dérivation des équations LES pour la phase dispersée requiert donc, outre la moyenne d’ensemble conditionnée par une réalisation fluide, l’application d’un filtre spatial LES classique. Il en résulte deux types de termes non fermés à modéliser, qui proviennent de la moyenne d’ensemble d’une part, et du filtrage spatial LES d’autre part. La mise en oeuvre numérique de ce système d’équations ainsi que son application à des géométries complexes nécessitent le développement, l’implantation et la validation de divers modèles :

- **Méthodes numériques** : la résolution numérique des équations particulaires en mode DNS, i.e. avant filtrage LES, s’avère complexe pour deux raisons principales. D’une part, leur dérivation ne fait pas apparaître naturellement de terme diffusif comme c’est le cas pour la phase gazeuse. D’autre part, la phase dispersée est fortement compressible, et ce d’autant plus que l’inertie des particules augmente. Il en résulte l’apparition de très forts gradients de densité par exemple, difficiles à représenter et à convecter sur une grille de calcul. La solution proposée par Kaufmann et al. (2006) consiste à introduire un terme de sous-maille dans l’équation de vitesse corrélée et ainsi, à résoudre les équations particulaires pour des grandeurs filtrées (densité, vitesses corrélée et décortélée). Si la stabilité de la méthode numérique s’en trouve accrue, il apparaît cependant une forte diffusion de la densité de particules. Dans cette étude, l’erreur de dispersion importante du schéma numérique jusqu’alors utilisé (LW) est mise en cause et il est montré que l’utilisation d’un schéma de type Taylor-Galerkin (TTGC) (Colin, 2000), non seulement moins dispersif mais également moins dissipatif, améliore significativement les résultats pour la phase dispersée. Par ailleurs, un modèle de dissipation artificielle basé sur celui de Jameson et al. (1981) et adapté à la phase dispersée complète le dispositif pour réaliser des calculs stables et précis. Enfin, un limiteur de flux pour les flux Euler de l’équation de transport de l’énergie décortélée des particules est utilisé pour garantir la positivité de cette quantité soumise à de fortes variations de cellule à cellule.
CONCLUSION

- **Modèles de sous-maille particulaires** : ils ont été proposés parallèlement à cette étude par Moreau (2006) qui a utilisé l’approche lagrangienne pour effectuer des DNS de THI chargée en particules. Un double filtrage, au sens moyenne d’ensemble puis LES, a permis de tester *a priori* plusieurs modèles pour les termes non fermés. Ceux issus de la moyenne d’ensemble ont été modélisés par analogie avec les fermetures de type RANS (Simonin, 1991) tandis que ceux résultant du filtrage spatial ont été modélisés par analogie avec les modèles de sous-maille développés pour les écoulements monophasiques compressibles. Dans ce travail, les modèles présentant le meilleur compromis entre d’une part la qualité des résultats *a priori* et d’autre part la facilité d’implantation numérique ont été retenus et intégrés au code AVBP_TPF.

- **Condition limite d’entrée particulaire** : les écoulements diphasiques considérés dans cette étude sont suffisamment dilués pour négliger les collisions inter-particulaires. Par ailleurs, la modélisation des interactions particules-parois n’est pas cruciale pour les configurations retenues. Dans celles-ci pourtant, les particules sont injectées dans la chambre avec de l’air par le biais de tubes. A défaut de calculer l’écoulement gaz-particules dans ces conduits, il est important de tenir compte du mouvement des particules dans les tubes pour écrire une condition aux limites adéquate en entrée de chambre. Les expériences nous indiquent que les fluctuations particulaires sont partiellement corrélées à celles du fluide. Les différences entre les deux phases proviennent principalement de l’inertie des particules, des collisions, même faibles, entre particules, et des interactions particules-parois. Ainsi, la condition aux limites développée dans cette thèse propose d’imposer, en plus de la vitesse partielle moyenne, une fluctuation de vitesse partielle qui se décompose par analogie avec la décomposition de Février et al. (2005), en une fluctuation spatialement corrélée et une fluctuation décorrélée. Seule la première contribution est alors partiellement corrélée à la fluctuation gazeuse. Le développement de cette condition aux limites s’est fait par étapes et la version la plus élaborée a été implémentée dans le code AVBP_TPF.

L’apport de ces différents modèles pour la compréhension et la simulation des écoulements gaz-particules s’est révélé essentiel pour la calcul des trois configurations retenues dans le cadre cette thèse.


La LES avec une approche Eulérienne du jet d’air turbulent vertical chargé en particules (Hishida et al., 1987) constitue à la connaissance de l’auteur la première tentative de ce genre dans la communauté diphasique. Ce calcul analysé dans le chapitre 5 permet d’affirmer la nécessité d’inclure les fermetures de sous-maille proposées par Moreau (2006). De même la condition aux limites d’entrée portant sur la fluctuation de vitesse particulaire décrite ci-dessus apparaît primordiale pour la juste prédiction de la dispersion des particules dans un tel champ gazeux turbulent. Cette configuration donne l’occasion d’effectuer deux types de calcul. Le premier calcul néglige les effets du mouvement décорré en ne résolvant que les équations de transport pour la densité et la vitesse corrélée des particules. Des comparaisons avec les résultats expérimentaux montrent que ce modèle simplifié permet de prédire correctement les flux moyens de masse et de quantité de mouvement des particules. En revanche, l’agitation des particules, qui ne tient compte dans ce calcul que de leur mouvement corrélé, est sous-estimée. Une évaluation a posteriori de la contribution du mouvement décorté est proposée en utilisant la corrélation de Vance et al. (2006). En sommant la contribution du mouvement corrélé issue de la LES et la contribution du mouvement décorté estimée a posteriori, le niveau d’agitation particulaire s’accorde avec les mesures expérimentales. Le second calcul tient compte de la dissipation du mouvement décorté dans l’équation de quantité de mouvement corrélé particulaire et propose de résoudre en outre l’équation pour l’énergie décortée des particules. Cependant ce modèle ne s’avère pas satisfaisant car il conduit à une relaminarisation de l’écoulement particulaire. Une série de tests a permis de remettre en cause le modèle de viscosité utilisé pour la fermeture des corrélations doubles : sa valeur semble trop élevée mais sa forme pourrait également, à terme, être discutée. Une nouvelle thèse portant sur la modélisation Eulérienne mésoscopique vient de débuter au sein du groupe EEC de l’IMFT et devrait apporter des réponses à ces questions.

Compte-tenu de ces résultats, le modèle LES Eulérien mésoscopique sans prise en compte directe du mouvement décorté, a finalement été mis en œuvre dans une géométrie réaliste
CONCLUSION

de chambre de combustion aéronautique. Le calcul d’un jet turbulent recirculant chargé en particules (Borée et al., 2001) fait l’objet du Chapitre 6 et permet de développer deux principaux points. D’une part, les résultats LES de l’écoulement monophasique s’avèrent fortement dépendants du maillage, du schéma convectif, ainsi que des conditions aux limites d’entrée et de paroi. L’influence de l’ensemble des paramètres est décrite et le calcul garantissant les prédictions les plus précises comparativement aux mesures expérimentales est comparé avec un calcul mené par V. Moureau avec le code CDP développé par l’université de Stanford. La précision du solveur gazeux d’AVBP_TPF, pour les grandeurs moyennes et fluctuantes, est ainsi démontrée. D’autre part, le développement d’un module lagrangien dans le code AVBP_TPF dans le cadre de la thèse de M. García a permis de comparer directement les descriptions Lagrangienne et Eulérienne mésoscopique dans cette configuration. Il ressort que les deux modèles s’accordent précisément sur la prédiction des grandeurs moyennes avec les mesures expérimentales tandis qu’une fois encore, l’agitation des particules est sous-estimée par le modèle Eulérien mésoscopique pour les mêmes raisons que dans le calcul du jet confiné.

Enfin, il convient de rappeler que cette étude a en grande partie été motivée par la nécessité de développer une description Eulérienne pour les écoulements diphasiques réactifs dans les chambres de combustion aéronautiques. Le modèle Eulérien mésoscopique sans prise en compte directe du mouvement décorrélé des particules a été couplé à des modèles d’évaporation de gouttelettes et de combustion dans le cadre de thèses menées parallèlement par M. Boileau et plus récemment par N. Lamarque, J. Lavédrine et M. Sanjose au CERFACS. Les calculs effectués ont permis de calculer des séquences d’allumage dans des chambres de combustion réalistes en tenant compte de la dispersion et de l’évaporation des gouttelettes de fuel. Dans cette optique, de nombreux points restent à étudier : la prise en compte du couplage inverse dans le modèle Eulérien mésoscopique (thèse de E. Massi Boscolo au sein du groupe EEC de l’IMFT), la polydispersion en sortie d’injecteur (thèse de J. Lavédrine au CERFACS), les collisions inter-particulaires (travaux de recherche de P. Fede à l’IMFT), l’influence des gouttes liquides dans la flamme (thèse de M. Sanjose au CERFACS) et la modélisation des films liquides aux parois (thèse de G. Desoutter à l’IFP) en sont quelques exemples.


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222


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Appendix
Appendix A

Bluffbody: additional graphs

For the sake of clearness, not all the graphs have been included in the discussion of Chapter 6. Hereafter, the missing ones are provided to complete the analysis.
Figure A.1 - **Convective scheme influence.** Radial profiles of mean axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1
lw
smagolwm
norfg – Solid line: Nst1
ltgc
smagolwm
norfg.

Figure A.2 - **Convective scheme influence.** Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1
lw
smagolwm
norfg – Solid line: Nst1
ltgc
smagolwm
norfg.
Figure A.3 - **Convective scheme influence.** Radial profiles of RMS radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1 ttgc_smgmo_lwm_norfg – Solid line: Nst1 ttgc_smgmo_lwm_norfg.

Figure A.4 - **Grid influence.** Radial profiles of mean axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1 ttgc_wale_lwm_rfgint – Solid line: Nst2 ttgc_wale_lwm_rfgint.
Figure A.5 - **Grid influence.** Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1 ttgc wale wnm rfgint – Solid line: Nst2 ttgc wale wnm rfgint.

Figure A.6 - **Grid influence.** Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1 ttgc wale wnm rfgint – Solid line: Nst2 ttgc wale wnm rfgint.
Figure A.7 - **Grid influence.** Radial profiles of RMS radial gas velocity at 7 stations along z axis. Symbols: experiment — Dashed line: Nst1 ttgc wale wnm rf gint – Solid line: Nst2 ttgc wale wnm rf gint.

Figure A.8 - **Grid influence.** Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst2 ttgc wale wnm rf gall – Solid line: St ttgc wale wnm rf gall.
Figure A.9 - **Grid influence.** Radial profiles of RMS radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst2 ttgc wale wnm rfga – Solid line: St ttgc wale wnm rfga.

Figure A.10 - **LES and wall modeling influence.** Radial profiles of mean non-dimension turbulent viscosity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1 ttgc smago lwm norfg – Solid line: Nst1 ttgc wale wnm norfg.
Figure A.11 - LES and wall modeling influence. Axial profiles of mean (a.), and RMS (b.), axial gas velocity. Symbols: experiment – Dashed line: \( Nst1_{ttgc, smago, lwm, norfg} \) – Solid line: \( Nst1_{ttgc, wale, wnm, norfg} \).
Figure A.12 - **LES and wall modeling influence.** Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_ttgc_smago_lwm_norfg – Solid line: Nst1_ttgc_wale_wnm_norfg.

Figure A.13 - **LES and wall modeling influence.** Radial profiles of RMS radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_ttgc_smago_lwm_norfg – Solid line: Nst1_ttgc_wale_wnm_norfg.
Figure A.14 - **Inner tube turbulent forcing influence.** Radial profiles of mean axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_ttge_wale_wnm_norf – Solid line: Nst1_ttge_wale_wnm_rfgint.

Figure A.15 - **Inner tube turbulent forcing influence.** Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_ttge_wale_wnm_norf – Solid line: Nst1_ttge_wale_wnm_rfgint.
Figure A.16 - **Inner tube turbulent forcing influence.** Radial profiles of RMS axial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_tge_wale_wnm_norfg – Solid line: Nst1_tge_wale_wnm_rf bigint.

Figure A.17 - **Inner tube turbulent forcing influence.** Radial profiles of RMS radial gas velocity at 7 stations along z axis. Symbols: experiment – Dashed line: Nst1_tge_wale_wnm_norfg – Solid line: Nst1_tge_wale_wnm_rf bigint.
Figure A.18 - **Coflow turbulent forcing influence.** Axial profiles of mean (a.), and RMS (b.), axial gas velocity. Symbols: experiment – Dashed line: Nst2_Itgc_wale_wnm_rfgint – Solid line: Nst2_Itgc_wale_wnm_rfgall.

Figure A.19 - **Coflow turbulent forcing influence.** Radial profiles of mean radial gas velocity at 7 stations along z axis. Symbols: experiment — Dashed line: Nst2_Itgc_wale_wnm_rfgint – Solid line: Nst2_Itgc_wale_wnm_rfgall.