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Intensification of Gas Fluidized and Spouted Beds

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**Development of a Robust Eulerian-Lagrangian Model for Process
Intensification of Gas Fluidized and Spouted Beds**

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Thèse présentée en vue de l'obtention du diplôme de *Philosophiæ Doctor*
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**Development of a Robust Eulerian-Lagrangian Model for Process
Intensification of Gas Fluidized and Spouted Beds**

présentée par **Toni EL GEITANI NEHME**

en vue de l'obtention du diplôme de *Philosophiæ Doctor*
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DEDICATION

To my dear father, without whom I wouldn't be here today.

To my loving mother, words cannot do her justice; she is the epicenter of love and the joy of life, a model of devotion and giving.

To my brother and sister, my support and companions in the joys and sorrows of life.

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to pursue my academic goals and make significant contributions to my field.

RÉSUMÉ

L'existence des écoulements multiphasiques, en particulier les écoulements solide-fluides, dans plusieurs applications industrielles, a conduit les chercheurs à investir beaucoup de temps pour comprendre les phénomènes sous-jacents qui régissent le comportement physique de ces écoulements. En génie chimique, les processus les plus connus impliquant de tels écoulements sont les lits fluidisés et les lits à jets, qui restent prévalents dans l'industrie en raison de leurs propriétés améliorées de transfert de masse et de chaleur. Cependant, ces lits sont complexes à concevoir et à exploiter.

Plusieurs études ont été menées pour permettre une conception améliorée et efficace de ces lits, dont beaucoup sont des expériences utilisant des techniques invasives ou non invasives. Néanmoins, les expériences présentent plusieurs limitations, telles que leur coût élevé et le temps nécessaire, ce qui les rend moins efficaces. C'est là que les méthodes numériques jouent un rôle en surmontant les limites des expériences, même si les expériences restent importantes pour la validation des modèles computationnels. Parmi ces méthodes, le modèle à deux fluides (TFM), qui est une approche eulérienne-eulérienne, est capable de modéliser les écoulements multiphasiques, mais sa précision est limitée puisqu'il traite les particules comme un continuum. Une autre approche, l'approche eulérienne-lagrangienne, implique l'application de la dynamique des fluides numérique (CFD) couplée à la méthode des éléments discrets (DEM). Cette méthode est de plus en plus utilisée comme elle simule les écoulements solide-fluide avec une meilleure précision. Néanmoins, elle présente plusieurs limitations, en particulier en termes de temps de calcul, ce qui rend la CFD-DEM inefficace pour la simulation de systèmes industriels de très grande taille.

Dans cette thèse, un modèle CFD-DEM à éléments finis d'ordre élevé est développé pour modéliser la fluidisation de particules solides dans des lits fluidisés et des lits à jets. Le modèle permet de prédire tous les régimes, depuis les écoulements laminaires à faibles nombres de Reynolds jusqu'aux écoulements turbulents à nombres de Reynolds élevés. Il permet une meilleure compréhension du comportement de fluidisation des particules et aborde plusieurs des limitations de la CFD-DEM, notamment les schémas de projection des particules sur la grille de la CFD et la limite du ratio entre la taille des particules et la taille des cellules.

Une nouvelle formulation à éléments finis pour les équations de Navier-Stokes volumiquement moyennées est introduite et stabilisée en utilisant la méthode de Galerkin avec stabilisation de la pression (PSPG) pour éviter les pressions parasites lors de l'utilisation d'interpolation polynomiale de même ordre, et la méthode de Galerkin avec stabilisation amont des lignes de

courant (SUPG) pour prévenir les oscillations dans les solutions des écoulements hautement convectifs à nombres de Reynolds élevés. Une stabilisation grad-div est introduite pour améliorer la conservation de la masse et capturer les chocs dans la solution. Une méthodologie utilisant la méthode de solution manufacturée est conçue pour vérifier la formulation stabilisée proposée en démontrant que le modèle préserve l'ordre de convergence de la discrétisation sous-jacente par éléments finis. Le schéma est ensuite validé par le biais d'une simulation de lit fixe.

Un nouveau solveur CFD-DEM non résolu, entièrement parallélisé et appliquant l'équilibrage dynamique des charges sur une architecture unifiée, est développé. Il intègre les solveurs CFD et DEM dans un logiciel unique, ce qui permet un couplage plus rapide et moins coûteux entre eux, et mène à des simulations plus efficaces, car l'équilibrage des charges assure une répartition uniforme du travail entre les processeurs; ce qui permet d'exploiter efficacement les ressources disponibles. La mise en œuvre du schéma de projection des particules, le calcul des interactions particule-fluide, l'interpolation des variables fluides aux positions des particules et le couplage entre les solveurs dans le modèle non résolu sont vérifiés et validés à l'aide de plusieurs cas de plus en plus complexes.

Lorsque les particules se trouvent partiellement dans une cellule, leur contribution volumique n'est pas évaluée avec précision, ce qui entraîne une prédiction inexacte de la fraction de vide et, par conséquent, des simulations inexactes. Cela affecte également la stabilité de la simulation et introduit des contraintes sur la taille des éléments ainsi que sur le pas de temps pour le couplage entre la CFD et la DEM. Habituellement, la fraction de vide locale est calculée à l'aide de méthodes approximatives simplifiées telles que la méthode centrée sur les particules (PCM). Des méthodes analytiques permettant de déterminer avec précision la fraction de vide existent; cependant, elles sont souvent irréalisables en raison de leurs coûts de calcul élevés et de leur inapplicabilité aux maillages non structurés. Une méthode centrée sur la quadrature (QCM) est proposée dans le but de mieux prédire le comportement des écoulements multiphasiques et de résoudre les limitations mentionnées. La capacité de cette méthode dans la CFD-DEM non résolue est démontrée avec divers cas.

En outre, le développement d'une nouvelle référence expérimentale permet la validation du modèle CFD-DEM non résolu ainsi qu'une étude détaillée de l'effet des propriétés de la surface DEM sur la fidélité des simulations. Grâce à des expériences de four rotatif solide-fluide à une échelle de laboratoire, différentes variables affectant les résultats de la simulation CFD-DEM sont étudiées et de meilleures prédictions sont obtenues en déterminant les facteurs importants affectant les résultats. Les résultats CFD-DEM dépendent fortement de la précision de la calibration des propriétés de surface DEM, de l'ordre du schéma de discrétisation

CFD et des interactions particule-fluide considérées.

Enfin, les limites du travail actuel, les travaux futurs possibles et les extensions sont brièvement discutés à la fin de cette thèse.

ABSTRACT

The existence of multiphase flows specifically solid-fluid flows in countless industrial applications such as fluid catalytic cracking units has led scientists and researchers to invest a lot of time trying to understand the underlying phenomena governing the physical behavior of such flows. In chemical engineering, the most known processes involving such flows are fluidized and spouted beds which remain prevalent in industries due to their improved mass and heat transfer properties. However, these beds are complex to design and operate.

Various studies have been performed to allow for improved and efficient design of such beds, many of which are experiments using either invasive or non-invasive techniques. Nonetheless, experiments suffer from several limitations, such as being expensive and time consuming which render them less effective. This is where numerical methods play a role in overcoming the limitations of experiments, even though experiments remain important for the validation of the computational models. Among these methods, the two fluid model (TFM) which is a Eulerian-Eulerian approach is capable of modelling multiphase flows, but its accuracy is limited as it treats the particles as a continuum. Another approach, most commonly known as the Eulerian-Lagrangian approach involves the application of computational fluid dynamics (CFD) coupled with the discrete element method (DEM). This method is increasingly being used as it simulates solid-fluid flows with better accuracy. Nevertheless, it suffers from several limitations, specifically computational time, which renders CFD-DEM inefficient for the simulation of very large industrial systems.

In this thesis, a high-order finite element CFD-DEM model is developed to model the fluidization of solid particles in gas fluidized and spouted beds. The model entails the prediction of all regimes from laminar flows at low Reynolds numbers to turbulent flows at high Reynolds numbers. It allows for a better understanding of the fluidization behavior of particles and tackles several of the limitations of CFD-DEM, notably the projection schemes of particles onto the CFD mesh and the particle to cell size ratio limit.

A new finite element formulation for the volume-averaged Navier-Stokes equations is introduced and stabilized using pressure-stabilizing Petrov-Galerkin (PSPG) for preventing spurious pressure when using equal order finite elements and streamline-upwind Petrov-Galerkin (SUPG) to prevent oscillations in solutions for highly convective flows at high Reynolds numbers. Grad-div stabilization is introduced to improve mass conservation and to capture shocks in the solution. A methodology using the method of manufactured solution is designed to verify the proposed stabilized formulation by demonstrating that the model preserves the

order of convergence of the underlying finite element discretization. The scheme is then validated through a packed bed simulation.

A novel unresolved CFD-DEM solver that is fully parallelized and supports dynamic load balancing on a unified architecture is developed. It integrates the CFD and DEM solvers into a single software resulting in faster and cheaper coupling between them allowing for more efficient simulations as load balancing ensures the even distribution of workloads among processors; thus, exploiting available resources efficiently. The implementation of the particle projection scheme, the calculation of particle-fluid interactions, the interpolation of fluid variables at the particles' locations, and the coupling between solvers in the unresolved model are verified and validated using several cases with increasing complexities.

When particles are partially located in a cell, their volume contribution is not evaluated accurately, leading to inaccurate prediction of the void fraction and, consequently, inaccurate simulations. This also affects the stability of the simulation and introduces constraints on the elements' size as well as the time step for the coupling between CFD and DEM. Usually, the local void fraction is calculated using simplified approximate methods such as the particle centered method (PCM). Analytical methods which accurately determine the void fraction exist; however, they are often unfeasible due to their increased computational costs and being inapplicable to unstructured meshes. A quadrature centered method (QCM) is proposed in an attempt to better predict the behavior of multiphase flows and to resolve the mentioned limitations. The capacity of this method in unresolved CFD-DEM is demonstrated with various test cases.

Furthermore, the validation of the unresolved CFD-DEM model along with a detailed study about the effect of DEM surface properties on the fidelity of the simulations is achieved through the development of a new experimental benchmark. Through lab scale solid-fluid rotary kiln experiments, different variables affecting the CFD-DEM simulation results are studied and better predictions are obtained by determining the important factors affecting the results. The CFD-DEM results are shown to depend strongly on the accuracy of the calibration of DEM surface properties, the order of the CFD discretization scheme, and the considered particle-fluid interactions.

Finally, the limitations of the current work, possible future works, and extensions are discussed briefly at the end of this thesis.

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LIST OF SYMBOLS AND ACRONYMS

ABS	Acrylonitrile Butadiene Styrene
BDF	Backward Differentiation Formulation
CFD	Computational Fluid Dynamics
CG	Coarse graining
CGM	Continuous Galerkin Methods
CPU	Central processing Unit
DEM	Discrete Element Method
DGM	Discontinuous Galerkin Methods
DIA	Digital Image Analysis
DNS	Direct Numerical Simulation
DPM	Discrete Particle Method
DPVM	Divided Particle Volume Method
DSMC	Direct Simulation Monte Carlo
FCCU	Fluid Catalytic Cracking Unit
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method
GLS	Galerkin Least Square
ILU	Incomplete Lower Upper
IRT	Infrared Thermography
LBB	Ladyzhenskaya–Babuska–Brezzi
LBM	Lattice Boltzmann Method
LDR	Light Dependent Resistor
LDV	Laser Doppler Velocimetry
LES	Large Eddy Simulation
LIF	Laser Induced Fluorescence
LSFB	Liquid Solid Fluidized Bed
MD	Molecular Dynamics
MFV	Minimum Fluidization Velocity
MMS	Method of Manufactured Solution
MPI	Message Passing Interface
NSERC	National Science and Engineering Research Council of Canada
NTC	Negative Temperature Coefficient

ODE	Ordinary Differential Equation
PAM	Point Approximate Approach
PCM	Particle Centroid Method
PIV	Particle Image Velocimetry
PSPG	Pressure-Stabilizing/Petrov-Galerkin
QCM	Quadrature Centered Method
RANS	Reynolds-Averaged Navier-Stokes
RMSE	Root Mean Squared Error
SGS	Sub-Grid Scale
SPM	Satellite Point Method
SUPG	Streamline-Upwind/Petrov-Galerkin
TFM	Two Fluid Model
VANS	Volume Averaged Navier-Stokes

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CHAPTER 1 INTRODUCTION

Multiphase flows exist naturally, from the wind gusts that carries dust particles with it to the river that pushes small pebbles along its way. These naturally occurring phenomena seems simple and modest in nature. However, examining the underlying physics that governs such flows is complex and non-trivial. Multiphase flows are defined as systems with two or more distinct phases flowing simultaneously within a mixture. When talking about multiphase flows, it is important to differentiate between them depending on the combination of phases [1]. Two phase flows can be divided into solid-gas, solid-liquid, liquid-gas, and liquid-liquid flows.

Solid-gas flows are defined by the motion of solid particles dispersed or suspended within the moving continuous gaseous phase. They are characterized according to their number density which is defined as the number of particles per unit volume. They are either dilute (low number density) or dense flows (high number density). In the dilute regime, the gas flow dominates the motion of particles which exhibit negligible effect on the gas phase. On the other hand, dense solid-gas flows are not only influenced by the motion of the gas. The motion of the particles is controlled by the particle-particle and particle-wall collisions where surface characteristics and material properties of both the particles and the wall play a role [1]. Solid-liquid flows transport solid particles that are dispersed in a liquid medium. As the density ratio between phases is lower than in solid-gas flows and the drag force between phases is significantly higher, solid-liquid flows are largely driven by pressure gradients [1]. Liquid-gas flows can be divided into three main configurations. The dispersed flow in which one phase is dispersed in the other, the separated flow in which the two phases are separated in layers of a single phase, and the transitional or mixed flow denoted by the transition from dispersed to separated flow and is characterized by the presence of both regimes. As bubbles (gas) or droplets (water) can deform freely within the continuous phase, they can take different geometrical shapes [1]. Liquid-liquid flows are defined as the motion of two immiscible liquids where both phases are treated as continuous media. Additionally, multiphase flows include three phases solid-liquid-gas flows where both the solid and the gaseous phases are taken to be the dispersed phases and the liquid phase is considered the continuous phase. These flows are more complicated compared to two phase flows due to the various phenomena altering the flow physics such as particle-particle, bubble-bubble, bubble-particle, fluid-particle, and fluid-bubble interactions [1]. This work lays particular emphasis on solid-gas multiphase flows.

Various technological applications deal with solid-gas multiphase flows. Among these applications, there exist particle-exhaust control systems, combustion systems such as furnaces and diesel engines where mixtures of solid particles or aerosols in air are present, drying systems, particle from effluent separation systems [2], conveying systems and systems with chemical reactions [3]. Additionally, the existence of solid-gas flows is more prevalent in certain industries such as power generation, oil and gas, and pharmaceuticals [3].

Solid-gas contactors such as fluidized beds and spouted beds are common in the industry. They are characterized by the different regions that arise during the fluidization process as shown in Figure 1.1. Fluidized beds are divided mainly into two regions, bubble phase which is mainly gas and emulsion phase which is mainly particles [4]. Spouted beds are divided into three well differentiated sections that are the spout which is the central core through which the gas flows, the fountain appearing above the bed surface which includes particles that are entrained by the spout and that travels down the annular region of the bed, and the annulus which is formed between the spout and the wall of the bed and includes the surrounding annular region [4].

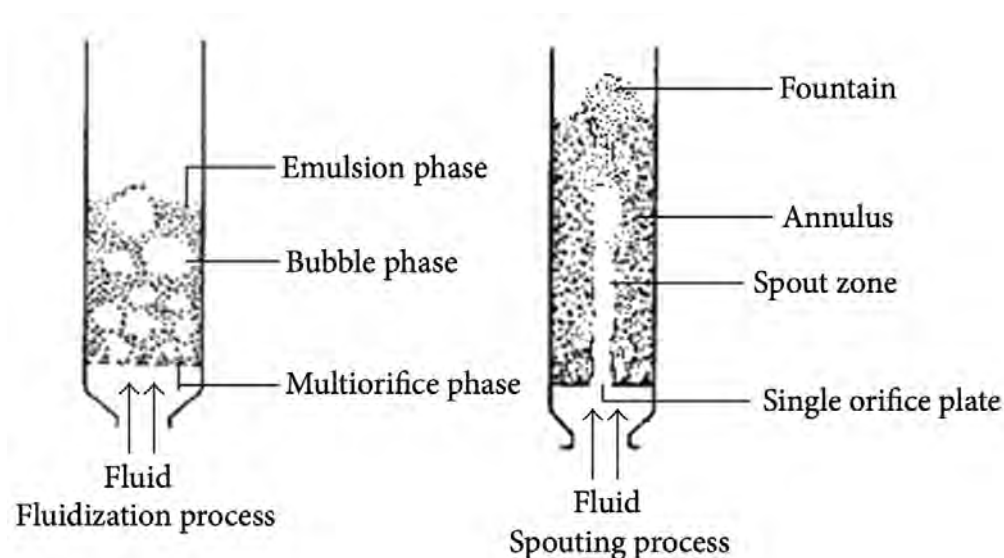


Figure 1.1 The different regions of fluidized and spouted beds [4].

Gas fluidized beds work through the application of a gas flow at the bottom of the bed through a multi-orifice distributor plate allowing the fine granular material inside the bed to fluidize. This can be achieved when the gas inlet velocity is greater than the minimum fluidization velocity (MFV) which is the minimum velocity required for the fluid to exert sufficient drag on the particles and allow them to overcome gravity [5]. Fluidized beds offer various distinct advantages which makes them desirable for a wide range of processes. First, they are characterized by high mass and heat transfer rates resulting in a uniform temperature

distribution [5,6]. Second, due to their maintained mass and temperature profiles, fluidized beds greatly improve the yield and efficiency for the various chemical and physical processes which include mass or heat transfer limited reactions. Also, fluidized beds allow to process components with a wide particle size distribution [6]. Moreover, such beds are advantageous in continuous processes as they offer the ability to add or remove particles from the bed without requiring shutdown of the process [6]. This explains why gas fluidized beds are widely used in chemical, petrochemical, metallurgical, environmental, energy industries and so on [5] in a large variety of applications such as fluidized catalytic cracking units (FCCUs), polyolefin production, the acrylonitrile process, etc [6]. On the other hand, fluidized beds suffer from certain limitations. They are complex in their design, building, operation and scale-up when compared to other types of beds such as packed beds or stirred tank reactors. Additionally, the vigorous motion of the particles make such beds more susceptible to erosion and particle attrition. Furthermore, the presence of droplets in solid-gas beds or bubbles in solid-liquid beds should be managed as they can reduce mass transfer between the different phases [6]. Nonetheless, gas fluidized beds remain widely used in industries as their benefits often outweigh their disadvantages by far.

Gas-spouted beds are different from gas fluidized beds in the way they operate. They are defined as solid-gas contactors where the gas enters through a single orifice located at the center of the base of the bed. This results in a cyclic motion of the fluidized particles [4]. During stable spouting, the solid particles are entrained by the high-velocity gas flow in the spout. This results in a stable spout and fountain formation in the bed which is characterized by homogeneous particle circulation and mass and heat transfers. However, the flow dynamics are altered during unstable spouting resulting in swirling, pulsating, and periodic movement of the fountain [7]. There are various applications of spouted beds discussed in the literature. Spouted beds are used in the food industry for drying fruits, vegetables, and grains where the vigorous movement of the particles within the bed allows the products to be dried without being damaged [8]. Increasingly, they are being used in thermo-chemical reaction applications such as the pyrolysis of biomass [9]. Spouted beds are a promising technology with several already working pilot plants. Still, its implementation in industry is limited and lacking [8].

The choice of spouted beds over fluidized beds depend mainly on the characteristics of the particles being used according to the Geldart classification as presented in Figure 1.2. In 1973, Geldart classified particles into four groups based on their behavior in gas fluidized beds: group A - aeratable, group B - bubbly, group C - cohesive, and group D - spoutable [10]. Some particles, such as Geldart D particles cannot be handled using fluidized beds and therefore they must be handled using spouted beds [11]. In general spouted beds showed better performance than fluidized beds for the handling of sticky solids. When particle

agglomeration occurs, de-fluidization of fluidized beds is observed, whereas it was avoided in spouted beds [12]. Finally, some particles cannot be fluidized such as those in group C, and therefore other types of solid-gas contactors such as rotary kilns should be employed for such particles.

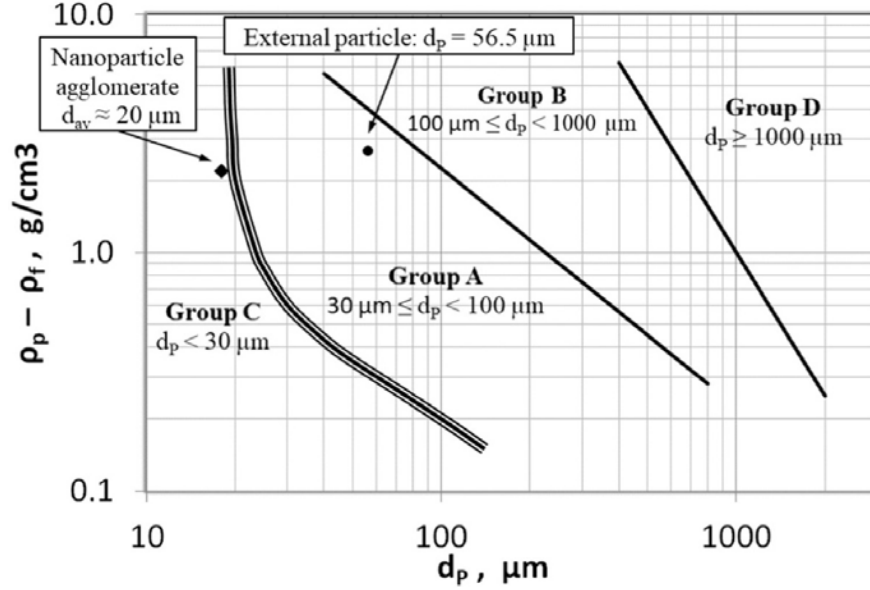


Figure 1.2 Geldart classification of particles based on the density difference between phases and the mean particle size [13].

As such, the Geldart classification becomes important in identifying the class of particles to be studied. This is necessary because if the particles to be modelled are of group C or group A particles, inter-particle forces such as electrostatic and van der Waals interactions could no longer be neglected and should be considered in the numerical model being developed. The particles of interest for the current work are group B and group D particles and therefore, inter-particle forces can be neglected while focusing mainly on hydrodynamic and collision forces.

Naturally, the physics involved in multiphase flows is multi-scale and as such the physical phenomena which occur within such flows are governed by a range of scales. From a chemical reaction engineering point of view, and by considering a chemical reactor as the system of interest, it can be determined that three scales exist as shown in Figure 1.3.

The single particle stands for the micro-scale on which particle-fluid interactions have been thoroughly investigated and led to the development of well established laws such as drag coefficient for momentum transfer. The reactor represent the macro-scale over which the temperature, pressure, and flow rates can be measured and controlled to achieve optimal conversion, energy efficiency, and pollutant emissions. In between these two scales, exists

the meso-scale where various heterogeneous structures such as bubbles and particle clusters affect the behavior of the flow. Within the meso-scale, individual particles behave differently than a single isolated particle and as such simple averaging of the behavior of a single particle does not allow the prediction or understanding of the meso-scale structures of the flow [14]. To this end, it is critical to find ways that allow the in-depth understanding of the meso-scale structures of multiphase flows.

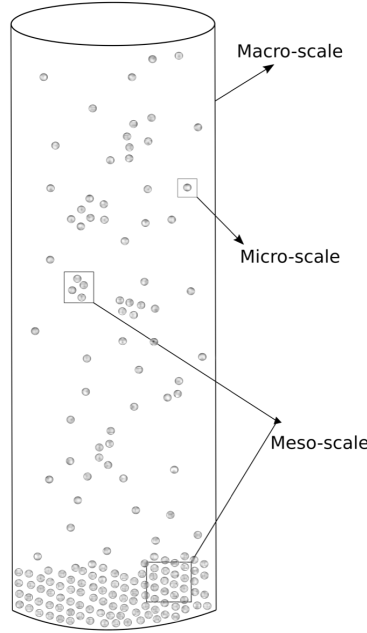


Figure 1.3 Different scales in a heterogeneous catalytic reactor.

As fluidized and spouted beds are prevalent in industries because of their various advantages, their intensification is a must to enhance processes and improve their efficiency. As such, accurately predicting the behavior of such beds is vital for their design, scale-up, optimization, and troubleshooting [3]. Due to the different scales that exist in such beds, accurately modelling their behavior is important to understand the underlying meso-scale phenomena which are difficult to study using experiments.

This project aims to develop a robust and reliable computational fluid dynamics-discrete element method (CFD-DEM) solver capable of accurately modelling multiphase flows specifically, solid-gas flows. The main objective of this thesis is the development of a numerical model capable of predicting the behavior of particles and flow regimes including turbulent structures in gas fluidized and spouted bed as a mean to understand and predict the dynamics of such beds. Therefore, going towards a computer assisted design of these unit operations. To achieve this, certain limitations of CFD-DEM would have to be tackled.

CHAPTER 2 LITERATURE REVIEW

The organization of the literature review is written in a manner that chronologically introduces the theories behind multiphase modelling. Therefore, an exhaustive list of topics including mathematical formulations as well as theoretical concepts is introduced.

Section 2.1 introduces the kinetic theory of gases. It gives a simplified explanation of the theory and discuss the discrete (microscopic) and continuum (macroscopic) behavior of a gas in the limits of the Knudsen number (Kn). The behavior of the solid phase is also described as well as the inter-phase coupling in solid-gas multiphase flows. Section 2.2 describes the governing equations of fluid dynamics which result in the Navier-Stokes equations. It introduces the concept of turbulence including the several approaches that can be implemented to calculate turbulent structures.

Section 2.3 discusses the various numerical methods that can be implemented to numerically solve the Navier-Stokes equations with a main focus on the finite element method (FEM) which will be used throughout this thesis. High-order schemes in the context of the finite element method are also introduced as well as the numerical method through which turbulence is modelled in this thesis.

In Section 2.4, the discrete element method (DEM) is introduced along with its two models, the hard-sphere model and the soft-sphere model. The focus is on the soft-sphere model which is the model of choice in this thesis as it allows multiple collisions and overlap of particles which is the case in dense systems unlike the hard-sphere model where collisions are instantaneous as in dilute systems. Section 2.5 introduces the two main approaches to model large scale multiphase flow problems, that are the two fluid model (TFM) and computational fluid dynamics-discrete element method (CFD-DEM). Finally, Section 2.6 discusses the main work that has been achieved so far in the simulation and modelling of fluidized and spouted beds.

2.1 Behavior of the Flow

The behavior of a multiphase flow depends on the behavior of individual phases as well as the inter-phase exchange between phases. This is because the concentration of one phase with respect to the other plays an important role in characterizing the multiphase behavior of the mixture. In order to accurately investigate processes involving multiphase flows, it is critical to account for the various mass, momentum, and energy exchanges that take place

between the phases. However, for the purpose of this thesis, mass and energy transfers are neglected as no chemical reactions occurs and since the dispersed phase is always solid. As such, the focus is on the hydrodynamics of multiphase flows.

2.1.1 Gas Phase

A gas flow can be described as a discrete phase or as a continuous phase depending on the Knudsen number (Kn) characterizing it. The kinetic theory of gases which is represented by the Boltzmann equation is often used for the continuous representation of particles where these particles are considered as rigid spherical gas molecules which can collide with each other and can relax to a Maxwellian equilibrium.

The Knudsen Number

The Knudsen number is a dimensionless number defined as the ratio of the molecular mean free path length (λ) to a physical length scale (L) often taken as a characteristic length of the geometry. It is defined as [5]:

$$\text{Kn} = \frac{\lambda}{L} \quad (2.1)$$

When $\text{Kn} < 0.01$, the gas is considered as a continuum and is described using the Navier-Stokes equations along with no-slip boundary conditions. The gas properties such as temperature, density and velocity can be described as continuous functions in space and time. When $0.01 < \text{Kn} < 0.1$, the Navier-Stokes equations still hold but no-slip boundary conditions do not always hold as there might exist partial slip between the gas and the boundary. No-slip boundary conditions assume the gas to have the same velocity as the boundary at the boundary, whereas slip or partial slip boundary conditions assume velocity difference between the gas and the boundary at the boundary. At these scales, numerical methods such as computational fluid dynamics (CFD) can be used to model the flow. For $\text{Kn} > 0.1$, the continuum assumption breaks down and the Navier-Stokes equations can no longer be used. The kinetic theory of molecular gases should be applied to describe the gas. At this scale, Molecular Dynamics (MD) and Direct Simulation Monte Carlo (DSMC) simulations are used to track the motion of gas molecules [5].

The Kinetic Theory of Molecular Gases

The kinetic theory is the foundation of fluid dynamics. Mainly, it is used to describe the macroscopic properties of a gas (pressure, temperature, thermal conductivity, viscos-

ity, etc.) from microscopic quantities (mass, velocity, kinetic energy, etc.) associated with the molecules which constitute the gas [15]. Maxwell laid the foundation of the modern kinetic theory of gases in 1867 when he proposed a general transport equation for arbitrary macroscopic quantities derived from the mean values of microscopic quantities. He assumed that the interaction potential between particles was derived from a repulsive force which was inversely proportional to the fifth power of the relative distance between the molecules. This type of potential is currently known as the Maxwellian potential [15].

Of central importance in the kinetic theory is the single particle distribution function $f(\mathbf{x}, \mathbf{v}, t)$ which can be defined as the number density of particles (or molecules) in the 6 dimensional phase space (μ -phase) spanned by the coordinates ($\mathbf{x}$) and velocities ($\mathbf{v}$) of the particles (or molecules) [5, 15]. It is given as:

$$f(\mathbf{x}, \mathbf{v}, t)d\mathbf{x}d\mathbf{v} = f(\mathbf{x}, \mathbf{v}, t)dx_1dx_2dx_3dv_1dv_2dv_3 \quad (2.2)$$

In 1872, Boltzmann proposed a non-linear integro-differential equation to represent the velocity distribution function in the μ -phase when there are collisions between molecules. It gives the temporal change of the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ in terms of a transport term related to the motion of particles and a collision term related to the encounters between particles. It is currently known as the Boltzmann equation and is given by:

$$\frac{\partial f}{\partial t} + \underbrace{v_i \frac{\partial f}{\partial x_i} + \frac{\partial f F_i}{\partial v_i}}_{\text{transport}} = \underbrace{C}_{\text{collision}} \quad (2.3)$$

where F_i is a specific external force acting on the particles and is independent from the particles' velocities. C is the collision operator and is difficult to calculate as it depends on the product of two distribution functions. It is determined using kinetic models such as the Bhatnagar–Gross–Krook (BGK) model which is one of the oldest models and gives the collision operator as:

$$C = \nu(f^{(0)}(\mathbf{x}, \mathbf{v}, t) - f(\mathbf{x}, \mathbf{v}, t)) \quad (2.4)$$

where ν represents a frequency which is of the order of the collision frequency and $f^{(0)}(\mathbf{x}, \mathbf{v}, t)$ is the Maxwellian distribution function and is given by:

$$f^{(0)}(\mathbf{x}, \mathbf{v}, t) = n \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} e^{-\frac{m}{2k_B T} \mathbf{V}^2} \quad (2.5)$$

where n is the number of particles or molecules, m is the mass of a molecule, k_B is the

Boltzmann constant, T is the temperature, $\mathbf{V}$ is the peculiar velocity defined as the velocity of the molecules ($\mathbf{v}$) relative to the hydrodynamic velocity of the gas ($\mathbf{u}$). Based on the definition of the distribution function, the macroscopic states of a gas such as mass density ρ , momentum density $\rho\mathbf{u}$, and total energy density $\rho\mathbf{E}$ can be obtained from the mass m , linear momentum $m\mathbf{v}$, and energy $m\mathbf{v}^2/2$ [15]:

$$\rho(\mathbf{x}, t) = \int m f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} \text{ - mass density,} \quad (2.6)$$

$$\rho\mathbf{u}(\mathbf{x}, t) = \int m\mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} \text{ - momentum density,} \quad (2.7)$$

$$\rho\mathbf{E}(\mathbf{x}, t) = \frac{1}{2} \int m\mathbf{v} \cdot \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} \text{ - energy density.} \quad (2.8)$$

where $\mathbf{E}$ is the total energy. The moment of the distribution function of order N can be written in the general form as a symmetric tensor of order N :

$$p_{i_1 i_2 \dots i_N}(\mathbf{x}, t) = \int m V_{i_1} V_{i_2} \dots V_{i_N} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} \quad (2.9)$$

where the second moment is written as:

$$p_{ij}(\mathbf{x}, t) = \int m V_i V_j f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} \quad (2.10)$$

which is called the pressure tensor [15]. The conservation of mass, momentum, and energy in a collision gives that the collision operator C should satisfy [5]:

$$\int C d\mathbf{v} = 0 \quad (2.11)$$

$$\int C \mathbf{v} d\mathbf{v} = 0 \quad (2.12)$$

$$\int C \mathbf{v}^2 d\mathbf{v} = 0 \quad (2.13)$$

Replacing C by its equivalent from the Boltzmann equation (2.3) results in:

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}) = 0 \quad (2.14)$$

$$\frac{\partial \rho_f \mathbf{u}}{\partial t} + \nabla \cdot (\rho_f \mathbf{u} \otimes \mathbf{u}) = -\nabla \cdot \mathbf{p} \quad (2.15)$$

where $\mathbf{p} = p_{ij}$ and ρ_f is the density of the fluid (gas). In order to obtain the expression for pressure, one has to solve the Boltzmann equation (2.3) which is not possible even for the simple BGK model. An approximate expression for the pressure tensor can be obtained us-

ing the Chapman-Enskog expansion in which the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ is expanded about the equilibrium distribution (Maxwellian distribution) function $f^{(0)}(\mathbf{x}, \mathbf{v}, t)$ where the expansion parameter is a variation of the hydrodynamic fields in time and space [5]. Replacing the obtained pressure expression in equation (2.15) allows to obtain the Navier-Stokes equations.

2.1.2 Solid Phase

The methods used to model granular flows are borrowed from that of a molecular gas where the solid particles are considered as the molecules in a gas. Two main approaches exist to model a solid phase: the Eulerian (continuous) approach and the Lagrangian (discrete) approach. For large scale systems, the Eulerian approach can be used and the governing equations for the solid resembles the Navier-Stokes equations for an ordinary gas flow. When the detailed physics of the granular flow needs to be investigated, the Lagrangian approach is used where the particles' motion is assumed to be well described by Newton's equations of motion [5].

A kinetic theory of granular flow (KTGF) has also been proposed to connect the micro-scale quantities of a granular flow to the macro-scale quantities. However, a granular flow differs significantly from a molecular gas flow. In molecular gas flows, collisions between molecules is elastic and the kinetic energy is conserved meaning that in the absence of external energy sources, there exists a well-defined equilibrium state. On the other hand, collisions between particles in granular flows are characterized by surface friction and elastic-plastic deformation, meaning that in the absence of external energy sources, there exist no equilibrium state as a granular system will continuously cool down due to the dissipation of kinetic energy which will slow down the particles. This effect of in-elasticity is the main difference between molecular gas and granular flows [5].

In the kinetic theory of granular flows, in order to model granular systems, an energy source term and a dissipative term should be added to the Boltzmann equation (2.3), resulting in a more complicated equation. Additionally, the effect of gravity can no longer be ignored and differences in particles' size will affect their distribution and will lead to the segregation of granular material (ex. the Brazil nut effect) [5].

2.1.3 Inter-phase Coupling in Solid-Gas Flows

One of the major difficulties arising from the modelling of multiphase solid-gas flows is the inter-phase coupling. This is because taking into account the effect of the fluid on the

motion of the particles and that of the particles on the flow of the fluid is not trivial. An important dimensionless number that allows the characterization of the inter-phase coupling in a mixture is the Stokes number (St) defined as the ratio of the characteristic time of the particle to the characteristic time of the flow and is given as [3]:

$$St = \frac{u \rho d_p^2}{18 \mu D} \quad (2.16)$$

where d_p is the particle diameter, μ and u are the fluid viscosity and mean velocity respectively and D is the diffusion coefficient. If $St \ll 1$, the particles would have enough time to respond to changes in the fluid velocity and both phases would nearly have the same velocity. On the other hand, if $St \gg 1$, the particles would not have enough time to respond to changes in the fluid velocity and thus the fluid velocity does not affect that of the particles [3]. This is summarized as the interaction between the solid and gas phases. These interactions can be described through various momentum coupling strategies shown in Figure 2.1.

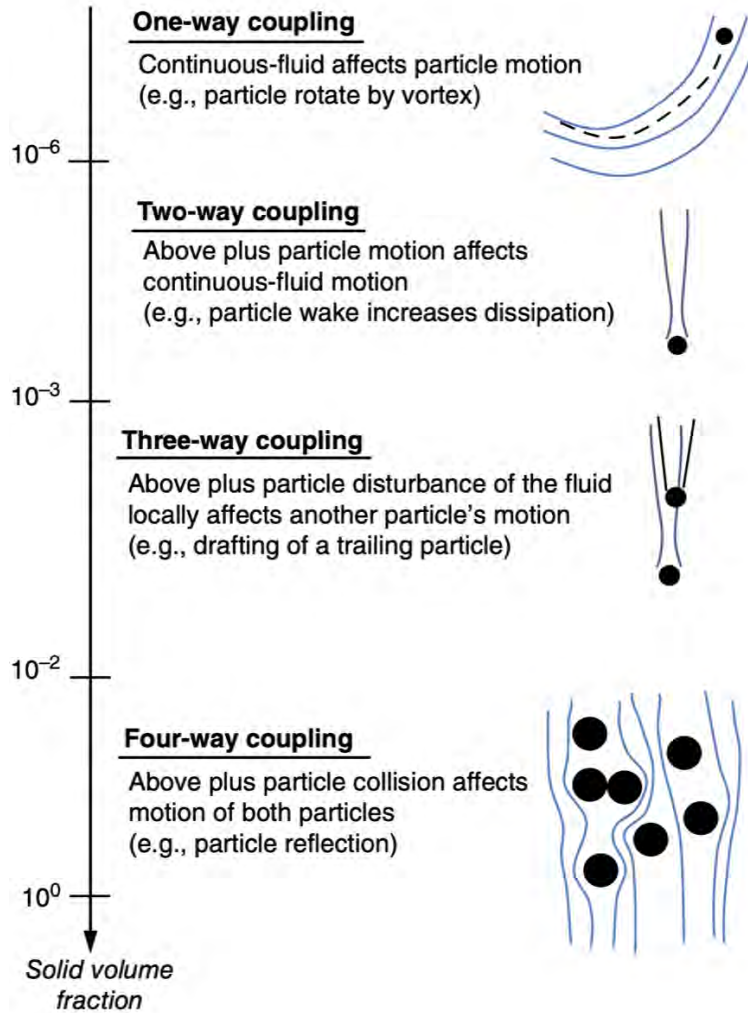


Figure 2.1 Various coupling strategies [3].

There are four categories characterizing the interaction between phases. The first three only include particle-fluid interactions while the fourth category include particle-particle interactions as well. The classification is dependent on the volume fraction of solid particles in the mixture. In general, more effects associated with different length and time scales are included in the model as we move upwards in the coupling categories necessitating a more complex numerical model to capture all structures within both phases [3].

One-Way Coupling

The motion of the solid phase is affected by the motion of the continuous phase while the opposite is not true, that is the effect of the particles' motion on the fluid can be neglected. In such case, the flow is treated as a pure fluid and can be solved independently from the equations of particle motion. On the other hand, the particles' equations need information about hydro-dynamical forces such as drag for solution [3].

Two-Way Coupling

When the phases exhibit mutual effects between their flows, the coupling is termed two-way coupling. In this case, the motion of particles affect the motion of the fluid and vice-versa. This can be for example in the case of particles inducing disturbances in the fluid flow and thus altering the fluid behavior [3].

Three-Way Coupling

In such cases, the disturbance in the fluid flow induced by a particle can affect the motion of another particle [3]. This result in an indirect effect between the two particles through the disturbance propagated in the fluid.

Four-Way Coupling

In such situations, solid-solid interactions come into play. In addition to solid-fluid interactions, particle-particle collisions also influences the overall motion of the phases. This is mainly prominent in applications where there exist dense flows such as the fluidization of particles [3]. As this thesis includes the modelling of solid-gas fluidized and spouted beds, this class is of the utmost importance to this work.

2.2 Fluid Mechanics

Fluid mechanics is a branch of continuum mechanics where matter is modelled from a mesoscopic viewpoint without considering its microscopic constituents [16]. It is mainly divided into two groups. Fluid statics involves studying the fluid at rest while fluid dynamics involves studying the effect of forces on the motion of the fluid. It is a concept used to study continuous media by moving away from their molecular nature through averaged equations. The equations of mass, momentum and energy conservation describe the continuous displacement of the fluid. As discussed in Section 2.1, the Knudsen number (Kn) is used to determine whether or not a fluid can be treated as a continuum. This assumption is valid when $\text{Kn} < 0.1$.

The partial differential equations describing a fluid motion in time and space are detailed in this Section. Their derivation is presented as well as all assumptions for incompressibility as this thesis deals solely with incompressible fluids.

2.2.1 Governing Equations

In an Eulerian reference frame, mass conservation is presented by the continuity equation whereas momentum conservation is presented by the Cauchy equation. The equations are presented in vector-tensor notation similar to the one used by Bird et al. [17]:

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}) = 0 \quad (2.17)$$

$$\frac{\partial \rho_f \mathbf{u}}{\partial t} + \nabla \cdot (\rho_f \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho_f \mathbf{g} \quad (2.18)$$

where ρ_f is the fluid's density, $\mathbf{u}$ is the fluid's velocity, $\mathbf{g}$ is the gravitational acceleration and $\boldsymbol{\sigma}$ is the Cauchy stress tensor and is given by:

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau} \quad (2.19)$$

where p is the pressure, $\mathbf{I}$ is the identity matrix, and $\boldsymbol{\tau}$ is the deviatoric stress tensor. The stress tensor for a compressible flow is expressed as:

$$\boldsymbol{\tau} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^\top) + \left(\frac{2}{3}\mu - \kappa \right) (\nabla \cdot \mathbf{u}) \mathbf{I} \quad (2.20)$$

where $\nabla \mathbf{u}$ is the velocity gradient tensor, $(\nabla \mathbf{u})^\top$ is the transpose of the velocity gradient tensor, $\nabla \cdot \mathbf{u}$ is the divergence of the velocity vector, μ is the dynamic viscosity of the fluid, and κ is the dilatational viscosity. In the case of a gas, the fluid is assumed to be mono-atomic and $\kappa = 0$. In case of an incompressible fluid, $\nabla \cdot \mathbf{u} = 0$ is satisfied by the continuity equation, and thus the term containing κ is discarded [17].

It is important to note that the compressibility of a fluid is not determined only by the type of fluid as is commonly thought of in the literature where gases are assumed to be compressible and liquids to be incompressible. This is because the compressibility is also determined by the nature of the flow. An incompressible flow is that having a low Mach number (Ma) where the Mach number is a dimensionless number defined as the ratio between the speed of the fluid and the speed of sound in that fluid (c) and it given as:

$$\text{Ma} = \frac{|\mathbf{u}|}{c} \quad (2.21)$$

$$c = \sqrt{\left(\frac{\partial p}{\partial \rho_f} \right)_s} \quad (2.22)$$

where c is determined as the isentropic derivative of the pressure with respect to density [17]. When $\text{Ma} < 0.3$, the change in the density of the fluid due to velocity is up to 5 % and the fluid is considered incompressible [18]. As such, in the context of this thesis, a gas specifically air in fluidized and spouted beds is considered to be incompressible or at a low Mach number. In such case, the Navier-Stokes equations for an incompressible Newtonian fluid are:

$$\nabla \cdot \mathbf{u} = 0 \quad (2.23)$$

$$\rho_f \frac{\partial \mathbf{u}}{\partial t} + \underbrace{\rho_f \nabla \cdot (\mathbf{u} \otimes \mathbf{u})}_{\text{advection}} = -\nabla p + \underbrace{\mu \nabla^2 \mathbf{u}}_{\text{diffusion}} + \rho_f \mathbf{g} \quad (2.24)$$

The first and second terms on the left of equation (2.24) represent the temporal evolution of the velocity and the advection of the fluid respectively. The second and third terms to the right are respectively the diffusion of the fluid represented by the laplacian and the gravitational acceleration.

The Navier-Stokes equations lack an independent equation for the pressure whose gradient contribute to the momentum equation. This equation allows the determination of the velocities, which leaves the continuity equation that does not include the pressure, to determine the pressure. In compressible flows, an equation of state relating the density to the pressure

is used. This is not the case for incompressible flows where the density is constant. In that case, and according to equation (2.22), the speed of sound c becomes infinite leading to an instantaneous propagation of pressure everywhere.

Combining the two governing equations allows to determine the pressure by taking the divergence of the momentum equation and using the continuity equation divergence free condition to simplify it. This results in a Poisson equation for the pressure [19] given by:

$$\nabla^2 p = \rho_f \nabla \cdot (\mathbf{g} - \mathbf{u} \cdot \nabla \mathbf{u}) \quad (2.25)$$

meaning that the pressure is not transient and is driven by the above Poisson equation which depends on the instantaneous velocity field. As the Navier-Stokes equations are solved and the velocity determined, the pressure can be instantaneously deduced from the velocity using equation (2.25). Thus, pressure is a Lagrange multiplier used to impose the mass conservation constraint as it is linked to the continuity equation and not to the momentum conservation equation.

2.2.2 Turbulence

Turbulence is found in our everyday surroundings such as the movement of strong winds or the water flowing through a waterfall where the flow is unsteady, irregular, random, and chaotic, and the motion of each water droplet is unpredictable. As such, the fluid velocity field varies significantly and irregularly in both time and space [20].

Turbulence can be defined as the motion of the fluid based on random and chaotic three-dimensional vorticity and it dominates all other flow phenomena when it is present [21]. The majority of engineering and naturally occurring flows are turbulent; however, it is not easily seen [20, 22]. Flows in pumps, compressors and pipe lines and around airplanes, automobiles, ships and submarines are generally turbulent flows. Additionally, the mixing of reactants in chemical reactors is turbulent. Turbulence plays an important role in most flows as it greatly enhances the transport and mixing of matter, momentum and heat in flows which is usually of great practical importance. Compared to laminar flows, it also increases wall shear stress and hence drag [20, 21].

The transition from laminar to turbulent flows was first demonstrated by Reynolds in 1883 [23], where he performed experiments of water flow along a pipe in which he steadily injected a dye along the centerline of the pipe [20]. He defined a dimensionless number characterizing the transition between laminar and turbulent regimes. This number is known as Reynolds number (Re) [24] and is defined as the ratio of inertial to viscous forces and is given as:

$$\text{Re} = \frac{\mathcal{U}\mathcal{L}}{\nu} \quad (2.26)$$

where $\mathcal{U}$ and $\mathcal{L}$ are the characteristic velocity and length scales of the flow, and ν is the kinematic viscosity of the fluid. If the Reynolds number is small ($\text{Re} < 2300$ for the pipe experiment), the flow is laminar and is driven by viscous forces, whereas if the Reynolds number is large ($\text{Re} > 4000$ for the pipe experiment), the flow is turbulent and is driven by inertial forces.

According to Richardson [25], turbulent flows are composed of eddies of different sizes where eddies are defined as “turbulent motions localized with a region of size ℓ , that is moderately coherent over this region. This region occupied by a large eddy can also contain smaller eddies” [20]. The eddies in the largest size range can be characterized by the length-scale ℓ_0 and the velocity $u_0 \equiv u(\ell_0)$ which are respectively comparable to the flow scale $\mathcal{L}$ and $\mathcal{U}$. The Reynolds number of these eddies $\text{Re}_0 \equiv u_0\ell_0/\nu$ is large and can be compared to Re and thus the viscosity’s direct effects are negligibly small [20].

Turbulent flows arise often from laminar flows with increasing Reynolds number resulting in the growth of small disturbances by taking energy from the laminar flow [21]. Large eddies are unstable and break up, transferring their energy to smaller eddies, which in turn break up to transfer their energy to successively smaller and smaller eddies until the Reynolds number ($\text{Re} \equiv u(\ell)\ell/\nu$) is sufficiently small (close to unity) that the eddy motion is stable and molecular viscosity is effective in dissipating the kinetic energy [20, 25]. In turbulence, there is three unique length (η), velocity (u_η) and time scales (τ_η) that characterize the very smallest dissipative eddies. These are known as the Kolmogorov scales [20]:

$$\eta \equiv \left(\frac{\nu^3}{\epsilon} \right)^{\frac{1}{4}} \quad (2.27)$$

$$u_\eta \equiv (\epsilon\nu)^{\frac{1}{4}} \quad (2.28)$$

$$\tau_\eta \equiv \left(\frac{\nu}{\epsilon} \right)^{\frac{1}{2}} \quad (2.29)$$

where ϵ is the dissipation rate determined by the transfer of energy from the largest eddies and scales independent of ν [20]. The Kolmogorov scales allows to readily determine the ratios of the smallest to largest scales using the scaling $\epsilon \sim u_0^3/\ell$:

$$\frac{\eta}{\ell_0} \sim Re^{-\frac{3}{4}} \quad (2.30)$$

$$\frac{u_\eta}{u_0} \sim Re^{-\frac{1}{4}} \quad (2.31)$$

$$\frac{\tau_\eta}{\tau_0} \sim Re^{-\frac{1}{2}} \quad (2.32)$$

where it is evident that at high Reynolds numbers, the velocity and time scales of the smallest eddies (u_η and τ_η) are small compared to those of the largest eddies (u_0 and τ_0).

2.3 Numerical Solution of Fluid Dynamics Governing Equations

Analytically solving the partial differential equations that govern the physical phenomena of a fluid system is unfeasible as an exact analytical solution for the Navier-Stokes equations is yet to be found. Therefore, it is necessary to convert them into a system of algebraic equations and to solve them computationally, thus the term computational fluid dynamics (CFD). In this section, three main numerical methods for solving the Navier-Stokes equations are presented: the finite difference method (FDM), the finite volume method (FVM), and the finite element method (FEM). These methods are distinct and each possess its own advantages and disadvantages.

FDM is one of the most commonly used methods. It works by approximating the derivatives in a given equation such as the transport equation using a Taylor series expansion. The time derivative can be discretized in a similar way to that of space [26]. This method is defined dimension by dimension which makes it easy to increase the elements' order to achieve high-order accuracy. However, it is fitted for rectangular or square geometries. Its implementation becomes problematic when the geometry includes curved boundaries since defining boundary conditions over the curve becomes difficult. Also, it isn't a viable method when local grid refinement or adaptive mesh refinement is needed to resolve local rapid variations in solutions [19, 26].

FVM converts the differential partial equations over differential volumes into discrete algebraic equations over non overlapping elements or finite volumes. It works by converting some terms in the conservation equations into face fluxes evaluated at the faces of the finite volume. This method is characterized by being strictly conservative since the flux entering a volume is identical to that leaving the adjacent volume. Moreover, this method is popular due to its flexibility which is associated with its discretization that is performed directly in the physical space without the need to transform between computational and physical coordinate sys-

tems. Finally, FVM allows easy non-invasive imposition of the boundary conditions since the unknown variables are not evaluated at the boundary faces of the volume elements but at their centroids [27].

As the finite element method (FEM) is the only method that will be used in this thesis, it will be discussed in detail explaining the continuous Galerkin methods (CGM). Additionally, within the context of FEM, high-order methods will be introduced. Furthermore, the way the compressibility constrain is applied will be discussed. At the end, methods for computationally modelling turbulence will be explained.

2.3.1 Finite Element Method

FEM is considered as a generalization of the classical variational (the Ritz) and weighted-residual (such as weak-form Galerkin least square, etc.) methods. The idea behind these methods is that the solution $\mathbf{u}$ of a differential equation can be expressed as a linear combination of unknowns c_j and approximation functions ϕ_j . c_j are then determined to satisfy the differential equation while ϕ_j which are usually polynomials, are selected to satisfy the boundary conditions of the problem [28]. The entire equation to be solved is then multiplied by a weight function w . In the Galerkin formulation, the weight function w is taken equal to the approximation functions ϕ_i . This choice is computationally advantageous as the matrix of the linear system to be solved becomes symmetric. For clarity, FEM will be explained by analyzing a problem for the determination of the steady-state velocity $\mathbf{u}$ distribution in a two-dimensional domain Ω , with boundary Γ .

Steps of Continuous Galerkin FEM The major steps involved in the analysis of a given problem using the finite element method are discussed in what follows.

1. **Discretization of the domain:** The finite element method includes discretizing the domain of the problem to simple geometric shapes, known as finite elements which possess certain geometric and physical features [28]. The domain of a known element is defined as Ω^e while its boundary is denoted by Γ^e . The assembly of all elements of the domain Ω are represented by Ω^h . Since the actual domain is geometrically complex, Ω^h may never be equal to the actual domain Ω .

An unknown physical quantity $\mathbf{u}$ can then be expressed as :

$$\mathbf{u} \approx \mathbf{u}^e = \sum_{j=1}^n \mathbf{u}_j^e \psi_j^e \quad (2.33)$$

where $\mathbf{u}^e$ is the approximation of $\mathbf{u}$ over the element Ω^e , $\mathbf{u}_j^e$ represents the values of $\mathbf{u}^e$ at the element nodes and is equivalent to the unknown c_j , and ψ_j^e are the approximation functions specific to this element and are equivalent to the approximation functions ϕ_j [28].

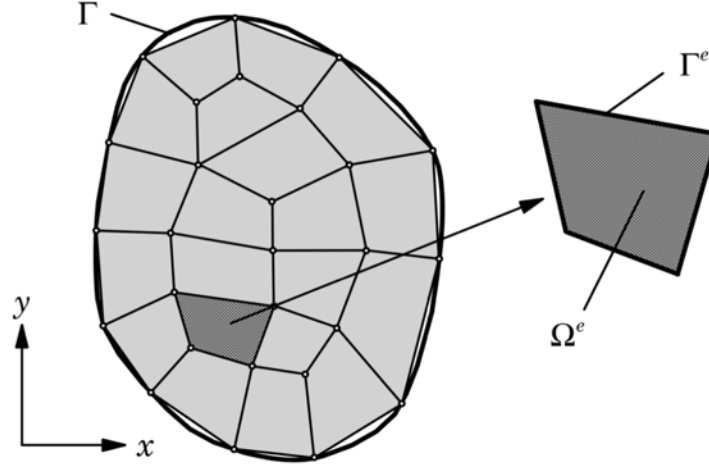


Figure 2.2 Finite element discretization of a given domain [28].

2. Construction of a statement and development of a finite element model:

The approximation functions are chosen in order to satisfy the boundary conditions of the problem, while the unknowns are determined in order to satisfy the governing differential equation in a weighted integral sense. Therefore, n algebraic equations composed of the nodal values ($\mathbf{u}^e$) are obtained and are referred to as the finite element model [28]. However, this model suffers from a drawback for second or higher order differential equations where the approximation functions ψ_j^e should be differentiable as many times as the actual solution $\mathbf{u}$ in the differential equation while the weight function w is not subject to differentiation. The weak form of the differential equation is constructed as a weighted-integral statement that combines both the governing differential equation as well as some types of boundary conditions. This form is important since it reduces the continuity requirement by moving part of the differentiation from $\mathbf{u}^e$ to the weight function w [28].

3. Assembly of the finite elements into a global system of algebraic equations:

In order to obtain the global system of equations representing the entire domain, the finite elements must be assembled. This leads to the following system: $\mathbf{K}\mathbf{X} = \mathbf{F}$, where $\mathbf{K}$ represents the system matrix, $\mathbf{F}$ the right hand side of the finite element equations,

and $\mathbf{X}$ the solution of the system. To assemble the matrix, we integrate the weak form over each element. The primary variable, the velocity $\mathbf{u}$, should be continuous at the nodes, and the secondary variable, the flux, should be balanced between the elements. This means that at the interface of the elements, the flux should be equal in magnitude and opposite in sign. The finite element formulations are classified in three categories: super-parametric, iso-parametric, and sub-parametric where the approximation used for the geometry is higher order, equal degree, or lower order than that used for the dependent variable respectively [28].

4. **Imposition of Initial and Boundary Conditions:** Suitable boundary and initial conditions are required to complete the description of any general initial and/or boundary value problem. In steady state problems, coherent initial conditions are important as they greatly help with convergence. Often, initial conditions are set by initiating the flow from an already established steady state or from rest where the fluid is not in motion. In all cases, the dependent variable should be known at time $t = 0$ for all spatial nodes and should satisfy the basic conservation equations (e.g., solving for velocity, the initial velocity field should be divergence free and have a compatible pressure field) [28]. Concerning boundary conditions, the velocity components or the total surface stress (σ_{ij}) should be specified at the boundary of a fluid. This translates mainly to two main boundary conditions:

Dirichlet or essential boundary condition:

$$\mathbf{u}_i = f_i^{\mathbf{u}}(s_k, t) \quad \text{on } \Gamma_{\mathbf{u}} \quad (2.34)$$

Neumann or natural boundary condition:

$$\mathcal{T}_i = \sigma_{ij}(s_k, t)\mathbf{n}_j(s_k) = f_i^{\mathcal{T}}(s_k, t) \quad \text{on } \Gamma_{\mathcal{T}} \quad (2.35)$$

where s_k are the coordinates along the boundary, t is the time, $\mathbf{n}_j$ is the outward unit normal to the boundary and Γ_f is the total boundary enclosing the domain Ω_f with $\Gamma_f = \Gamma_{\mathbf{u}} \cup \Gamma_{\mathcal{T}}$. No slip boundary condition at fixed boundaries is applied when $f_i^{\mathbf{u}} = 0$. When fluid enters or exit the domain Ω_f , $f_i^{\mathcal{T}} = \text{constant}$. When the fluid slips across the surface boundary, a slip boundary condition can be obtained by replacing the tangential Dirichlet boundary condition with a traction condition of the form:

$$\alpha \sigma_{ij} \mathbf{n}_j t_i = (\mathbf{u}_i - \mathbf{u}_i^s) t_i \quad (2.36)$$

$$\mathbf{u}_i \mathbf{n}_j = 0 \quad (2.37)$$

where α is the slip coefficient, t_i is the components of the tangent vector to the surface, and $\mathbf{u}_i^s$ is the velocity of the surface [28].

5. **Solution of the equations:** For most practical problems, the finite element model involves solving a large and sparse system of non-linear algebraic equations. Usually, the non-linear equations are linearized prior to solving using Taylor expansion for example. The non-linear equations are solved using Newton's method while the linear set of equations that arise from them are solved using direct methods such as Gauss elimination or Kyrlov methods. They are termed direct methods since the solution of the matrix is obtained via a fixed number of steps. Iterative Kyrlov methods such as the generalized minimal residual method (GMRES) provide approximate solution which improves with continued iterations. Initially, the number of iterations to achieve a certain accuracy is unknown. These methods are well suited for large problems and are compatible with parallel computer architectures [28].
6. **Post-processing of the solution and the quantities which are of interest.**

Continuous Galerkin Methods

The method implemented in this thesis is the continuous Galerkin finite element method. There exist several weaknesses in the continuous Galerkin method (CGM), specifically arising instabilities in the approximate solution for advection or convection dominated problems. Using Petrov-Galerkin stabilization techniques allows to stabilize the continuous Galerkin finite element method. On the other hand, the finite volume method does not suffer from this limitation; however, extending it to high-order spatial approximations is difficult. As we are interested in high-order simulations, the Continuous Galerkin method is used.

High-Order Methods

For computational fluid dynamics, there exists low and high-order numerical methods that can be implemented to solve the governing equations. The definition of high-order methods is methods possessing an order of accuracy greater than 2 [29]. The use of low order methods is usually prevalent in simulation due to them being reliable and robust. Even though high-order methods achieve higher accuracy for the same computational cost, they are less used due to their complexity and because they are less robust. Steady state convergence is more difficult and challenging to reach with high-order simulations, and for worse cases, the solution may even diverge [29]. Additionally, high-order methods lacks in general the robust and versatile shock capturing capabilities found in lower order methods. Moreover, spatial

operators in high-order schemes are much stiffer than those of low order schemes. However, high-order methods have shown promise in efficiently solving problems with a requirement for high accuracy such as vortex dominated flows, numerical simulation of turbulence, and large eddy simulations [29].

The advantage of these methods is their relatively small error. When the error in the solution of a method decreases with the size of the mesh h based on $e \propto h^{k+1}$, then the method error is said to be of order $k + 1$. Moreover, for the same number of degrees of freedom (DOFs), high-order methods produce solutions with less errors compared to lower order methods. When dealing with explicit methods, high-order schemes usually have smaller Courant–Friedrichs–Lewy (CFL) number than low order methods. The CFL number is a condition for the stability of different numerical methods that are often unstable. It is often overcome by using an implicit scheme [29].

In the context of the finite element method, high-order implementation is applied by increasing the order of the approximation polynomials (ϕ) within an element to obtain higher order convergence. As such, a polynomial of degree k results in an order of convergence $k+1$. Thus, a linear approximation function resulting in a second order scheme is termed low order and any higher order approximation function will result in what is termed as high-order schemes.

2.3.2 Applying the Incompressibility Constraint

Both velocity and pressure need to be solved for when modelling a fluid. In general, two categories of methods can be used to solve the Navier-Stokes equations: splitting methods and monolithic methods. Splitting methods involves the separation of the velocity and pressure unknowns for solving them sequentially. Monolithic methods involves the discretization in space and time of the governing equations to obtain a global system including both the velocity and pressure unknowns to solve them simultaneously [26, 30].

Splitting Methods

Splitting methods are divided into three main categories: pressure-correction schemes, velocity-correction schemes and consistent splitting schemes. They involve decomposing the Navier-Stokes equations into a convection-diffusion problem for the velocity and a Poisson problem for the pressure. Pressure-correction schemes divide each time step into two main sub-steps. The first sub-step accounts for the viscous effects where the pressure is either ignored or treated explicitly and the second sub-step account for incompressibility where the pressure is corrected using the provisional velocity obtained in the previous sub-step. Velocity-correction

schemes switches the sub-steps of the pressure-correction schemes where the viscous term is ignored or treated explicitly in the first sub-step and the velocity is accordingly corrected in the second sub-step. Consistent splitting schemes are similar to pressure-correction schemes where the pressure is treated explicitly to calculate the velocity in the first sub-step and then updating the pressure using the Poisson pressure equation [30].

Among these methods, the most famous implemented algorithm is the SIMPLE (Semi-Implicit Method for Pressure-Linkage Equations) [31] algorithm which allows the determination of a divergence free velocity by decoupling the momentum and pressure equation resulting in a Poisson equation for the pressure. The algorithm steps are as follows [32]:

1. Guess the pressure field p^* .
2. Solve the momentum equation to obtain the velocity field $\mathbf{u}^*$ corresponding to the guessed pressure field p^* .
3. Solve the pressure correction equation to obtain a correction for pressure p' .
4. Calculate the pressure p by adding p' to p^* .
5. Calculate $\mathbf{u}$ from its starred value using the velocity-correction equations.
6. Treat the corrected pressure as the new guessed pressure p^* and repeat all steps starting from step 2 until the convergence of the solution.

Several attempts have been made to improve this algorithm. The SIMPLE revised (SIMPLER) [33] algorithm evaluated the pressure using an extra equation, the SIMPLE consistent (SIMPLEC) [34] algorithm requires no under-relaxation of the pressure as consistent approximations are made in the derivation of the pressure-correction equation, the modified SIMPLER (MSIMPLER) algorithm [35] involves a minor modification in the pressure-correction equation of the SIMPLER algorithm and the PISO (Pressure Implicit with Splitting of Operators) algorithm [36] involves two or more correction steps to solve the pressure-correction equation.

Monolithic Methods

Lethe uses a monolithic or coupled approach in numerically solving the transient incompressible Navier-Stokes equations. Therefore, a detailed description of this method is important to understand how the solution of these equations is undertaken. Contrary to the splitting

methods, a single linearized system of equations for both pressure and velocity is solved at each Newton's iteration:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^\top & \mathbf{C} \end{bmatrix} \begin{bmatrix} \delta \mathbf{u} \\ \delta p \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_u \\ \mathbf{R}_p \end{bmatrix} \quad (2.38)$$

where $\delta \mathbf{u}$ and δp are the step change vectors of the velocity and pressure components defined on the finite element mesh at each iteration. The matrix block $\mathbf{A}$ depend on $\mathbf{u}$ due to the non-linear convective term in the momentum equation. The $\mathbf{C}$ block is equal to 0 in classical finite element but becomes non-zero when stabilized techniques are used. Vectors $\mathbf{R}_u$ and $\mathbf{R}_p$ are the residual of the coupled Navier-Stokes equations as a function of pressure p and velocity $\mathbf{u}$. The ordinary differential equation is discretized in time using finite difference methods of first order or higher order schemes, such as the backward difference (BDF) or using singly-diagonal implicit Runge-Kutta methods of arbitrary order (SDIRK) [26].

The main difficulty with this finite element formulation is the choice of interpolation functions for pressure and velocity. The use of the same order interpolation functions for both velocity and pressure lead to highly oscillatory pressure fields. In order to overcome this problem, two options are considered in the implementation of the incompressible Navier-Stokes solver. First, the use of mixed finite element formulation where different interpolation functions are used for pressure and velocity to obey the Ladyzhenskaya-Babuska-Brezzi (LBB) condition, prevents spurious pressure in the solution. In general, the mixed finite element formulations applies a pressure interpolation function that is one order of magnitude lower than the velocity interpolation function. Another option is the use of a stabilized finite element formulation while keeping equal order interpolations for velocity and pressure [26]. The stabilization technique for pressure is known as pressure stabilizing Petrov-Galerkin (PSPG). The implementation of streamline upwind Petrov-Galerkin (SUPG) prevents oscillatory solutions resulting from the large convective term in high Reynolds number flows.

Comparing both methods, the stabilized finite element formulation requires the adjusting of stabilization parameters which is often a delicate problem, contrary to the mixed formulation that is parameters free. Additionally, equal order interpolation is often more costly from the pressure point of view without further gains in accuracy as the finite element mesh is generally determined based on the velocity behavior [26]. However, this is not clear for turbulent flows.

2.3.3 Turbulence Modelling

Turbulence plays a dominant role in a vast majority of naturally occurring and industrial flows [22]. Before going into the methods for turbulence modelling, it is important to mention

the notion of homogeneous and isotropic turbulence. By considering a flow with a velocity field $\mathbf{u}(\mathbf{x}, t)$ and pressure $p(\mathbf{x}, t)$, homogeneous turbulence is defined as the flow where $\mathbf{u}(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ are homogeneous, that is $\mathbf{u}(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ are invariant under a shift in position $(\mathbf{x} + \mathbf{X}, t)$ where $\mathbf{X}$ is the shift in position. Homogeneous turbulence could be approximated in wind-tunnel experiments [20]. Defining homogeneous turbulence as statistic invariance under translation, isotropic turbulence is defined as statistic invariance under rotation where $\mathbf{u}(\mathbf{x}, t)$ can be replaced by $\bar{\mathbf{u}}(\bar{\mathbf{x}}, t)$ where $\bar{\mathbf{x}}$ and $\bar{\mathbf{u}}$ denote the position and velocity in any coordinate system obtained by rotation of the coordinate system. Isotropy is extremely important in turbulence as much of the turbulence theory centers on it [20].

In this section, three main methods for modelling turbulence are discussed. In order of accuracy, they are the Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and the Reynolds-Averages Navier-Stokes (RANS) simulation. In the context of this work, LES will be implemented and as such, LES will be explained in detail while the other methods will be described in brief.

Direct Numerical Simulations

In DNS, all the scales down to the Kolmogorov scale of motion are resolved when solving the Navier-Stokes equations, taking appropriate initial and boundary conditions for the flow considered. This leads to a simulation producing a single realization of the flow. It is the simplest modelling approach possessing unrivalled accuracy and level of description. However, it is limited in its use since it is the most computationally expensive method. Additionally, computational power increases drastically with an increase in the Reynolds number as the increase is proportional to the cube of the Reynolds number. As such, its implementation is limited to low and moderate Reynolds numbers. Homogeneous turbulence is the simplest class of flows that can be studied using DNS [20].

Explicit Large Eddy Simulations

LES allows to directly represent the larger three-dimensional unsteady turbulent motion while the effects of the smaller scale motions are modelled. This makes the method computationally cheaper than DNS but more expensive than RANS. The four main steps of LES are:

1. Decomposing the velocity field using a filtering operation where Reynolds decomposition for the velocity results in:

$$\mathbf{u}(\mathbf{x}, t) = \bar{\mathbf{u}}(\mathbf{x}, t) + \mathbf{u}'(\mathbf{x}, t) \quad (2.39)$$

where $\bar{\mathbf{u}}(\mathbf{x}, t)$ is the filtered velocity field and $\mathbf{u}'(\mathbf{x}, t)$ is the residual velocity field. The general filtering operation is defined as:

$$\bar{\mathbf{u}}(\mathbf{x}, t) = \int G(\mathbf{r}, \mathbf{x}) \mathbf{u}(\mathbf{x} - \mathbf{r}, t) d\mathbf{r} \quad (2.40)$$

with $G(\mathbf{r}, \mathbf{x})$ satisfies the normalization condition:

$$\int G(\mathbf{r}, \mathbf{x}) d\mathbf{r} = 1 \quad (2.41)$$

Among the most commonly used filters are the box filter, the Gaussian filter, and the sharp spectral filter in 1 D and their extensions in 3D [20].

2. The filtered equations for the evolution of the filtered velocity field can be obtained from the incompressible Navier-Stokes equations where the momentum equation includes the residual or sub-grid scale (SGS) stress tensor that arises from the residual motions. Using Einsteins notation, these equations are [22]:

$$\partial_i \bar{u}_i = 0 \quad (2.42)$$

$$\partial_t (\rho \bar{u}_i) + \partial_j (\rho \bar{u}_i \bar{u}_j) = - \underbrace{\partial_i \bar{p}}_{\text{isotropic stress}} + \underbrace{2\partial_j (\mu \bar{S}_{ij})}_{\text{viscous stresses}} - \underbrace{\partial_j (\tau_{ij})}_{\text{apparent stresses}} \quad (2.43)$$

where the viscous stress stems from the momentum transfer at the molecular level, the apparent stress stems from the momentum transfer by the fluctuating velocity field, and the isotropic stress stems from the mean pressure field. $\bar{S}_{ij}$ and τ_{ij} are given by:

$$\bar{S}_{ij} = \frac{1}{2} (\partial_i \bar{u}_j + \partial_j \bar{u}_i) \quad (2.44)$$

$$\tau_{ij} = \rho_f (\overline{u_i u_j} - \bar{u}_i \bar{u}_j) \quad (2.45)$$

where $\bar{p}$ is the filtered pressure, $\bar{S}_{ij}$ is the filtered or resolved strain rate tensor, and τ_{ij} is the unknown SGS stress tensor which represents the SGS motions effects on the resolved LES fields. This tensor is modelled using the SGS model in order to solve the governing equations.

3. The obtained system is open as the apparent stress tensor requires knowledge of the unfiltered velocity field that is unknown. A closure model for the filtered velocity allows the modelling of the apparent stress tensor using an eddy-viscosity model proposed by Smagorinsky in 1963 and which forms the basis for many more advanced models [20].

This model describes the apparent stress tensor as [20, 22]:

$$\tau_{ij} = 2\mu_t \bar{S}_{ij} + \frac{1}{3}\delta_{ij}\tau_{ll} \quad (2.46)$$

where μ_t is the eddy viscosity. By substituting equation (2.46) in equation (2.43), the equation to be solved is obtained:

$$\partial_t (\rho \bar{u}_i) + \partial_j (\rho \bar{u}_i \bar{u}_j) = -\partial_i \bar{p} + 2\partial_j [(\mu + \mu_t) \bar{S}_{ij}] \quad (2.47)$$

where a modified pressure $\bar{P} = \bar{p} + \frac{1}{3}\tau_{ll}$ is introduced, thus the pressure obtained from the above equation is not only the static pressure. The simplest model to determine the eddy viscosity is Smagorinsky's model and is given by:

$$\begin{cases} \mu_t = \rho (C_S \bar{\Delta})^2 S \\ S = (2\bar{S}_{ij}\bar{S}_{ij})^{\frac{1}{2}} \\ \Delta = (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}} \end{cases} \quad (2.48)$$

where C_S is the Smagorinsky constant dependent on the flow type. However this model, although mostly successful is too dissipative which makes it not suitable for transition simulations. Additionally, the value of C_s needs to be adjusted for different flows [22]. One way to improve this, is the use of a dynamics model which allows to compute C_s locally in space and time during the simulation [22].

4. Finally, the model filtered equations are solved numerically for $\bar{\mathbf{u}}(\mathbf{x}, t)$ thus providing an approximation for the large scale motions in one realization of the turbulent flow [20].

Implicit Large Eddy Simulations (ILES): In the context of this thesis, implicit large eddy simulations (ILES) is implemented through the use of stabilized finite element techniques. Using this technique, no SGS model will be added to the discretized Navier-Stokes equations and the modelling of SGS will be obtained from the numerical truncation error resulting from the discretization of the governing equations [37]. Implicit filtering results in certain disadvantages such as solutions are always mesh dependent [22]. Methods for ILES depend mainly on the numerical method used. For examples, ILES methods implemented in FVM are different from those implemented for FEM. In FEM, they are represented by residual based methods and stabilized methods.

Stabilized formulation such as streamline-upwind Petrov-Galerkin (SUPG) and pressure-stabilizing Petrov-Galerkin (PSPG) are some of the most significant stabilized formulations

that found usage in a large range of applications as they stabilize the method without introducing excessive dissipation and they prevent numerical oscillations and other instabilities in solving problems at high Reynolds numbers. Additionally, they improve the convergence rate in iterative solvers of large matrix systems [38].

These stabilization techniques include a stabilizing parameter τ which is often dependent on the local length scale (element length) and the local Reynolds number. In a study performed by Akin et al. [38], it was found that the viscosity introduced by SUPG stabilization is on average less than 1% of the Smagorinsky eddy viscosity except in regions with very high vorticities where the SUPG viscosity was on average 5 % greater than the Smagorinsky eddy viscosity [38]. As such, it is expected that SUPG stabilization will perform similarly to explicit LES in capturing turbulence especially in regions with not very high vorticities since the artificial viscosity introduced using SUPG is of similar magnitude as that of the Smagorinsky eddy viscosity.

Reynolds-Averaged Navier-Stokes Simulations

The RANS approach solves the Navier-Stokes equations for the mean velocity field while the apparent stress tensor commonly referred to as Reynolds stresses is determined using a turbulence model usually via a turbulent-viscosity hypothesis where μ_t from equation (2.46) is specified as a product of a velocity $\mathbf{u}^*$ and a length ℓ^* [20]:

$$\mu_t = \rho_f \mathbf{u}^* \ell^* \quad (2.49)$$

where in algebraic models ℓ^* is generally specified on the basis of the geometry of the flow. $\mathbf{u}^*$ and ℓ^* are respectively related to the turbulent kinetic energy k and the turbulent dissipation rate ϵ for the $k - \epsilon$ model and to the turbulent kinetic energy k and the specific dissipation rate ω for the $k - \omega$ model for which modelled transport equations are solved [20].

2.4 Discrete Element Method

The discrete element method (DEM) is a Lagrangian approach in which the transient behavior of a system of a large number of distinct bodies is studied by solving Newton's second law. These bodies continuously collide and rebound. In multiphase flows, the fluid interacts with distinct bodies in the system. Additionally, these bodies and the fluid interact with the walls of the domain [3]. In DEM, bodies are considered as either rigid or deformable. The choice depends mainly on the operating conditions and on available computational resources. They are known as the hard-sphere (rigid) and soft-sphere (deformable) formulations. In a dilute

system, the hard-sphere formulation is more computationally efficient as the contact time between bodies is much shorter than the mean time between successive collisions and as such contacts can be considered instantaneous and pairwise. The particle travels freely under the effect of external forces and translational velocities until colliding with another particle. In this case, the velocity and position of the particles are only evaluated after the collision occurs. Using the momentum conservation laws, the post-collision velocities are calculated from pre-collision velocities. This is why this model is considered very efficient in certain dilute systems [3]. For dense systems where multiple contacts exist between particles over several time steps, a soft-sphere formulation is more appropriate.

The work in this thesis is focused only on the soft-sphere model since it covers most granular and multiphase flows and it can be modified to suit the hard-sphere approach whereas the inverse is not true. Moreover, it allows straight-forward modelling of time progressive phenomena such as particle breakage. Additionally, due to developments in computational resources, it can simulate a large system with hundreds of thousands of distinct bodies in a reasonable time [3]. Therefore, only the soft-sphere model will be described in detail.

2.4.1 Soft-Sphere Model

The collision forces obtained during contact between particles establish the formulation of the soft-sphere model which is presented in Figure 2.3.

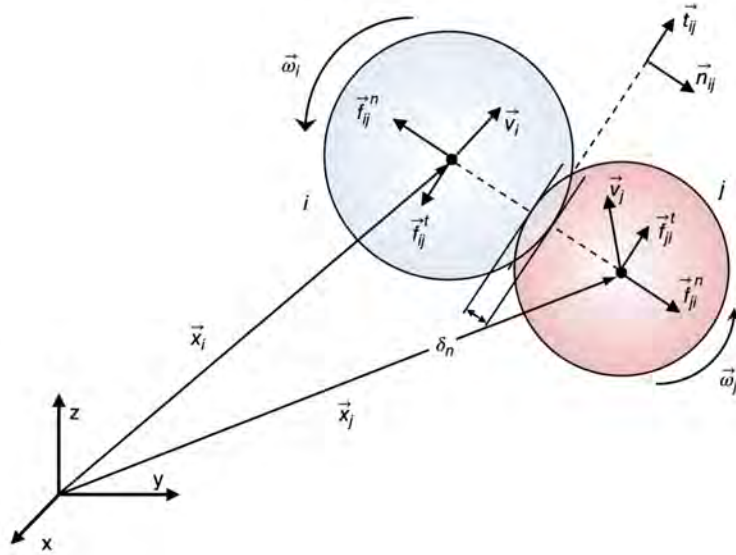


Figure 2.3 Schematic of colliding particles i and j and the forces acting on them due to collision [3].

The contact model is considered the core of the DEM where artificial overlaps and a set of imaginary springs and dash-pots are used for the modelling of contact forces and torques resulting from particle collisions [39].

The force of collision is obtained using the overlap between the particles in contact. During collision, this overlap and the collision force change. Applying Newton's second law of motion, the acceleration and the forces acting on the particles are balanced, and by integrating Newton's second law equation, new velocities and positions are obtained at each time step. The time step for such simulation should be small enough so that the contact between particles is processed in several time intervals. The critical time step based on the Rayleigh analysis is given by:

$$\Delta t_{crit} = \left(\frac{\pi r_i}{0.1631\nu_i + 0.8766} \sqrt{\frac{\rho_i}{G_i}} \right) \quad (2.50)$$

where ρ_i is the particle's density, G_i is the particle's shear modulus, ν_i is the particle's Poisson's ratio, and r_i is the particle's radius. Usually, the DEM time step is taken to be a fraction of the Rayleigh time step in the range of 10-20 % of the Rayleigh time step. This often leads to very small time steps which makes the simulation of a system of millions of particles to be unfeasible within a reasonable computational time frame. As such, artificially softening the particles by lowering the Young's modulus allows the use of larger time steps and decreases the computational time significantly [39].

During each time step, there should be relaxation of old collisions and the finding of new collisions [3]. Since most collisions are inelastic, the imaginary springs and dash-pots between overlapping particles allow for the restitution and dissipation of a part of the kinetic energy [39].

Whether the system consists of solid particles or granular material, its dynamics are governed by Newton's second law of motion for the center of mass of each particle and by Euler's second law of motion for the change in angular momentum of spherical particles [3]. These equations are:

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \mathbf{f}_{c,ij}^{p-p} + \sum_k \mathbf{f}_{l,ik}^{p-p} + \sum_w \mathbf{f}_{iw}^{p-w} + \mathbf{f}_i^{f-p} + \mathbf{f}_i^{ext} \quad (2.51)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_j (\mathbf{M}_{ij}^t + \mathbf{M}_{ij}^r) \quad (2.52)$$

where $\mathbf{v}_i$ the translational velocity of center of mass and $\boldsymbol{\omega}_i$ the rotational velocity around the center of mass are the state variables of the particle. Particle-particle interaction forces are divided into collision forces $\mathbf{f}_{c,ij}^{p-p}$ acting on particle i by particle j and long distance forces $\mathbf{f}_{l,ik}^{p-p}$ such as van der Waals interaction between particles i and k . Long distance forces are not considered in the context of this thesis as they are thought to have a negligible effect in fluidized and spouted beds. $\mathbf{f}_{iw}^{p-w}$ are particle-wall contact forces acting on particle i by wall w . The summation is performed on all particles in the contact list j and w . $\mathbf{f}_i^{f-p}$ represents all fluid interactions with particle i , and $\mathbf{f}_i^{ext}$ represents all external forces acting on particle i due to uniform or non-uniform external fields such as the gravitational force. $\mathbf{M}_{ij}^t$ is the tangential torque that occurs due to particles' collision. This causes the rotation of the particles. $\mathbf{M}_{ij}^r$ is known as the rolling friction or the rolling resistant torque since it always opposes the particle's rotation [3].

When two particles are in contact, they overlap. This overlap which models the deformation of these particles has two components, the normal and tangential portions. The normal unit vector passes through the centers of the two particles while the tangential unit vector is orthogonal to the normal unit vector [39]. Thus, the contact force between the two particles can be written as:

$$\mathbf{f}_{c,ij} = \mathbf{f}_{c,ij}^n + \mathbf{f}_{c,ij}^t \quad (2.53)$$

where $\mathbf{f}_{c,ij}^n$ is the normal contact force and $\mathbf{f}_{c,ij}^t$ is the tangential contact force.

Contact forces belong to one of two groups: continuous potential force displacement models and non-continuous force displacement models. The former include forces such as the Lennard-Jones potential which have a non-zero force at the beginning and end of collision and thus is physically unrealistic in granular flows. On the other hand, non-continuous models have a zero repulsive force if particles are not in contact and as such are more realistic to model granular materials. Non-continuous force displacement models are divided into three groups: linear visco-elastic models, non-linear visco-elastic models, and elastic perfectly plastic models [3].

Linear Visco-Elastic Models

Among linear visco-elastic models, the linear spring dash-pot (LSD) is widely used since it is easy to implement and it is applicable to multiple collisions and non-spherical particles. Also, by using a small value of the spring stiffness, larger time steps could be used which

makes calculations faster. However, this may lead to unrealistic results since it might affect the maximum overlap and the repulsive contact force between particles.

The collision force in both normal and tangential directions is given by:

$$\mathbf{f}_{c,ij}^n = -k_n \delta_{n,ij} - \eta_n \mathbf{v}_{rn,ij} \quad (2.54)$$

$$\mathbf{f}_{c,ij}^t = -k_t \delta_{t,ij} - \eta_t \mathbf{v}_{rt,ij} \quad (2.55)$$

where k_n and k_t are the normal and tangential spring constants, η_n and η_t are the normal and tangential damping coefficients, $\delta_{n,ij}$ and $\delta_{t,ij}$ are the normal and tangential overlap [3] and $\mathbf{v}_{rn,ij}$ and $\mathbf{v}_{rt,ij}$ are the velocity of particle i relative to particle j in the normal and tangential directions respectively. The spring constants as well as the damping coefficients are often calculated using correlations that relate the Young's modulus, the Poisson's ratio, the restitution coefficient, the diameter and the density of the particles [3].

Non-Linear Visco-Elastic Models

Non-linear visco-elastic models present a higher accuracy in calculating collision forces since the linear relationship between the normal overlap and the normal elastic collision force does not represent adequately the force displacement for the contact between two particles. The first proposed model was the Hertz model which was further improved by Mindlin and Deresiewics (MD theory).

The collision force in the normal direction is given by:

$$\mathbf{f}_{c,ij}^n = -k_n \delta_n^{3/2} - \eta_n \delta_n^\alpha \mathbf{v}_{rn,ij} \quad (2.56)$$

where $\alpha = 1/2$ for the Kuwabara and Kono [40] (KKn) model and $\alpha = 1/4$ for the Tsuji et al. [41] (TTIn) model. The tangential contact force is similar to that used for the linear model where in this case the tangential spring constant (k_t) is a function of the normal overlap $\delta_{n,ij}$ [3].

Elastic Perfectly Plastic Models

The elastic perfectly plastic model includes collision in the normal direction between particles composed of elastic material where the kinetic energy of collision dissipates due to the stress wave propagation along the particles. The amount of energy dissipated depends mainly on the mechanism of collision. The collision is divided into two phases: the loading phase in

which compression occurs and the unloading phase in which restitution occurs. For elastic deformation, the particle shape is preserved after collision, but for plastic deformation, the particle is plastically deformed and this deformation is irreversible. Plastic deformation occurs when the impact velocity is high enough to initiate it [3].

The collision force in both normal and tangential directions is given by:

$$\mathbf{f}_{c,ij}^n = \begin{cases} -k_l \delta_{n,ij} & v_{rn,ij} \geq 0 \\ -k_{ul} (\delta_{n,ij} - \delta_{0,ij}) & v_{rn,ij} < 0 \end{cases} \quad (2.57)$$

$$\mathbf{f}_{c,ij_{new}}^t = \mathbf{f}_{c,ij_{old}}^t + k_t \Delta \delta_{t,ij} \quad (2.58)$$

where k_l and k_{ul} are the loading and unloading spring stiffness respectively, $\delta_{0,ij}$ is the residual overlap after completing the unloading phase, $\Delta \delta_{t,ij}$ is the tangential increment. The tangential force is calculated using an incremental approach where the old tangential force is used to calculate the new tangential force.

It is important to note that for all presented models, the tangential force equations presented are valid when Coulombs criterion is not violated, that is $\mathbf{f}_{c,ij}^t < \mu_d \mathbf{f}_{c,ij}^n$ where μ_d is the coefficient of dynamic friction between particles i and j . If $\mathbf{f}_{c,ij}^t \geq \mu_d \mathbf{f}_{c,ij}^n$, then Coulomb's criterion is violated and gross sliding occurs resulting in a new expression for the tangential force:

$$\mathbf{f}_{c,ij}^t = -\mu_d \mathbf{f}_{c,ij}^n \text{sgn}(\delta_{t,ij}) \quad (2.59)$$

2.5 Numerical Modelling for Multiphase Flows

Two main types of models exist for the simulation of the solid phase: the continuous Eulerian models and the discrete Lagrangian models. The most commonly used models for solid-gas multiphase flows are the Eulerian-Eulerian two-fluid model (TFM) and the Eulerian-Lagrangian Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) model. In this section, both models are described with a strong emphasis on CFD-DEM as it is the method of choice implemented in this thesis.

2.5.1 Two Fluid Model

In the TFM, the particles are considered as a second continuous phase and the notion of discrete particles does not exist. The motion of both the fluid and solid phases is modelled from a continuum point of view in what is called a Eulerian-Eulerian approach [3]. In such approach, computational fluid dynamics (CFD) is used to solve for the local mass and momentum conservation of both phases through time.

The TFM approach is computationally simple and inexpensive, thus it is used more often in commercial packages. However, it is not applicable to all flow conditions and has greatly reduced accuracy. Due to the increase in computational power, TFM is able to model the behavior of multiphase flows of systems at the process (industrial) scale depending on the turbulent nature of the flow. Closure relations used for the effective pressure, viscosity, and fluid-solid forces are obtained from the kinetic theory and from some numerical data that is collected from more detailed scale models. The TFM approach relies to a large extent on these closure relations which can greatly affect the accuracy and the robustness of the simulations [5].

Governing Equations

In the TFM, the governing equations of continuity and momentum for the fluid phase include an additional fluid-solid interaction term when compared to the regular equations. They are represented by:

$$\frac{\partial (\varepsilon_f \rho_f)}{\partial t} + (\nabla \cdot \varepsilon_f \rho_f \mathbf{u}) = 0 \quad (2.60)$$

$$\frac{\partial (\varepsilon_f \rho_f \mathbf{u})}{\partial t} + (\nabla \cdot \varepsilon_f \rho_f \mathbf{u} \mathbf{u}) = -\varepsilon_f \nabla p - \beta (\mathbf{u} - \mathbf{v}) - \nabla \cdot (\varepsilon_f \bar{\boldsymbol{\tau}}) + \varepsilon_f \rho_f \mathbf{g} \quad (2.61)$$

where $\mathbf{v}$ is the velocity of the solid phase, β is the momentum transfer coefficient, and $\bar{\boldsymbol{\tau}}$ is the viscous stress tensor defined by:

$$\bar{\boldsymbol{\tau}} = - \left(\lambda_f - \frac{2}{3} \mu_f \right) (\nabla \cdot \mathbf{u}) \bar{\mathbf{I}} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^\top) \quad (2.62)$$

where λ_f is the fluid bulk viscosity [5].

For the solid particle phase, the governing equations of continuity and momentum are rep-

resented as:

$$\frac{\partial (\varepsilon_s \rho_s)}{\partial t} + (\nabla \cdot \varepsilon_s \rho_s \mathbf{v}) = 0 \quad (2.63)$$

$$\frac{\partial (\varepsilon_s \rho_s \mathbf{v})}{\partial t} + (\nabla \cdot \varepsilon_s \rho_s \mathbf{v} \mathbf{v}) = -\varepsilon_s \nabla p - \nabla p_s + \beta (\mathbf{u} - \mathbf{v}) - \nabla \cdot (\bar{\boldsymbol{\tau}}_s) + \varepsilon_s \rho_s \mathbf{g} \quad (2.64)$$

where $\varepsilon_s = 1 - \varepsilon_f$ and ρ_s is the density of the solid phase where the local mass per unit volume is defined as $\rho_s \varepsilon_s$. p_s , the effective solid pressure and $\bar{\boldsymbol{\tau}}_s$, the effective solid stress tensor implicitly include the particle-particle interactions where the notion of particles has disappeared completely in the TFM [5].

2.5.2 Computational Fluid Dynamics-Discrete Element Method

In the CFD-DEM approach, the fluid is modelled as a continuum using CFD while the particles are modelled as discrete entities using DEM. This enables increased accuracy in predicting the behavior of the solid phase as the position and velocity of individual particles are tracked. However, this increased accuracy comes at the expensive of computational efficiency as CFD-DEM is more computationally demanding than TFM where both phases are modelled as continuum.

Resolved and Unresolved CFD-DEM

There exists two types of CFD-DEM coupling: resolved and unresolved shown in Figure 2.4. In resolved CFD-DEM, the fluid mesh is discretized to a smaller scale than the particle size. The flow around each particle is fully resolved and the two phases are coupled through the no slip boundary condition at the particle surface. It allows detailed fluid profiles to be integrated to obtain the total hydrodynamic forces as well as forces acting on the particles. Among these methods and in the context of FEM, a sharp-interface immersed boundary method can be used to impose the boundary conditions on complex geometries including particles [42]. In unresolved CFD-DEM, the particle size is finer than the fluid mesh. The volume averaged Navier-Stokes equation are solved for the fluid where several solid particles occupy the same fluid cell. The two phases are coupled through explicit expressions for each solid-fluid interaction force such as drag, virtual mass, and Saffman lift [43] which are derived from particle-resolved simulations. Additionally, coupling is done through the calculation of the void fraction which allows the fluid to be aware of the solid phase.

Since resolved CFD-DEM accounts completely for the flow around each particle without

requiring additional models for the solid-fluid coupling, it is more accurate than unresolved CFD-DEM. However, it is computationally intensive and is limited by the number of particles in a system that can be simulated. With the largest resolved CFD-DEM system comprised of 350 000 particles on a very large cluster, it stands incomparable to unresolved CFD-DEM where systems with more than 50 million particles can be simulated [43].

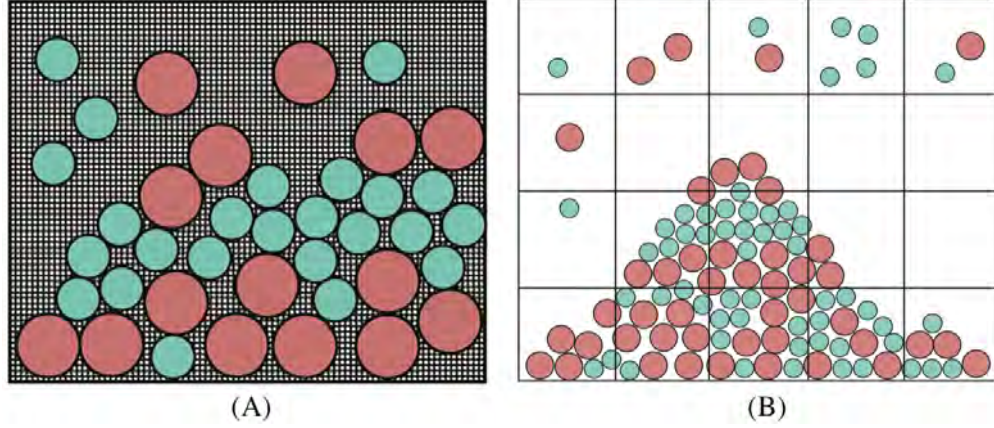


Figure 2.4 (A) Resolved CFD-DEM (B) Unresolved CFD-DEM [43].

Since most chemical processes involve the presence of a large number of particles (much greater than 350 000), resolved CFD-DEM becomes an unattractive method for the simulation of such processes. This is where unresolved CFD-DEM has shown extremely high potential for the modelling of industrial scale solid-fluid flows in fluidized and spouted beds despite the additional complexity due to the coupling procedure between CFD and DEM.

In the subsequent sections, unresolved CFD-DEM is discussed in detail as it is the main method implemented in this work. The governing equation for the fluid flow as well as the coupling strategy between the phases in terms of solid-fluid interactions and void fraction calculation are demonstrated. The solid phase motion, governed by the discrete element method (DEM) has been described in detail in Section 2.4 and therefore will not be discussed here.

The Volume-Averaged Navier-Stokes Equations

The volume-averaged Navier-Stokes equations are the governing equations for the fluid phase in unresolved CFD-DEM simulations. They take into account the dependency of the fluid volume within a computational cell on the solid phase volume occupying it. They are obtained through a definition of the void fraction where the fluid void fraction (ε_f) and the solid void

fraction ε_s are related to each other by the following relation:

$$\varepsilon_f = 1 - \varepsilon_s \quad (2.65)$$

In this section, we present the VANS equations for the fluid phase using the same forms as presented by Zhou et al. [44]. All three forms have the continuity equation in common where it remains unchanged and is given by:

$$\frac{\partial}{\partial t} (\varepsilon_f) + \nabla \cdot (\varepsilon_f \mathbf{u}) = 0 \quad (2.66)$$

The difference in the three formulations lies in the form of the momentum equation:

Form A (Set II):

$$\rho_f \left(\frac{\partial}{\partial t} (\varepsilon_f \mathbf{u}) + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) = -\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) - \mathbf{F}_{pf}^{II} + \rho_f \varepsilon_f \mathbf{g} \quad (2.67)$$

$$\mathbf{F}_{pf}^{II} = \frac{1}{V_\Omega} \sum_i^{n_p} (\mathbf{f}_{pf,i}) \quad (2.68)$$

Form B (Set I):

$$\rho_f \left(\frac{\partial}{\partial t} (\varepsilon_f \mathbf{u}) + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) = -\nabla p + \nabla \cdot (\boldsymbol{\tau}_f) - \mathbf{F}_{pf}^I + \rho_f \varepsilon_f \mathbf{g} \quad (2.69)$$

$$\mathbf{F}_{pf}^I = \frac{1}{V_\Omega} \sum_i^{n_p} (\mathbf{f}_{pf,i} + \mathbf{f}_{\nabla p,i} + \mathbf{f}_{\nabla \cdot \boldsymbol{\tau},i}) \quad (2.70)$$

Simplified Form B (Set III):

$$\rho_f \left(\frac{\partial}{\partial t} (\varepsilon_f \mathbf{u}) + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) = -\nabla p + \nabla \cdot (\boldsymbol{\tau}_f) - \mathbf{F}_{pf}^{III} + \rho_f \varepsilon_f \mathbf{g} \quad (2.71)$$

$$\mathbf{F}_{pf}^{III} = \frac{1}{\varepsilon_f V_\Omega} \sum_i^{n_p} (\mathbf{f}_{pf,i}) - \frac{1}{V_\Omega} \sum_i^{n_p} \rho_f V_{p,i} \mathbf{g} \quad (2.72)$$

with

$$\mathbf{f}_{pf,i} = \mathbf{f}_{d,i} + \mathbf{f}_{vm,i} + \mathbf{f}_{B,i} + \mathbf{f}_{Saff,i} + \mathbf{f}_{Mag,i} \quad (2.73)$$

where $\mathbf{F}_{pf}$ is the momentum transfer between the solid and the fluid phases, V_Ω is the volume of the fluid element Ω , V_p is the volume of the particle i , n_p is the number of particles in the fluid volume V_Ω , $\mathbf{f}_{d,i}$ is the drag force, $\mathbf{f}_{\nabla p,i}$ is the pressure force, $\mathbf{f}_{\nabla \cdot \boldsymbol{\tau},i}$ is the shear force, $\mathbf{f}_{vm,i}$ is the virtual mass force, $\mathbf{f}_{B,i}$ is the Basset force, $\mathbf{f}_{Saff,i}$ is the Saffman lift force and $\mathbf{f}_{Mag,i}$ is the Magnus lift force [44].

The simplified form B (set III) is valid and applicable only under the condition:

$$\rho_f (1 - \varepsilon_f) \left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) \right) = 0 \quad (2.74)$$

Thus, this form is not general and can only be used when the fluid circulating between the particles is steady and uniform [44], therefore it will not be considered in this thesis as the applications to be studied involve unsteady flows. These models have been discussed in detail by Bouillard et al. [45] and Gidaspow [46]. With few algebraic manipulations, form A and B of the VANS equations can be shown to be mathematically equivalent. However, what differentiates the two models is the manner in which incompressibility is applied. In model A, the void fraction ε_f multiplies the pressure gradient directly which alters the pressure equation to be solved and results in the pressure being shared between the fluid and solid phases. On the other hand, model B solves the pressure in a traditional way resulting in the pressure to be attributed solely to the fluid phase [44]. The application of these two models and their comparison have been studied for pneumatic conveying [47] and fluidization processes [45] where no significant difference have been shown between models A and B. As can be seen in equations (2.68) and (2.70), model B requires the explicit addition of the pressure and shear forces while model A does not. This makes model B stiffer and more difficult to converge compared to model A which explains the attractiveness of model A for use in commercial software due to its stability [45]. Nonetheless, since model B possesses all real characteristics, it is deemed to be a well-posed model, even though according to Enwald et al. [48], well-posedness for a multi-dimensional initial-boundary value problem have not been proved.

Void Fraction Calculation Schemes

In order to define the fluid volume fraction ε_f and calculate the momentum exchange term $\mathbf{F}_{pf}$, the particle volume must be projected into the CFD mesh. This projection should ensure several properties such as mass conservation, stable CFD simulations, and an acceptable computational cost [43]. Different methods exist to project the particles where each results

in a different projection scheme [49]. Each method possesses its own advantages and suffers from certain limitations. The most commonly used void fraction schemes are discussed in this section and they are the particle centered method (PCM), the MFIx divided particle volume method (DPVM) where MFIx is an open-source CFD-DEM package [50], the cube DPVM, the corrected cube DPVM, the statistical kernel, and the satellite point method (SPM) [49]. Only PCM and SPM will be detailed in this section as they will be implemented in this project.

PCM The particle centered method is the simplest projection method to calculate the void fraction in a fluid cell. It considers the entire volume of the particle to be in the cell in which the particle's center lies. This means that no calculation of the intersection between the particle and the cell boundaries is performed. The void fraction using PCM is given by:

$$\varepsilon_f = 1 - \frac{\sum_i^{n_p} V_p}{V_\Omega} \quad (2.75)$$

SPM The satellite point method refines the particle into smaller sub-particles and treats each individual sub-particle the same way as the PCM. It is more accurate than the PCM and allows for better performance for smaller Δx but suffers from the same disadvantages. As the number of particles increase, this method become much more computationally expensive than the PCM. The void fraction using the SPM is given by:

$$\varepsilon_f = 1 - \frac{\sum_i^{n_p} \sum_j^{n_{sp}} V_{sp}}{V_\Omega} \quad (2.76)$$

where n_{sp} and V_{sp} are the number and volume of sub-particles in each particle respectively. It is important to note that a void fraction projection method that is mass conservative, computationally efficient, and continuous in both time and space where it is well-posed in the limit where $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$ does not exist. The work done in this thesis allowed for the development of such projection scheme.

Particle-Fluid Interactions

The different hydrodynamic forces which result from the interactions between the solid and fluid phases are represented in what follows.

Drag force It is the resistance to the flow force that is experienced by a particle due to the fluid flow around it in steady state and it acts in the opposite direction of the flow.

$$F_D = \frac{1}{2} \rho_f C_D A_p |\mathbf{u} - \mathbf{v}| (\mathbf{u} - \mathbf{v}) \quad (2.77)$$

where $\mathbf{u}$ is the fluid velocity, $\mathbf{v}$ is the particle velocity, A_p is the particle's cross-sectional area, and C_D is the drag coefficient and is dependent on the Reynolds number, Mach number, the particle's Reynolds number ($Re_p = \rho_f d_p |\mathbf{u} - \mathbf{v}| / \mu_f$), the particle shape and orientation, turbulence, and evaporating droplets. Many correlations for the drag force exist where most of them are based on the Navier-Stokes equations [43].

Some of the correlations represented by Marchelli et al. [51] are listed for the following representation of the drag force:

$$F_D = m_p \frac{\mu_f}{\rho_p d_p^2} (\mathbf{u} - \mathbf{v}) D \quad (2.78)$$

where m_p is the particle's mass.

Wen-Yu drag model:

This model assumes the porosity coefficient to be constant with a value of -3.65 which is valid for small and large Reynolds numbers but not for intermediate ranges [51].

$$D = 18 \varepsilon_f^{-3.65} \left(1 + 0.15 (Re_p)^{0.687} \right) \quad (2.79)$$

Gidaspow drag model:

This is the most popular model for fluidized and spouted beds where it is a combination of the Wen-Yu and the Ergun models allowing to switch between them when the void fraction is lower than 0.8, thus it can work well in both dense and dilute regions [51]. Nonetheless, this model suffers from a discontinuity at $\varepsilon_f = 0.8$ where the models are switched. As such, its use should be avoided in fluidized and spouted beds where the void fraction of 0.8 exists.

$$D = \begin{cases} 18\varepsilon_f^{-3.65} \left(1 + 0.15 (Re_p)^{0.687}\right) & \text{for } \varepsilon_s \leq 0.2 \\ 150 \frac{\varepsilon_s}{\varepsilon_f^2} + 1.75 \frac{Re_p}{\varepsilon_f} & \text{for } \varepsilon_s > 0.2 \end{cases} \quad (2.80)$$

Di Felice drag model:

Di Felice showed that the coefficient of ε_f should not be constant but is a function of Re_p only and is represented by the coefficient β .

$$D = 0.75 C_D Re_p \varepsilon_f^{2-\beta} \quad (2.81)$$

where $C_D = \left(0.63 + \frac{4.8}{\sqrt{\varepsilon_f Re_p}}\right)^2$ is the drag coefficient proposed by Dallavalle and the coefficient of ε_f is:

$$\beta_{Di\ Felice} = 3.7 - 0.65 \exp\left(-\frac{(1.5 - \log_{10}(\varepsilon_f Re_p))^2}{2}\right) \quad (2.82)$$

Rong drag model:

This model is an enhancement of the Di Felice drag model where the only difference lies in the β coefficient. Through Lattice-Boltzmann simulations, it was shown that β is a function of the porosity as well as the particle's Reynolds number [51].

$$\beta_{Rong} = 2.65 (\varepsilon_f + 1) - (5.3 - 3.5\varepsilon_f) \varepsilon_f^2 \exp\left(-\frac{(1.5 - \log_{10}(\varepsilon_f Re_p))^2}{2}\right) \quad (2.83)$$

For $\varepsilon_f = 0.4$, Rong and Di Felice models produce the same results [51].

Beetstra drag model:

This model was developed through Lattice-Boltzmann simulations of fluid flows through arrays of spheres at several porosity values and Reynolds Numbers up to 1000 [51].

$$D = 18\varepsilon_f F_B \quad (2.84)$$

$$F_B = 10 \frac{\varepsilon_s}{\varepsilon_f^2} + \varepsilon_f^2 (1 + 1.5\sqrt{\varepsilon_s}) + \frac{\left(\frac{0.413Re_p}{24\varepsilon_f^2}\right) \left(\frac{1}{\varepsilon_f} + 3\varepsilon_f\varepsilon_s + 8.4Re_p^{-0.343}\right)}{1 + 10^{3\varepsilon_s}Re_p^{-0.5-2\varepsilon_s}} \quad (2.85)$$

Basset force This force is commonly known as the history term since it accounts for the viscous effects which depend on the historical acceleration of the particle in the unsteady state. The boundary layer surrounding the particle undergoes a temporal delay when the relative velocity changes with time. The model based on the integral of past particle acceleration is most common and is given by:

$$F_{Basset} = \frac{3}{2}d_p^2\sqrt{\pi\rho_f\mu_f} \left[\int_{t_0}^t \frac{(\mathbf{u} - \mathbf{v})}{\sqrt{t - t'}} dt' + \frac{(\mathbf{u} - \mathbf{v})_0}{\sqrt{t}} \right] \quad (2.86)$$

where the subscript $(\mathbf{u} - \mathbf{v})_0$ is the initial velocity difference, t' is the past time, and dt' is the time step between t and t' . This force is usually negligible in gaseous flows and when the acceleration of the particle is small [52].

Lift force Lift forces are generated by either particle rotation, velocity profile gradients, or shapes of the particles. Two different representations are often used to express lift forces. The first model assumes that lift and drag forces are proportional to each other:

$$F_L = \frac{1}{2}C_L\rho_f\mathbf{u}^2A_p \quad (2.87)$$

where C_L is the lift coefficient [43].

The second representation of the lift force separates it into Saffman type and Magnus type forces:

- **Saffman lift force:** This force occurs when a pressure distribution results from a gradient in the velocity across the particle surface where the highest velocity region corresponds to the lowest pressure and vice versa. As a result, a net lift force is generated on spheres and rotation may be induced for non spherical particles [43]. It is given by [52]:

$$\mathbf{f}_{Saff} = 1.61C_{Saff}d_p^2(\mu_f\rho_f)^{1/2}|\boldsymbol{\omega}_f|^{-1/2}[(\mathbf{u} - \mathbf{v}) \times \boldsymbol{\omega}_f] \quad (2.88)$$

where $\boldsymbol{\omega}_f$ is the vorticity of the fluid and

$$\boldsymbol{\omega}_f = \nabla \times \mathbf{u} \quad (2.89)$$

$$C_{Saff} = \begin{cases} \left(1 - 0.3314\alpha^{1/2}\right) \exp\left(\frac{-Re_p}{10}\right) + 0.3314\alpha^{1/2} & \text{for } Re_p \leq 40 \\ 0.0524(\alpha Re_p)^{1/2} & \text{for } Re_p > 40 \end{cases} \quad (2.90)$$

$$\alpha = \frac{d_p}{2|\mathbf{u} - \mathbf{v}|} |\boldsymbol{\omega}_f| \quad (2.91)$$

- **Magnus lift force:** This force is generated as a result of a pressure differential on the surface of the particle where particle rotation leads to a velocity gradient. It is a function of $\mathbf{u}$, $\mathbf{v}$, and ω_p , the angular velocity of the particle [43]. It is given by [52]:

$$\mathbf{f}_{Mag} = \frac{1}{2} \rho_f A_p C_{LR} |\mathbf{v} - \mathbf{u}| (\mathbf{v} - \mathbf{u}) \quad (2.92)$$

where the lift coefficient C_{LR} is given by Rubinow and Keller [53] as:

$$C_{LR} = \frac{d_p \omega_p}{|\mathbf{u} - \mathbf{v}|} \quad (2.93)$$

where ω_p is the particle's angular velocity.

Undistributed flow It includes forces generated due to pressure gradient ($F_{\nabla p}$) and shear stress ($F_{\nabla \cdot \boldsymbol{\tau}}$). Its presence is related to particles being subjected to gravity and acceleration in the fluid. Also, in fluidized beds, pressure drop is affected by particle-particle and particle-wall friction. The force is represented as [43]:

$$F_{ud} = F_{\nabla p} + F_{\nabla \cdot \boldsymbol{\tau}} \quad (2.94)$$

where

$$F_{\nabla p} = -V_p \left(\frac{\partial p}{\partial x} \right) = -\frac{1}{6} \pi d_p^3 \nabla p \quad (2.95)$$

and

$$F_{\nabla \cdot \boldsymbol{\tau}} = V_p \left(\frac{\partial \tau}{\partial x} \right) = -\frac{1}{6} \pi d_p^3 \nabla \cdot \boldsymbol{\tau} \quad (2.96)$$

Virtual mass force This force is exerted by the particle on a fluid with a smaller velocity than that of the particle. It is only considered in unsteady flows when the velocities of the particle and the fluid are not equal. Its general form is defined as [43]:

$$F_{vm} = \frac{\rho_f V_p}{2} \left(\frac{d\mathbf{u}}{dt} - \frac{d\mathbf{v}}{dt} \right) \quad (2.97)$$

Based on the following definition of the different forces, not all of them will be implemented in the model because only some are important for fluidized and spouted beds and they include: the drag force, the pressure, and the shear stress. The lift force is implemented to extend the gas fluidized and spouted beds to liquid fluidized and spouted beds as when the viscosity of the fluid increases, this force becomes important.

Current Limitations of Unresolved CFD-DEM

Unresolved CFD-DEM suffers from a range of limitations which greatly reduces its applicability. These limitations can be summarized by the following.

1. **Computational cost:** Since the trajectory of each particle is calculated at each time step, DEM is computationally expensive where systems larger than 10^8 particles can require weeks of simulation time on large computer clusters [39]. This mainly limits the size of the system that can be studied since the computational cost increases exponentially with the number of particles. This limitation is exacerbated in CFD-DEM where additional computational cost related to solving the VANS equations as well as coupling the CFD and DEM for each solid particle should be accounted for [43].
2. **Time step of integration:** The choice of the time step should be done to satisfy certain requirements for accurately capturing the collision dynamics. Thus, this choice is related to numerical error, stability of the explicit time integration scheme, the overall computational time, and contact mechanics where the time step should be chosen small enough so that the surface waves occurring during collision between two particles do not propagate further than the distance between their centers within a few time steps [39].

3. **Fluid-solid coupling step:** The stability of this step is related to the relaxation time of the particle. This step represents the effect of the fluid on the the DEM equations which describe the movement of individual particles. This stability requirement reduces to the particle relaxation time in the case of a single isolated particle in the limit of Stokes flow [54].
4. **Projection onto the mesh:** When projecting a particle onto the CFD mesh, it is important that the void fraction and momentum terms are continuously differentiable in space and time [39]. Unresolved CFD-DEM requires that the flow field be divided into cells (elements) which should be larger than the particle size (usually the element size is limited to a minimum of three times the particle diameter). As the mesh size decreases, the projection of the particle onto the mesh becomes a large source of error and numerical instability. This is problematic for turbulent flows, which require fine meshes, or for geometries with narrow regions and with complex flow physics [3] such as the spout region in a spouted bed.
5. **Surface properties and shape parameters:** Some parameters such as the density, Young's modulus, and Poisson ratio are based on material properties. Other parameters such the coefficients of sliding and rolling friction and the coefficient of restitution depend on surface properties such as roughness and on the shape of the particle. Such parameters have to be calibrated for each type of solid used as well as for each flow configuration. This affects the results of the CFD-DEM simulations to a certain extent [43].
6. **Shape of the particles:** Regular DEM usually considers spherical solid particles; however, there exists a large number of applications where different shapes of particles are used. Even though several extensions have been proposed to account for the non-sphericity of the particles, none has been able to achieve adequate results so far [39]. Some examples include the non-spherical particulate systems (NSPS) [55] and the use of super-quadric equation which allow the description of particles with concave and convex shapes [56].
7. **Turbulence modelling:** Simulations using steady CFD-DEM modelling is not logical since they do not reflect actual flow regimes where commonly turbulence exists. Therefore, the employment of turbulence methods such as unsteady Reynolds Averaged Navier-Stokes (URANS), direct numerical simulations (DNS), or large eddy simulations (LES) becomes important for reaching more realistic solutions [43].

In the context of this thesis, the following limitations of unresolved CFD-DEM will be tackled: computational cost through the implementation of a unified CFD-DEM architecture which support parallelization and load balancing, turbulence modelling through the use of ILES by stabilization techniques and high-order schemes, surface properties by studying the effect of such properties on fluidization regimes, and the projection onto the mesh through the development of a new space and time continuous void fraction scheme and the use of high-order schemes.

High-order methods have the potential of achieving higher accuracy for coarser meshes while being more cost efficient than lower order methods [57]. Furthermore, these methods are highly appropriate for large eddy simulation (LES), which can accurately predict the behavior of the larger eddies that occur in turbulent flows. However, high-order methods are not available in any commercial software and, so far, their use has been limited to the aerospace industry. Consequently, their great potential for the simulation of solid-gas and solid-liquid flows through CFD-DEM remains untapped.

2.6 Advances of Fluidized and Spouted Beds

Throughout the years, there have been several advances in the field of solid-fluid fluidization. Both experiments and modelling have been crucial for better understanding the underlying phenomena governing the behavior of fluidized and spouted beds.

Experimental investigation have played an important role in understanding the intricate dynamics and behaviors exhibited by fluidized and spouted beds. Numerous researchers have performed experiments to characterize the hydrodynamics, heat and mass transfer, and particle behavior within these multiphase systems. In a notable study by Li et al. [58], a turbulent fluidized bed was employed and was studied using a Laser Doppler Velocimetry (LDV) to investigate the effect of operating conditions, such as the superficial gas velocity, initial bed height, and particles sizes on the particle velocity and annular film thickness. Their experimental results provided valuable insights into the effect of particle size distribution on the bed behavior and led to the development of a correlation for the estimation of the annular film thickness. Furthermore, several researchers have used advanced non-invasive measurement techniques, such as particle image velocimetry (PIV) and laser induced fluorescence (LIF), to capture the complex flow structures and particle dynamics within fluidized and spouted beds. Among these, Laverman et al. [59] coupled PIV with a Digital Image Analysis (DIA) technique to estimate the solid circulation patterns and bubble properties with high spatial and temporal resolution. Tsuji et al. [60] investigated heat transfer in a gas fluidized bed using a combination of PIV and infrared thermography (IRT). These experimental studies have

been crucial in validating and refining the numerical models, as well as advancing the understanding of fluidized and spouted bed systems, leading to improved design and operational strategies for industrial applications.

Similarly, simulations have played a crucial role in the study and analysis of fluidized and spouted beds, providing valuable insights into their complex behavior and improving their design and operational efficiency. Over the years, various numerical and computational fluid dynamics (CFD) models have been developed to simulate these multiphase systems. Gao et al. [61] validated a three-dimensional Eulerian-Eulerian model, investigated the hydrodynamics of a gas fluidized beds, and compared the gas and solid residence time where it was found that the solid mean residence time is much longer than that of the gas. Different applications of fluidized beds were studied using CFD-DEM such as biomass gasification in fluidized bed reactors [62], segregation and dispersion of solids in liquid fluidized beds [63], heat transfer modelling in gas-solid fluidized beds [64], heat transfer modelling in fluidized beds with an immersed probe [65], fluid catalytic cracking of gas-solid reacting flows [66] and tube erosion in fluidized beds [67]. Large scale simulations of fluidized granular systems were also performed using the Compute Unified Device Architecture (CUDA) technology which is able to perform massively-parallel DEM simulations on a single Graphic Processing Unit (GPU) [68]. Additionally, several researchers have explored the use of advanced turbulence models, such as large eddy simulation (LES), to capture the intricate flow characteristics within fluidized and spouted beds. For instance, Gupta et al. [69] employed a LES-based approach to investigate the transient flow characteristics of gas-solid flows in a bubbling fluidized bed for the gasification of rice husk. Compared to fluidized beds, studies on spouted beds are discussed to a lesser extent in the literature. One interesting study conducted the modelling of the hydrodynamics of a lab-scale double slot rectangular spouted bed with a partition plate using parallel CFD-DEM. The MFIX DEM codes were used in the coupling approach of CFD-DEM. In order to increase the load balance of CPUs in the parallel computations, the authors developed a uniform domain decomposition strategy and coupled it into the MFIX-DEM code [70]. Other CFD-DEM studies on spouted beds include the simulation of gas solid turbulent flow in a cylindrical spouted bed with a canonical base [71] and the modelling of circulation frequencies and residence times in prismatic spouted beds [72].

Overall, these studies demonstrate the importance of both experiments and simulations in understanding the complex phenomena occurring in fluidized and spouted beds, thus facilitating their optimization and the development of operational strategies for these multiphase systems.

CHAPTER 3 THESIS OBJECTIVES AND ORGANIZATION

In this chapter, the literature review will be examined to identify existing gaps and to determine the unexploited regions in the state of the art of solid-gas fluidization. Then, the objectives of the research performed in this thesis are introduced followed by a section detailing the organization of the different chapters which is guided by the research objectives.

3.1 Gaps in the Literature

Several important gaps in solid-gas multiphase flows exist in the literature. Among these, most are related to the CFD side. For example, the choice of the VANS model to be used is rarely discussed in CFD-DEM articles where usually there is no mention of the model at all. Despite the fact that the literature introduce both models A and B in dedicated papers such as the article by Zhou et al. [44], a complete discussion on their instantaneous and averaged physical behaviors, as well as their computational robustness, stability, and efficiency has not been fully and completely addressed. Specifically, in the context of the finite element method, no prior detailed representation of the weak form of the models as well as their stabilization techniques have been done. An article by Srivastava et al. [73] previously derived the weak form of model A but their derivation was incomplete as the weak form of the pressure formulation lacked a term which rendered the model mathematically incorrect. Also, the finite element stabilization techniques allow to implicitly apply LES to model turbulence. This has been discussed by Adams and Hickel [37].

Moreover, high-order methods have not been used in CFD-DEM mainly because they lack the robustness of lower order methods and they require more computational power. Nonetheless, unresolved CFD-DEM is known to suffer from the limitation of particle to cell size ratio, where mesh cells cannot be smaller than three times the particle diameter [3]. This is a limitation inherent to unresolved CFD-DEM where when this size ratio is not respected, many particle projection schemes become inaccurate and result in large errors of the void fraction. Sometimes, a better accuracy is required in resolving the fluid which is not possible in current unresolved CFD-DEM. High-order methods can be an attractive solution that allows to obtain better accuracy on the fluid side without refining the mesh by simply increasing the order of the interpolation polynomials.

Furthermore, all CFD-DEM solvers in the literature are often parallelized separately and then coupled together using a coupling inter-phase. This causes a bottleneck in the transfer

of information between the CFD and DEM processors. As such, improved speeds due to parallelization are reduced because of this coupling. In addition, some of these software support load balancing which distributes the work loads evenly among processors; however the coupling inter-phase usually does not support this feature which further reduces the possibility of speedup.

Additionally, most if not all available software sets the first term of the continuity equation to zero when solving the VANS equations because the time derivative of the void fraction is unstable. This is due to the projection schemes of the void fraction which are not continuous in time and can lead to the explosion of this term as the time step tends to zero. Several analytical void fraction schemes exist that can remedy this issue [74–77]; however they are computationally unfeasible or extremely expensive for large systems. This limits their applicability for industrial scale problems.

Concerning DEM limitations, the surface properties of particles and walls such as the coefficients of rolling and sliding friction as well as the coefficient of restitution are often taken to be those calibrated in dry conditions. This works in solid-gas flows; however, when the fluid is no longer a gas, these properties change and should be re-calibrated as they affect the results and prediction accuracy of the CFD-DEM model. A complete discussion about the dependency of such parameters on the fluid choice has not been presented in the context of unresolved CFD-DEM.

3.2 Research Objectives

The main objective of this thesis is the development of a robust high-order unresolved CFD-DEM model that is capable of simulating the dynamics of fluidized and spouted bed.

This objective is divided into several sub-objectives, each contributing to the overall achievement of the main objective. These sub-objectives are defined below.

1. Develop a stabilized finite element model for the solution of the VANS equations. The applied stabilization techniques include PSPG/SUPG stabilization which allows to implement ILES.
2. Create a procedure using the method of manufactured solutions to verify the mathematical implementation of the solver through three different test cases. The validation of the solver is afterwards implemented through comparison with an empirical correlation for pressure drop.
3. Develop a high-order parallelized unresolved CFD-DEM solver for the prediction of

solid-gas flows where the high-order VANS solver is coupled with the DEM solver.

4. Improve the speed of the coupled solver through unified load balancing strategies between the CFD and DEM.
5. Validate the unresolved CFD-DEM solver through various test cases which include comparison with empirical correlations as well as experimental data.
6. Develop a void fraction projection (particle projection) scheme that is mass conservative, computationally efficient, and continuous in both space and time to improve the stability of the solver and the accuracy of the results obtained.
7. Investigate the surface properties of particles through experiments of a rotating drum with various fluid viscosities.

3.3 Organization of the Thesis

The subsequent chapters of this thesis aim at attaining the objectives mentioned in section 3.2. They are discussed in the order in which they were achieved. Chapter 4 discusses the methodology undertaken in this work. It introduces the open-source software Lethe which is the framework in which the totality of the work has been performed. Additionally, the verification and validation strategy of the developed numerical model is discussed.

Chapter 5 (Article 1) introduces the finite element discretization of models A and B of the VANS equations along with the stabilization techniques implemented in this work. The verification of the model is carried out using the method of manufactured solutions (MMS) where different orders of convergence are proven to be achievable using the proposed formulation. Finally, the validation of the model is performed using a packed bed test where the pressure drop in the bed for different drag models and finite element orders is compared against the empirical Ergun correlation.

In Chapter 6 (Article 2), the coupling between the developed VANS solver and the DEM solver is implemented. Load balancing for improved parallelization of the coupled CFD-DEM solver is applied and a strong scaling study is carried out to determine the speedup capabilities of the solver. The new model is validated using several test cases which include the sedimentation of a single particle, the fluidization of particles, the Rayleigh-Taylor instability, and the spouting of particles.

Chapter 7 (Article 3) aims at developing a new analytical void fraction scheme in an attempt to remedy some of the limitations of unresolved CFD-DEM, specifically, the continuity and

computational cost of the projection scheme and the coupling of the averaging volume and the mesh elements. The scheme is normalized to ensure proper mass conservation and is validated using a particle's sedimentation case, a Boycott effect case, and a flat fluidized bed case.

Chapter 8 (Article 4) introduces a simple and time efficient gas-solid and liquid-solid rotary kiln benchmark for the purpose of creating a validation case for unresolved CFD-DEM software. It gives insight on the importance of proper calibration of DEM surface properties in solid-liquid flows as well as on the importance of the lift force.

Appendix C represents an article in which the author of this thesis is the second author. It is written mainly by Victor Oliveira Ferreira as part of his PhD. It aims at extending the existing solid-gas CFD-DEM solver developed in Chapter 6 to solid-liquid simulations through the addition of the lift force which becomes no longer negligible. The in-depth validation of liquid fluidized bed simulations is done using a collection of experimental data.

CHAPTER 4 METHODOLOGY

This section introduces the methodology used for the achievement of this work. Since the specific methodology of each chapter is detailed within the corresponding chapter itself, it will not be introduced in this section. The open source software Lethe which is used to achieve the majority of the work in this thesis is introduced detailing its functionalities and specifications. Additionally, the process of verification and validation used is discussed. Finally, the post-processing of data is also briefly introduced.

4.1 Lethe

Lethe is an open-source CFD, DEM, and CFD-DEM software which uses high-order continuous Galerkin formulation to solve the incompressible Navier-Stokes equations as well as other governing equations (e.g. VANS). It is mainly written in object-oriented C++ and is based on the differential equations analysis library (deal.II) [78] which is a C++ library for the computational solution of partial differential equations using adaptive finite elements. Lethe uses Trilinos [79] for its sparse linear algebra routines and p4est [80] for its distributed adaptative quadrees and octrees. It is entirely hosted on github and available through the following link: <https://github.com/lethe-cfd/lethe>.

4.1.1 Lethe-CFD

Lethe-CFD employs the finite element method to discretize and solve problems involving continuous phases. It is generally intended for fluid mechanics problems. It mainly uses structured meshes (tensor elements), while some of its solvers supports simplex meshes (tetrahedral elements) as well. It assembles and solves the governing equations using the monolithic approach discussed in section 2.3.2 where the pressure and velocity fields are solved simultaneously. Lethe is fully parallelized and supports dynamic load balancing through deal.II [78]. It uses PSPG/SUPG or GLS stabilization to stabilize the finite element formulation and to model turbulence through implicit LES. The stability of the CFD solver is independent of the Courant–Friedrichs–Lewy (CFL) number as our solver is monolithic. The time-stepping schemes of various orders supported in Lethe are the backward difference (BDF) and the singly-diagonal implicit Runge-Kutta methods (SDIRK). The linear solvers supported are a direct solver and several iterative solvers: a biconjugate gradient stabilized solver (BICGSTAB), a generalized minimal residual solver (GMRES) with incomplete lower

upper (ILU) preconditioning, and an algebraic multigrid solver (AMG) with ILU preconditioning. The non-linear solver supported in Lethe uses the Newton-Raphson method with a line-search strategy.

4.1.2 Lethe-DEM

Lethe-DEM employs the discrete element method to track the position and velocity of solid particles. It enables the user to specify the surface and physical properties of the particles and walls and allows for particles' size distribution. Particle contact detection can be done in one of two options: constant or dynamic. In constant contact detection, contact search occurs at a specific frequency where the contact frequency is chosen such that the particles do not travel more than half a cell between two contact detection steps. In dynamic contact detection, the contact search occurs if the maximum displacement of a particle exceeds the smallest contact search criterion defined as the minimum of the smallest cell size in the triangulation or the radius of the spherical region in fine search. Lethe-DEM supports a linear particle-particle contact model and three non-linear particle-particle contact models: Hertz, Hertz Mindlin limit overlap, and Hertz Mindlin limit force. It also supports one linear particle-wall contact model and one non-linear particle-wall contact model. Two integration methods are available in Lethe for the integration of Newton's equations: the Euler integration scheme which is first order accurate and the Verlet integration scheme which is second order accurate. Finally, two rolling resistance models for particles' angular velocity are implemented in Lethe-DEM. They are constant resistance and viscous resistance. The rolling resistance can also be removed completely.

4.1.3 Lethe-CFD and Lethe-DEM Coupling

It is a solver with a unified architecture which inherits from the VANS solver and incorporates in its fluid solving steps, a DEM iterator where multiple DEM iterations occur for each CFD iteration depending on a coupling frequency specified by the user. As such, both the CFD and the DEM iterations occur on the same mesh and processors, thus improving computational efficiency and information propagation between both solvers. Due to the unified architecture, the coupling solver allows the calculation of the void fraction without the need to obtain particles' information from the DEM solver separately. Additionally, particle-fluid interactions are calculated and stored at the same time for both the fluid and the solid phases without necessitating the information to be sent to the DEM solver separately.

4.2 Verification and Validation Strategy

The development of any complex numerical model necessitates a rigorous procedure of verification and validation to ensure that the model and its results are correct for its use. Verification is defined as ensuring that the computer program of the model and its implementation is correct whereas validation is defined as possessing a satisfactory range of accuracy consistent with the intended application of the model [81]. The methods applied in this thesis follow the model development process shown in Figure 4.1 which summarizes the steps to be implemented for producing a reliable model.

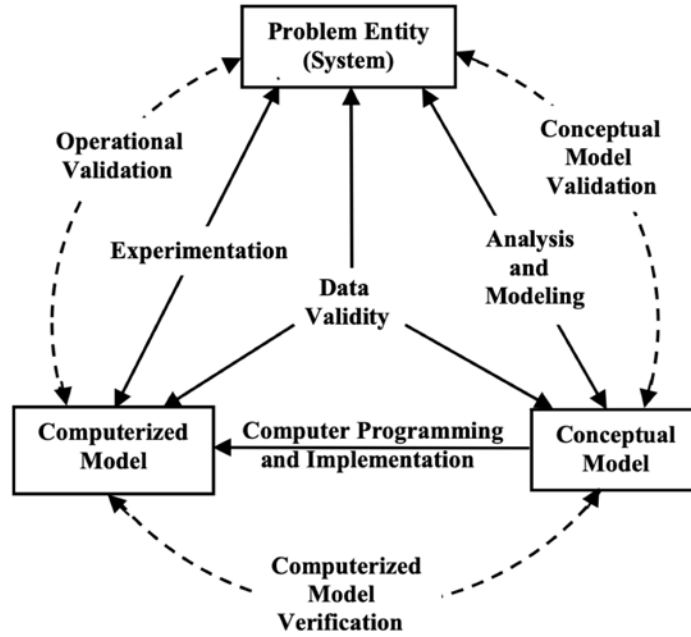


Figure 4.1 The model development process [81].

The problem entity represents the system to be modelled, that is a fluidized or spouted bed representing a multiphase system; the conceptual model represents the mathematical representation of the multiphase system such as the governing equations (e.g. VANS); and the computerized model represents the implementation of the conceptual model on a computer such as the unresolved CFD-DEM solver within Lethe [81].

In general, the verification and validation procedures are performed gradually and progressively as no analytical solution exist for the coupled unresolved CFD-DEM solver which makes the verification of such coupling non-trivial. The verification of the VANS solver is achieved primarily through the use of the method of manufactured solutions (MMS). It entails developing an analytical solution that is infinitely differentiable for a purely mathematical

case and using this case for the verification of the accuracy and order of convergence of the solver. A Python script is used to create the analytical test cases. The VANS solver is later validated using a packed bed simulation. The CFD-DEM solver is verified using a particle sedimentation test case where an analytical solution can be conceived for the sedimenting particle's velocity and position and compared with the solver's results. The model is then validated by comparing its results to empirical correlations and experimental results.

4.3 Post-processing

Visualization of the simulation results has been carried out using the open-source software Paraview which is a multiple-platform application for interactive, scientific visualization. Lethe outputs its results in files with vtu extension which can be easily visualized in Paraview. Quantitative data from the simulations were extracted using PyVista which is a 3D visualization and mesh analysis tool in Python. The extracted data were then used to create plots. The plots in this thesis have been created using the Matplotlib library available within Python.

CHAPTER 5 ARTICLE 1 : A HIGH-ORDER STABILIZED SOLVER FOR THE VOLUME AVERAGED NAVIER-STOKES EQUATIONS

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Declaration: The author of this thesis has contributed to the literature review, code development, simulation and modelling, analysis of the results and the writing of the article.

Abstract: The Volume-Averaged Navier-Stokes equations are used to study fluid flow in the presence of fixed or moving solids such as packed or fluidized beds. We develop a high-order finite element solver using both forms A and B of these equations. We introduce tailored stabilization techniques to prevent oscillations in regions of sharp gradients, to relax the Ladyzhenskaya-Babuska-Brezzi inf-sup condition, and to enhance the local mass conservation and the robustness of the formulation. We calculate the void fraction using the Particle Centroid Method. Using different drag models, we calculate the drag force exerted by the solids on the fluid. We implement the method of manufactured solutions to verify our solver. We demonstrate that the model preserves the order of convergence of the underlying finite element discretization. Finally, we simulate gas flow through a randomly packed bed and study the pressure drop and mass conservation properties to validate our model.

5.1 Introduction

Multi-phase flows are systems with two or more distinct phases flowing simultaneously within a mixture. Their classification depends on the combination of phases involved: solid-gas, solid-liquid, immiscible liquid-liquid, or liquid-gas flows [1]. Solid-gas flows play a key role in the dynamics of fluidized and packed bed reactors, spouted beds, pneumatic conveyors and other technological applications. For the solid-fluid flows in most chemical engineering processes, it is well known that the phenomena that occur at the particle scale greatly influence the macroscopic behavior of the process [5]. Generally, the design and scale-up of these beds are based on expensive and time-consuming pilot-scale tests. Therefore, modeling has become an important topic for researchers due to its contribution to our understanding of the processes involved as well as its predictive capabilities of solid-fluid flows in engineering-scale equipment. It has numerous advantages such as allowing the understanding of various phenomena occurring in processes, enabling sensitivity analysis on different input parameters,

and testing several configurations and operational conditions at a much cheaper cost than experimental work [3, 82]. In order to study such systems, the volume-averaged Navier Stokes (VANS) equations are used as they ensure that the volume of fluid that can occupy a cell and the volume of solids occupying it respect the continuity equation, thus ensuring mass conservation. Since in CFD-DEM, the fluid is modeled at a scale larger than that of the particles (mesoscopic), the governing equations for the fluid phase (VANS) are obtained based on local averaging methods as in the Two Fluid Model (TFM) [83].

Mainly, there exist two forms of the VANS equations: Model A (Set II) and Model B (Set I) [44, 46]. Model A is derived from Model B by decomposing the particle-fluid interactions into two components: a component accounting for the macroscopic variations in the fluid stress tensor on a large scale, and another component accounting for the variations in the point stress tensor when the fluid passes around particles [44]. It is the most widely used set of equations as it is implemented in several commercial software such as FLUENT and CFX [44]. Gidaspow derived a Model C which replaces the solid velocity in Model B with the relative velocity. According to Gidaspow [46], in order to be invariant under a change of frame of reference, entropy production should be a function of relative velocity and not of individual phase velocities. Zhou et al. [44] simplified Model B (Set I) under the assumption $\rho_f(1 - \varepsilon_f)[\frac{\partial \mathbf{u}_f}{\partial t} + \nabla \cdot (\mathbf{u}_f \mathbf{u}_f)] = 0$ in order to obtain Set III. The main difference between these models is that the solid-fluid interaction forces in Set I are explicit while in Set III, they are implicit. However, Set III is not general but conditional as it is only valid when the assumption is satisfied [3]. This assumption does not hold for numerous solid-fluid flows of interest and, as such, this model should not be considered.

Many numerical methods exist for solving these equations, but the majority of solvers for the VANS equation use the Finite Volume Method (FVM) [27] or the Lattice Boltzmann Method (LBM) [84, 85]. However, the Finite Element Method (FEM) is an attractive candidate to solve these equations because of its inherent capacity for higher order formulations. It is considered a generalization of the classical variational (the Ritz) and weighted-residual (such as weak-form Galerkin Least Square (GLS), etc.) methods.

High-order formulations are methods possessing an order of accuracy greater than two [29]. When the error in the solution e obtained with a method decreases with the size of the mesh h such that $e \propto h^{k+1}$, then the method's error is said to be of order $k+1$. The use of low order methods is usually prevalent in simulations due to them being robust. Even though high-order methods can achieve higher accuracy for the same computational cost, they are less used due to their complexity and because they are often considered less robust [86]. Steady-state convergence is more difficult and challenging to reach with high-order simulation, and

for worse cases, the solution may even diverge [29]. However, high-order methods have shown promise in efficiently solving problems with a requirement for high accuracy such as vortex dominated flows, numerical simulation of turbulence, and large-eddy simulations [29,87]. The advantage of these methods is their relatively small error [88].

In this paper, we build a high-order FEM stabilized VANS solver as a first step in realizing a coupled CFD-DEM solver within the open-source software Lethe [89]. We present a fully implicit finite element VANS solver. Thus, it does not require any stability condition. Moreover, the formulation we introduce is well posed in the presence of smooth void fraction or by using void fraction smoothing and it is globally mass conservative as it accounts for the time variation of the void fraction in the continuity equation. The order of our solver is arbitrary and we prove that it can support a large scale of high-order methods. In our solver, we calculate the void fraction in each cell using the Particle Centroid Method (PCM), then we project it onto the FEM mesh. When desired, we apply a smoothing factor to resolve the oscillations arising from the discontinuous void fraction and a primal-dual active set method to bound the void fraction. We use the continuity equation as the basis of the grad-div stabilization in order to improve local mass conservation. Using two different drag models, we calculate the drag force on individual particles which contributes to the particle-fluid interactions in the VANS equations. Through the method of manufactured solutions (MMS), we verify the solver by analyzing the order of convergence in space and time. Finally, we simulate a packed bed and study the pressure drop across the bed. We compare the results with the pressure drop obtained from the Ergun equation in order to validate our model.

5.2 Governing Equations

As forms A and B of the VANS equations are the most commonly known models, we represent them in Eqs. (5.1), (5.2) and (5.3). The conservative form of the continuity equation for an incompressible fluid remains the same for both models:

$$\rho_f \frac{\partial(\varepsilon_f)}{\partial t} + \rho_f \nabla \cdot (\varepsilon_f \mathbf{u}) = m' \quad (5.1)$$

where ρ_f is the fluid density, which is assumed to be constant, $\mathbf{u}$ is the fluid velocity, ε_f is the fluid's void fraction, and m' is the volumetric source of mass [46]. The difference between the two models lies in the formulation of the momentum equations. The conservative form of Model A of the incompressible VANS equations is defined as:

$$\rho_f \left(\frac{\partial(\varepsilon_f \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) = -\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf} + \rho_f \varepsilon_f \mathbf{f} \quad (5.2)$$

The conservative form of Model B of the incompressible VANS equations is:

$$\rho_f \left(\frac{\partial (\varepsilon_f \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) = -\nabla p + \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf} + \rho_f \varepsilon_f \mathbf{f} \quad (5.3)$$

with

$$\boldsymbol{\tau}_f = \nu \left((\nabla \mathbf{u}) + (\nabla \mathbf{u})^T \right) - \frac{2}{3} \nu \nabla \cdot \mathbf{u} \mathbf{I} \quad (5.4)$$

where p is the pressure, $\boldsymbol{\tau}_f$ the deviatoric stress tensor, $\nu = \frac{\mu_f}{\rho}$ the kinematic viscosity, $\mathbf{f}$ the external force(ex. gravity), and $\mathbf{F}_{pf}$ is the momentum transfer term between the solid and fluid phases and includes forces such as drag, virtual mass, Basset force, Saffman lift, and Magnus lift [90]. $\mathbf{I}$ is the identity or unit matrix. In the case of incompressible fluid, $\nabla \cdot \boldsymbol{\tau} = \nu (\nabla^2 \mathbf{u})$ in Eq. (5.4).

Each form leads to a different pressure equation. In Form A, ε_f is taken into account on the continuous equation and alters the saddle point problem for the pressure since ε_f multiplies the pressure gradient directly while in form B, ε_f is lumped with the momentum coupling term [43]. Both models are mathematically equivalent and differ in the way they implement incompressibility. Form B of the equations achieves a realistic representation of the system where the total pressure drop occurs in the fluid phase and no pressure drop occurs in the solid phase. This is not true for the other model [46]. This is because Form B uses pressure at previous times to calculate subsequent pressure values. Also, Form B possesses all real characteristics rendering the model well-posed as described by Gidaspow [46]. On the other hand, and according to Bouillard et al. [45], Form A of the VANS equations represents an ill-posed initial value problem that possesses complex characteristics which make this model conditionally stable. We solved both Form A and Form B of the VANS equations and compared the results obtained from both models.

In order to obtain the weak form of the VANS equations, we determine its non-conservative form. Using the incompressibility constraint, we simplify our problem even further as the density becomes constant.

$$\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot \varepsilon_f \mathbf{u} = \frac{m'}{\rho_f} \quad (5.5)$$

Form B:

$$\begin{aligned} \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \left(\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot \varepsilon_f \mathbf{u} \right) = \\ \frac{1}{\rho_f} \left(-\nabla p + \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf} \right) + \varepsilon_f \mathbf{f} \end{aligned} \quad (5.6)$$

Form A:

$$\begin{aligned} \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \left(\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot \varepsilon_f \mathbf{u} \right) = \\ \frac{1}{\rho_f} \left(-\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf} \right) + \varepsilon_f \mathbf{f} \end{aligned} \quad (5.7)$$

Since the continuity equation is used along with the momentum equation to solve the fluid flow, the left hand side term in brackets of Eqs. (5.6) and (5.7), which represents the continuity equation can be replaced by the mass source term. We also expand the term $(\nabla \cdot \varepsilon_f \mathbf{u})$.

$$\frac{\partial \varepsilon_f}{\partial t} + \varepsilon_f \nabla \cdot \mathbf{u} + \mathbf{u} \nabla \varepsilon_f = \frac{m'}{\rho_f} \quad (5.8)$$

Form B:

$$\begin{aligned} \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \underbrace{\left(\frac{\partial \varepsilon_f}{\partial t} + \varepsilon_f \nabla \cdot \mathbf{u} + \mathbf{u} \nabla \varepsilon_f \right)}_{m'} = \\ \frac{1}{\rho_f} \left(-\nabla p + \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf} \right) + \varepsilon_f \mathbf{f} \end{aligned} \quad (5.9)$$

Form A:

$$\begin{aligned} \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \underbrace{\left(\frac{\partial \varepsilon_f}{\partial t} + \varepsilon_f \nabla \cdot \mathbf{u} + \mathbf{u} \nabla \varepsilon_f \right)}_{m'} = \\ \frac{1}{\rho_f} \left(-\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf} \right) + \varepsilon_f \mathbf{f} \end{aligned} \quad (5.10)$$

The equations were solved by the finite element method using stabilization techniques which allows to circumvent the limitations of the classical Galerkin approach and satisfies the Ladyzhenskaya–Babuska–Brezzi (LBB) inf–sup condition. For a more detailed explanation, we refer the reader to the Lethe paper [89,91].

5.3 Finite Element Formulation for the VANS Equations

We implement a stabilized formulation in order to solve the VANS equations. Two stabilizing terms, streamline-upwind/Petrov-Galerkin (SUPG) and pressure-stabilizing/Petrov-Galerkin (PSPG) were added. PSPG helps relax the LBB condition and allows the use of equal order elements while the SUPG term stabilizes unresolved boundary layers [89]. The grad-div stabilization was added to ensure local mass conservation.

5.3.1 The Stabilized Formulation

The detailed weak form of the VANS equations can be expressed by setting $\nabla \cdot \boldsymbol{\tau} = \nu (\nabla^2 \mathbf{u})$.

$$\int_{\Omega} \left(\frac{\partial(\varepsilon_f)}{\partial t} + \varepsilon_f \nabla \cdot \mathbf{u} + \mathbf{u} \nabla \varepsilon_f \right) q d\Omega + \sum_K \int_{\Omega_K} \mathcal{SR} \cdot (\tau_u \nabla q) d\Omega_k = 0 \quad (5.11)$$

Form B:

$$\begin{aligned} & \int_{\Omega} \left(\varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} \right) \cdot \mathbf{v} d\Omega + \frac{1}{\rho_f} \left(\int_{\Omega} \nu (\nabla \mathbf{u}) \nabla \mathbf{v} d\Omega + \int_{\Omega} m' \mathbf{u} \cdot \mathbf{v} d\Omega \right. \\ & \left. - \int_{\Omega} p \nabla \cdot \mathbf{v} d\Omega + \int_{\Omega} \frac{\mathbf{F}_{pf}}{V_{\Omega}} \cdot \mathbf{v} d\Omega \right) - \int_{\Omega} \varepsilon_f \mathbf{f} \cdot \mathbf{v} d\Omega + \sum_K \int_{\Omega_K} \mathcal{SR} \cdot (\tau_u \mathbf{u} \cdot \nabla \mathbf{v}) d\Omega_k = 0 \end{aligned} \quad (5.12)$$

and

$$\mathcal{SR} = \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \nabla \cdot \mathbf{u} + \frac{1}{\rho_f} \left(m' \mathbf{u} + \nabla p - \nu (\nabla^2 \mathbf{u}) + \frac{\mathbf{F}_{pf}}{V_{\Omega}} \right) - \varepsilon_f \mathbf{f} \quad (5.13)$$

Form A:

$$\begin{aligned} & \int_{\Omega} \left(\varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} \right) \cdot \mathbf{v} d\Omega + \frac{1}{\rho_f} \left(\int_{\Omega} \left(\varepsilon_f \nu (\nabla^2 \mathbf{u}) + \nu \nabla \mathbf{u} \nabla \varepsilon_f \right) \cdot \mathbf{v} d\Omega + \right. \\ & \left. \int_{\Omega} m' \mathbf{u} \cdot \mathbf{v} d\Omega - \int_{\Omega} \left(\varepsilon_f p \cdot \nabla \mathbf{v} + p \nabla \varepsilon_f \cdot \mathbf{v} \right) d\Omega + \int_{\Omega} \frac{\mathbf{F}_{pf}}{V_{\Omega}} \cdot \mathbf{v} d\Omega \right) - \\ & \int_{\Omega} \varepsilon_f \mathbf{f} \cdot \mathbf{v} d\Omega + \sum_K \int_{\Omega_K} \mathcal{SR} \cdot (\tau_u \mathbf{u} \cdot \nabla \mathbf{v}) d\Omega_k = 0 \end{aligned} \quad (5.14)$$

and

$$\mathcal{SR} = \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \nabla \cdot \mathbf{u} + \frac{1}{\rho_f} \left(m' \mathbf{u} + \varepsilon_f \nabla p - \varepsilon_f \nu (\nabla^2 \mathbf{u}) + \frac{\mathbf{F}_{pf}}{V_\Omega} \right) - \varepsilon_f \mathbf{f} \quad (5.15)$$

and $\mathcal{SR}$ is the strong residual associated with the PSPG and SUPG stabilizations. $\mathbf{q}$ and $\mathbf{v}$ are the test functions of the finite element method. V_Ω is the volume of the domain Ω . The stabilization parameter τ_u is defined by Tezduyar [91] and is explained in detail in the Lethe paper [89]. Two forms of τ_u were implemented depending on whether the equations solved are stationary or time dependent. For transient simulations, τ_u is defined as:

$$\tau_u = \left[\left(\frac{1}{\Delta t} \right)^2 + \left(\frac{2|\mathbf{u}|}{h_{conv}} \right)^2 + 9 \left(\frac{4\nu}{h_{diff}^2} \right)^2 \right]^{-1/2} \quad (5.16)$$

while for stationary problems, τ_u is:

$$\tau_u = \left[\left(\frac{2|\mathbf{u}|}{h_{conv}} \right)^2 + 9 \left(\frac{4\nu}{h_{diff}^2} \right)^2 \right]^{-1/2} \quad (5.17)$$

where Δt is the time step, h_{conv} and h_{diff} are the size of the element related to the convection transport and diffusion mechanism respectively [89].

The weak form of Model A has been derived in another work [73]. However, the derivation is incomplete as the weak form of the pressure formulation lacks a term. The weak form of the pressure term is defined as:

$$\int_\Omega (\varepsilon_f \nabla p) \cdot \mathbf{v} d\Omega = \int_\Omega (\varepsilon_f p \cdot \nabla \mathbf{v} + p \nabla \varepsilon_f \cdot \mathbf{v}) d\Omega \quad (5.18)$$

The second term on the right hand side is missing in the weak form of Srivastava et al. [73]. Even though this term does not appear to have any physical meaning, its presence is important to make the equation mathematically correct and equivalent to that of Model B as well as to obtain the correct pressure drop in coupled simulations.

5.3.2 Grad-div Stabilization

In order to improve mass conservation in incompressible flow simulations and to stabilize our system at higher Re values, we apply grad-div stabilization to the VANS equations similarly to how it was applied to the Navier Stokes equations in Lethe [89]. However, the void fraction should be accounted for when considering the VANS equations. The resulting stabilization

term added to the weak form of the VANS momentum equation is expressed as:

$$\sum_K \int_{\Omega_k} \gamma \left(\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}) \right) (\nabla \cdot \mathbf{v}) d\Omega_k \quad (5.19)$$

where γ is a parameter related to the augmented Lagrangian formulation [89]. This γ parameter is defined differently by multiple authors in the literature. We chose to implement the formulation derived by Olshanskii et al. [92] where $\gamma = \nu + \mathbf{u}h$ m^2/s where h is the size of the element. The system we are solving is generally stiff and higher Re values make it more difficult to solve. A constant value of γ was initially used where we noticed that it didn't completely help in solving the issue, especially at a high Re number. Therefore, the formulation given by Olshanskii et al. [92] is used to stabilize the fluid flow. It is important to note that using heavy grad-div stabilization ($\gamma \gg 1$) significantly improves the mass conservation and does not affect the accuracy of the approximated solution [93]. Appendix A shows a simple test case with a sharp void fraction gradient which results in shocks in the velocity field. This was achieved by using a step function for the void fraction. We compare the velocity fields obtained using different combinations of stabilization terms. Before we implemented the grad-div stabilization, mass was not correctly conserved locally at the location of void fraction discontinuity where we had large velocity gradients. The application of this stabilization technique helps enhance the local conservation of mass. This conservation becomes much better as we refine the simulation mesh. This can be attributed to the element dependent γ . Refining the mesh also results in better oscillation control and reduces the distance over which the oscillations propagate.

5.4 Numerical Implementation

5.4.1 Void Fraction Calculation

We consider two cases for the calculation of the void fraction. In the case of the manufactured solutions (MMS), we calculate the void fraction from an analytical expression that satisfies the VANS equation. In the case where particles exist, we calculate the void fraction in a finite element as:

$$\varepsilon_f = \frac{v_{element} - v_{particles}}{v_{element}} \quad (5.20)$$

where $v_{element}$ is the volume of the finite element and $v_{particles}$ is the volume of all particles present within the element.

In order to determine the volume of particles in an element, we use the particle centroid

method (PCM) even though it possesses several limitations, due to its simplicity [83]. It assumes the volume of the particle to be located at its centroid. However, this method entails some disadvantages mainly the large fluctuation of the void fraction with time when particles' centers cross cell boundaries [49]. Another important limitation we should account for is the ratio of cell size to particle size which should be large enough in order to make the PCM accurate. But using a cell size which is much larger than particle size will prevent us from capturing the fluid flow field [49]. Therefore, there is a trade-off between cell size and particle size in unresolved CFD-DEM. This latter issue can be mitigated by increasing the order of the scheme instead of refining the mesh.

The void fraction obtained using the PCM method is calculated at each cell of the FEM mesh. However, for the assembly of the finite element system, we need the values of the void fraction at the nodes of the mesh. This is equivalent to finding the coefficients ε_j as to minimize the following equation [94]:

$$\min_{\varepsilon \in \mathbb{R}} \frac{1}{2} \sum_i \left(\sum_j \varepsilon_j \varphi_j - f_i \right)^2 \quad (5.21)$$

where ε_j is the projected void fraction on the finite element mesh and f_i is the calculated void fraction in each cell. We, therefore, applied $\mathcal{L}^2$ projection in order to project the calculated void fraction onto the quadrature points. This is done by assembling and solving the following finite element system:

$$\int_{\Omega} \varphi_i \varepsilon_j \varphi_j d\Omega = \int_{\Omega} f_i \varphi_i d\Omega \quad (5.22)$$

In certain applications where the void fraction is discontinuous or semi-discontinuous such as in a packed bed, we observe high gradients in the void fraction which results in high velocity gradients and leads to undesired oscillations in the flow field at high Reynolds number. In order to circumvent this problem, we apply to the left hand side of Eq. (5.22) a smoothing term similar to a Poisson equation to smooth the void fraction field. This smoothing term can be expressed as:

$$\iint_{\Omega} L^2 \nabla \varphi_i \nabla \varphi_j \varepsilon_j d\Omega \quad (5.23)$$

where L is the smoothing length chosen to be a multiple of the particle's diameter. In our case, L is chosen to be twice the particle's diameter. The resulting void fraction distribution is sufficiently smooth resulting in an enhanced convergence of the non-linear solver. However, implementing grad-div stabilization allows us to reduce the smoothing length required.

The projection of the void fraction solves one of the limitations of the PCM method, where now the void fraction becomes continuous in space between elements. However, the resulting values of the projected void fraction may exceed the value of 1 at certain locations (where there are strong gradients). Therefore, in order to ensure a realistic representation of the void fraction throughout the simulation domain, we bound the $\mathcal{L}^2$ system with a lower bound of 0.36, which represents the void fraction in a non-uniform packing and an upper bound of 1.

The $\mathcal{L}^2$ projection is bounded using a primal-dual active set method detailed in step-41 of the deal.II tutorials where we introduce a Lagrange multiplier λ in order to bound the problem [78]. This method allows us to keep the nature of the $\mathcal{L}^2$ projection as a quadratic optimization problem with n variables, but now with n bound constraints on these variables. This is applicable in the case of bi/tri-linear elements. In the case of bi/tri-quadratic elements, this method becomes expensive and exhaustive since high-order elements do not have their minimum and maximum attained at the nodes. We used the following two bounds for our problem:

$$\varepsilon_{min} \leq \varepsilon_j \leq \varepsilon_{max} \quad (5.24)$$

where $\varepsilon_{max} = 1$ is the maximum void fraction in the absence of particles while ε_{min} is the minimum void fraction and can be set by the user. This method, however, might reduce the mass conservation of our system as it slightly changes the mass preservative properties of the $\mathcal{L}^2$ projection. Therefore, we made it possible to enable or disable the bounding of the void fraction by the user.

5.4.2 Fluid-Particle Interactions

As an initial implementation of our FEM-VANS code, we determine that the drag force is the only non-negligible force. This is because the Basset and virtual mass forces are only significant in unsteady flows while the lift force is not significant in packed beds [83]. However, since we are only simulating steady flow with a large number of particles, these forces become insignificant and can therefore be neglected.

When many particles exist in the fluid, the influence of particles on the drag of a neighboring particle should be taken into account. The drag for this type of flow can be calculated using:

$$\mathbf{F}_D = \beta(\mathbf{u}_f - \mathbf{u}_p) \quad (5.25)$$

where $\mathbf{u}_p$ is the particle velocity, and β is the interphase momentum exchange coefficient and is determined by several correlations found in the literature. Among these correlations,

widely used models include the Gidaspow model [46] which combines the Ergun equation [95] for $\varepsilon_f < 0.8$ and the Wen-Yu model [96] for $\varepsilon_f \geq 0.8$, Syamlal and O'Brien model [97], Di Felice Model [98], Koch and Hill model [99], Rong et al. model [100] and Beestra et al. model [101]. For more information about the different drag models, we direct the reader to the article by Norouzi et al. [102] and the article by Bérard et al. [43]. Gidaspow explains that the interphase momentum exchange coefficient β differs between models A and B according to [46]:

$$\beta_B = \frac{\beta_A}{\varepsilon_f} \quad (5.26)$$

In our study, the drag force is calculated as a summation over particles of individual particle forces. We studied several drag models in order to evaluate the drag force. The drag force for Model B is calculated as:

$$\mathbf{F}_{pf_B} = \sum_{n=1}^{np} \frac{1}{2} \rho_f C_D A_{ref} |\mathbf{u}_{f,p} - \mathbf{u}_p| (\mathbf{u}_{f,q} - \mathbf{u}_{p,avg}) \quad (5.27)$$

and by using Eq. 5.26, we deduce that the drag force for model A is determined as :

$$\mathbf{F}_{pf_B} = \frac{\mathbf{F}_{pf_A}}{\varepsilon_f} \quad (5.28)$$

where n_p is the total number of particles in the cell, $\mathbf{u}_{f,p}$ is the interpolated fluid velocity at the particle's location calculated at the previous time step, $\mathbf{u}_{f,q} = \mathbf{u}_f$ is the fluid velocity at the quadrature point, and $\mathbf{u}_{p,avg}$ is the average particles' velocity in the cell both calculated at the current time step. This decomposition of the velocities allows us to consider the influence of the drag in the Jacobian of the matrix and makes the solid-fluid coupling semi-implicit thus resulting in faster and more robust convergence. A_{ref} is the particle's reference area which is taken as the cross-sectional area:

$$A_{ref} = \pi r_p^2 \quad (5.29)$$

where r_p is the particle's radius and C_D is the drag coefficient and is determined depending on the model used.

For the Di Felice model [98], the drag coefficient is:

$$C_{DA} = \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 \varepsilon_f^{2 - \left[3.7 - 0.65e^{\left(\frac{-(1.5 - \log_{10}(Re_p))^2}{2} \right)} \right]} \quad (5.30)$$

and Re_p is the particle Reynolds number and is expressed as:

$$Re_p = \frac{\rho_f |\mathbf{u}_f - \mathbf{u}_p| d_p}{\mu_f} \quad (5.31)$$

while for the Rong et al. model [100], the drag coefficient is defined as:

$$C_{DA} = \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 \varepsilon_f^{2-\left[2.65(\varepsilon_f+1) - (5.3-3.5\varepsilon_f)\varepsilon_f^2 e^{\left(\frac{-(1.5-\log_{10}(Re_p))^2}{2} \right)} \right]} \quad (5.32)$$

For a packed bed, the particles are at rest and therefore, $\mathbf{u}_p = 0$.

5.5 Verification of the Stabilized VANS Scheme by the Method of Manufactured Solutions

The Method of Manufactured Solutions (MMS) is a procedure which allows for the verification of a code's accuracy by manufacturing an analytical problem with an exact solution. Since the verification is purely mathematical, the solution does not have to be physically realistic; however, it has to be sufficiently complex in order to ensure a complete verification [103]. With the help of a Python script and through symbolic manipulation, we created several test cases with increasing complexity in order to fully verify all aspects of the VANS equations. We adopted a similar approach as presented by Blais et al. [90]. From Eqs. (5.1), (5.2), and (5.3), we identify two source terms that should be accounted for in the MMS. The mass source term (m') and the momentum source term $\mathbf{G}$. We define the momentum source term for each form as:

$$\mathbf{G}_B = \rho_f \left(\frac{\partial (\varepsilon_f \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) - m' \mathbf{u} + \nabla p - \nabla \cdot (\boldsymbol{\tau}_f) - \mathbf{F}_{pf} - \varepsilon_f \mathbf{f} \quad (5.33)$$

$$\mathbf{G}_A = \rho_f \left(\frac{\partial (\varepsilon_f \mathbf{u})}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right) - m' \mathbf{u} + \varepsilon_f \nabla p - \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) - \mathbf{F}_{pf} - \varepsilon_f \mathbf{f} \quad (5.34)$$

No particles are considered in the MMS cases, and therefore, $\mathbf{F}_{pf} = 0$. Four test cases were created for the verification of our code. All test cases presented in the following section can be found in the lethe repository on Github at <https://github.com/lethe-cfd/lethe-utils/tree/master/cases/vans>.

We performed the simulations with a mesh ranging from 256 cells to 4096 cell on a fixed

domain of simulation $\Omega = [-1, 1] \times [-1, 1]$. Different orders for the velocity and pressure shape functions are used in order to determine whether or not our solver conserves the order of accuracy. Convergence is reached when the residual of the non-linear solver becomes inferior to 10^{-8} . We calculate the order of convergence by a least-square linear regression of the Euclidean norm of the error with respect to the mesh size as was done by Blais et al. [90].

$$|E|_2 = \sqrt{\int_{\Omega} |e_q|^2} \quad (5.35)$$

where $|E|_2$ is the $\mathcal{L}^2$ norm of the error and e is the error at the quadrature points q .

We create four cases with increasing complexity to consider different possible scenarios. The 0th case includes a constant void fraction and a steady state divergence-free velocity profile. Due to its simplicity, it is not presented in this paper. For all other cases, the pressure, void fraction and velocity fields are chosen to be sufficiently differentiable. The 1st case investigates a spatially varying void fraction and a divergence free steady velocity. This is the only case that is studied for both Model A and Model B of the VANS equations to ensure both models are mathematically correct. Since the difference between the models is only related to the derivation of the pressure and stress tensor weak forms and in order to avoid repetition, we only present the other test cases for Model B. The 2nd case investigates a non-divergence free steady velocity. The 3rd case investigates a spatially and time varying void fraction as well as a transient velocity field.

The code was run for various finite element orders for velocity and pressure to determine whether or not the chosen order is well preserved within our implementation. The orders used were Q1-Q1, Q2-Q1, Q2-Q2, Q3-Q2, and Q3-Q3. The void fraction order is chosen to be equal to that of the velocity. For the transient case, and due to the large simulation time associated with higher orders, the study is limited to a highest order of Q2-Q2.

5.5.1 Case 1: Steady State Divergence-free Flow Problem

The velocity ($\mathbf{u}$), pressure (p) and void fraction (ε) for this case are defined in equations 5.36-5.38. In this case, there is no mass source term since mass conservation is satisfied. All fields are steady in this case, and the velocity field is divergence free which results in the normal stresses in the viscous stress tensor being zero. The velocity, pressure and void fraction fields are shown in Figure 5.1 for Model B. The convergence plots for models B and A are shown in Figure 5.2 and Figure 5.3 respectively.

$$\mathbf{u} = \begin{bmatrix} -2\sin^2(\pi x)\sin(\pi y)\cos(\pi y) \\ 2\sin(\pi x)\sin^2(\pi y)\cos(\pi x) \\ 0 \end{bmatrix} \quad (5.36)$$

$$p = \sin(\pi x)\sin(\pi y) \quad (5.37)$$

$$\varepsilon = \frac{1}{2} + \frac{1}{4}\sin(\pi x)\sin(\pi y) \quad (5.38)$$

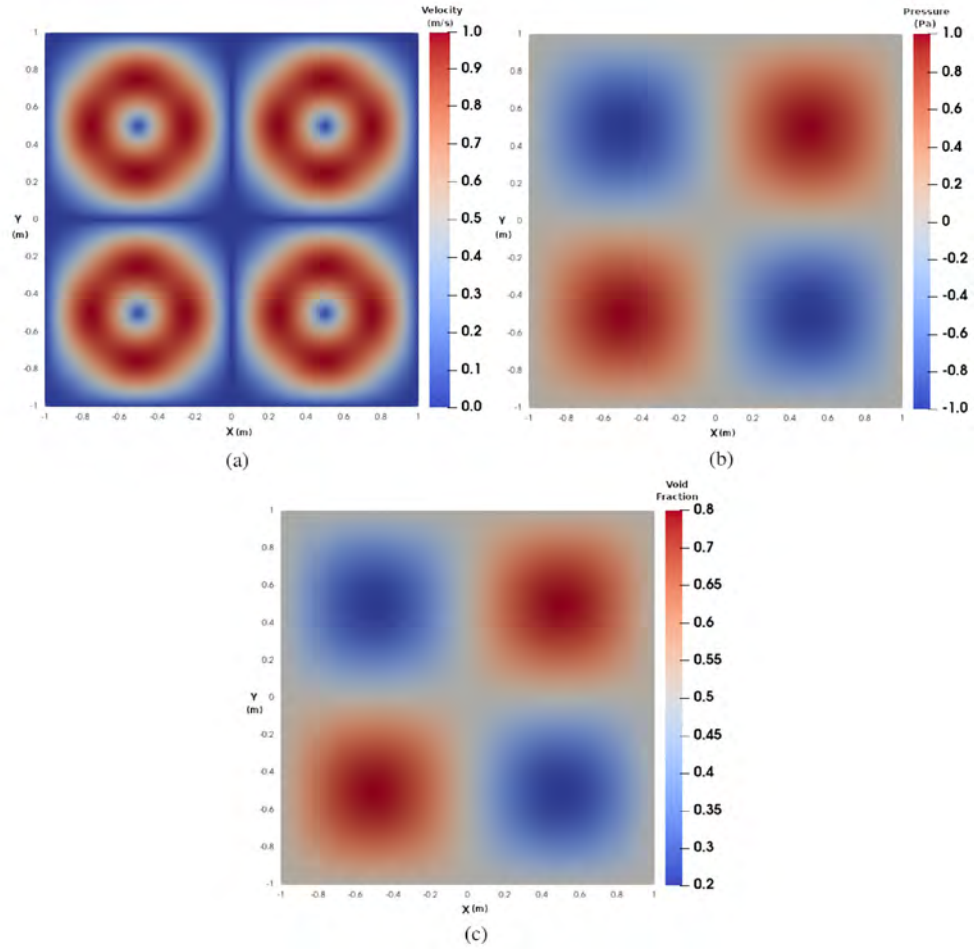
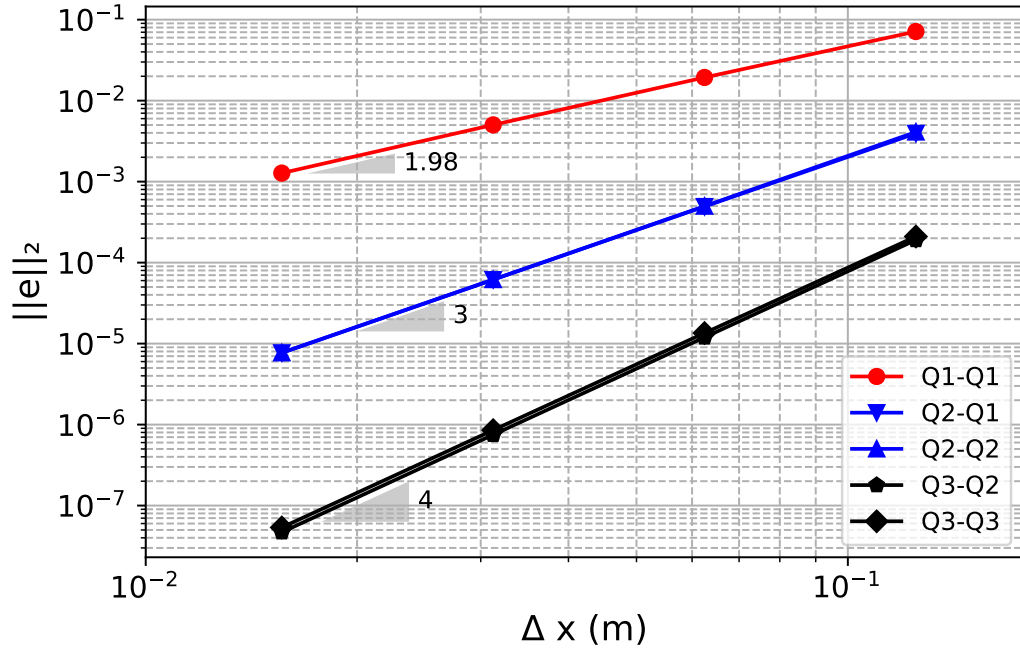
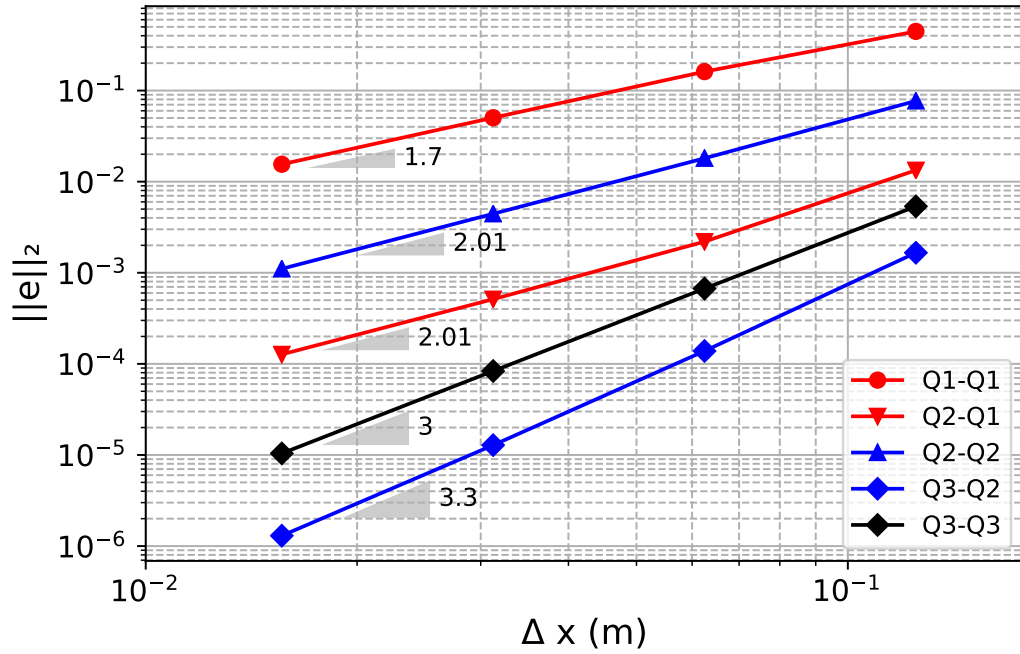


Figure 5.1 Case 1 analytical solution for (a) velocity, (b) pressure and (c) void fraction using model B with 4096 cells and Q1-Q1 elements.

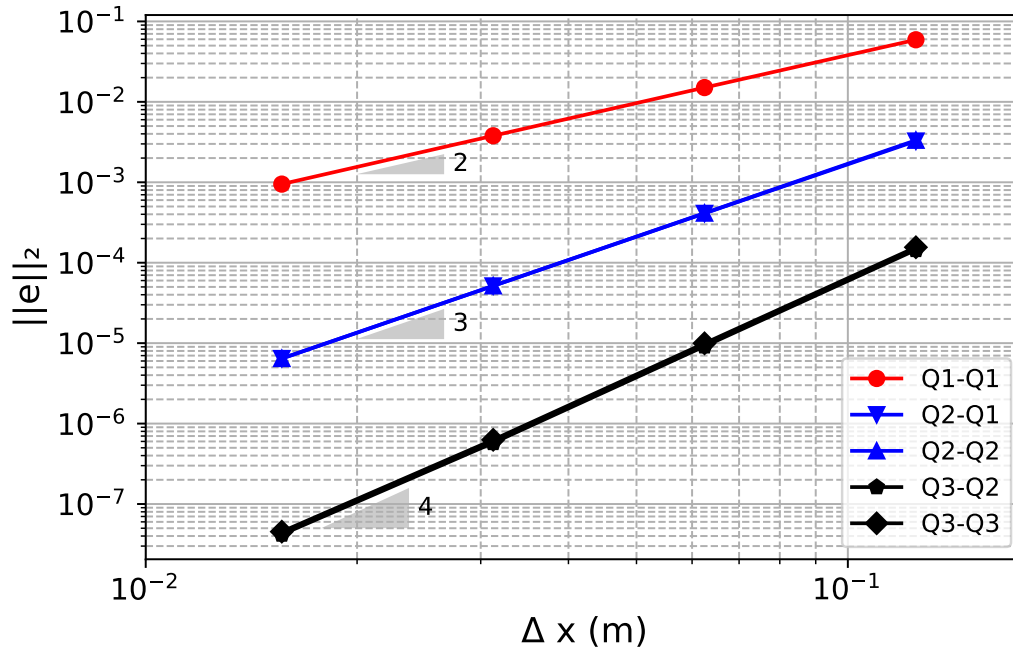


(a)

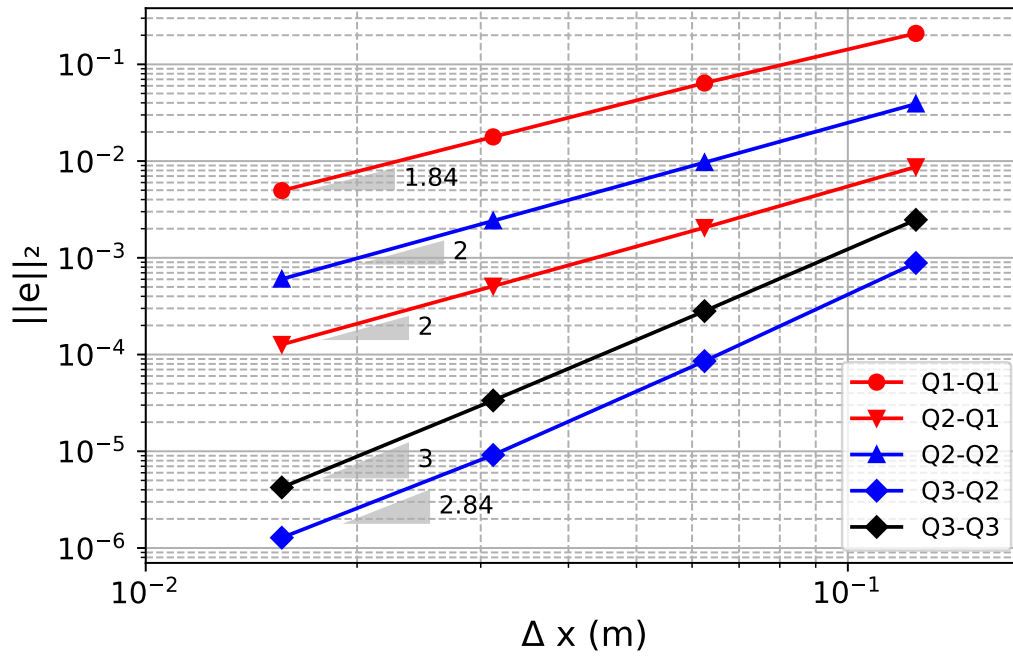


(b)

Figure 5.2 Case 1 convergence plots for (a) velocity and (b) pressure using Model B with respect to mesh size.



(a)



(b)

Figure 5.3 Case 1 convergence plots for (a) velocity and (b) pressure using Model A with respect to mesh size.

5.5.2 Case 2: Steady State Non Divergence-free Flow Problem

The velocity, pressure and void fraction for this cases are defined as:

$$\mathbf{u} = \begin{bmatrix} \frac{1}{e} e^{\sin(\pi x) \sin(\pi y)} \\ \frac{1}{e} e^{\sin(\pi x) \sin(\pi y)} \\ 0 \end{bmatrix} \quad (5.39)$$

$$p = \frac{1}{2} + \frac{1}{2} \sin(\pi x) \sin(\pi y) \quad (5.40)$$

$$\varepsilon = \frac{1}{e} e^{-\sin(\pi x) \sin(\pi y)} \quad (5.41)$$

In this case, mass conservation is inherently satisfied by the velocity field. Therefore, there is no mass source term. All fields are steady; however, the velocity field is not divergence free which results in the presence of all components of the stress tensor in the VANS equations. The velocity, pressure and void fraction fields are shown in Figure 5.4. The convergence plot is shown in Figure 5.5.

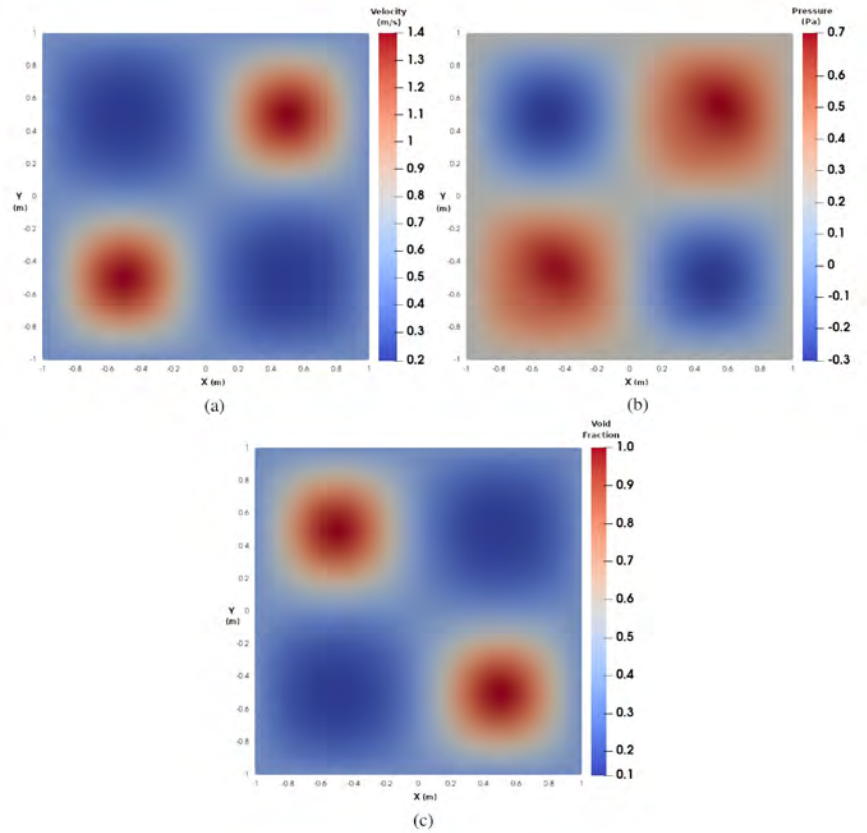
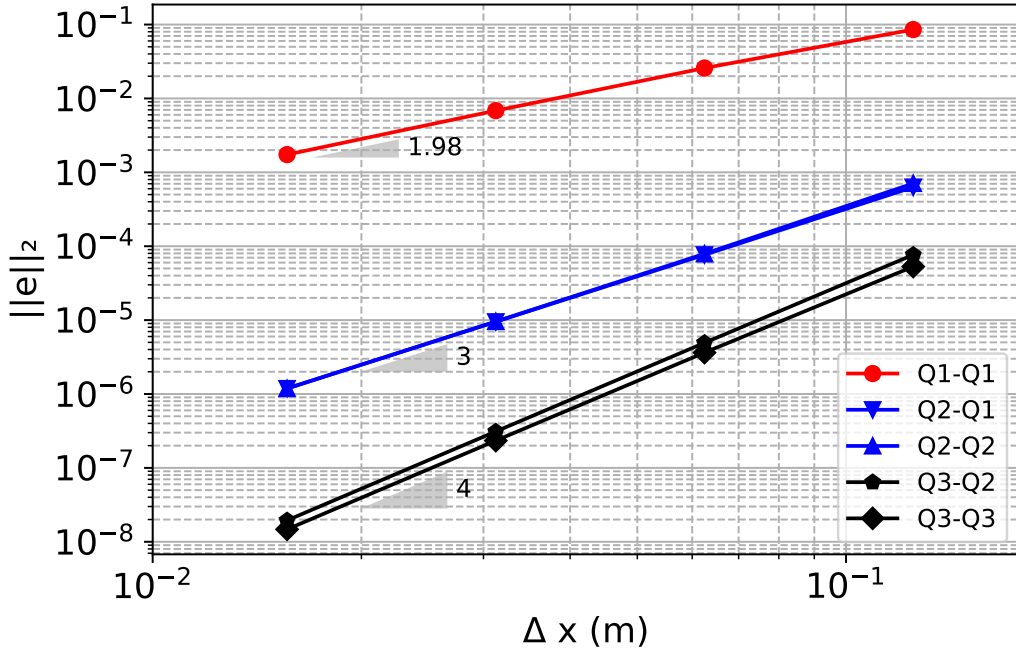
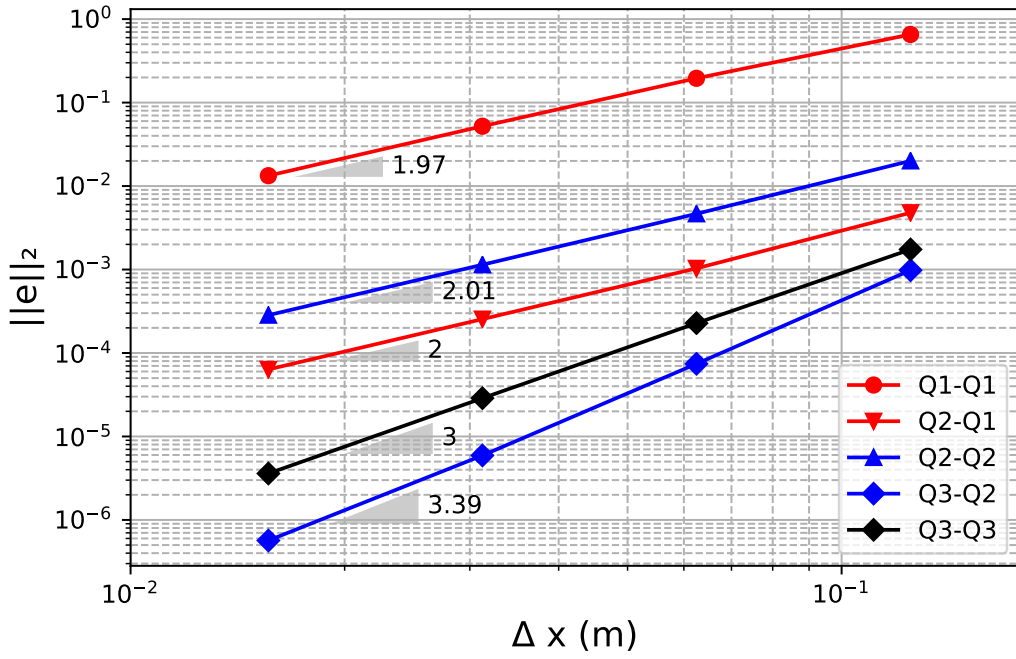


Figure 5.4 Case 2 analytical solution for (a) velocity, (b) pressure and (c) void fraction using model B with 4096 cells and Q1-Q1 elements.



(a)



(b)

Figure 5.5 Case 2 convergence plots for (a) velocity and (b) pressure using Model B with respect to mesh size.

5.5.3 Case 3: Unsteady Non Divergence-free Flow Problem

This case is defined as:

$$\mathbf{u} = \cos(2\pi t) \begin{bmatrix} \cos(\pi x)\cos(\pi y) \\ \cos(\pi x)\cos(\pi y) \\ 0 \end{bmatrix} \quad (5.42)$$

$$p = 0 \quad (5.43)$$

$$\varepsilon = \frac{1 - 0.1\cos(2\pi t)e^{-\sin(\pi x)\sin(\pi y)}}{e} \quad (5.44)$$

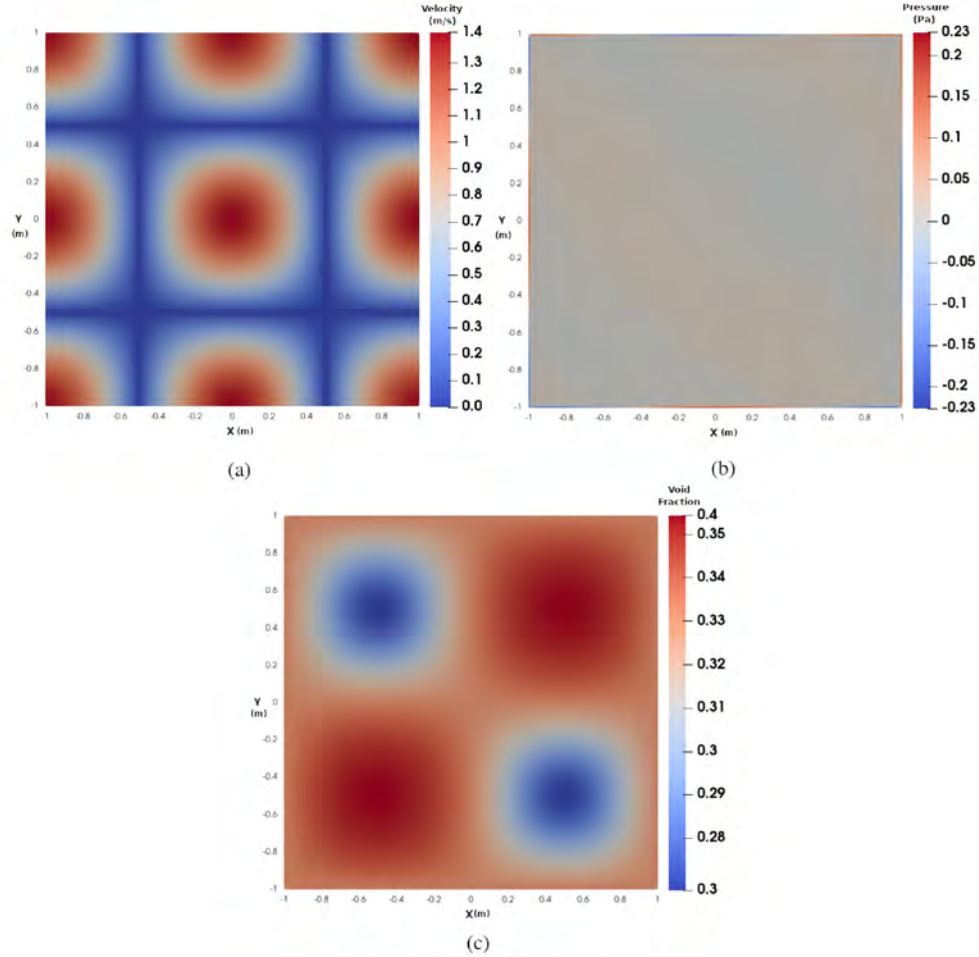
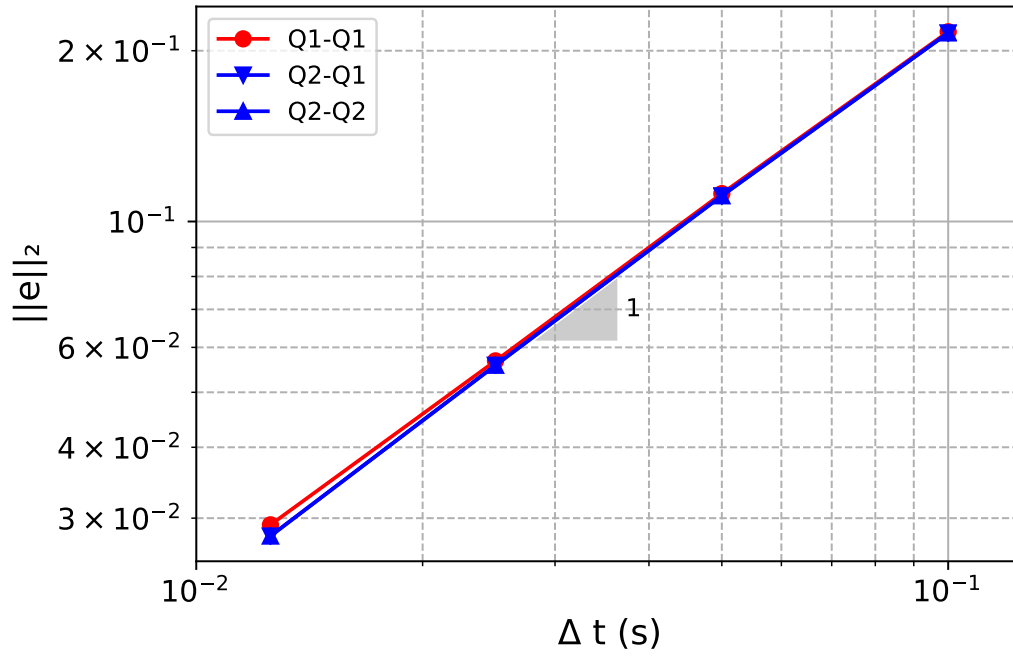
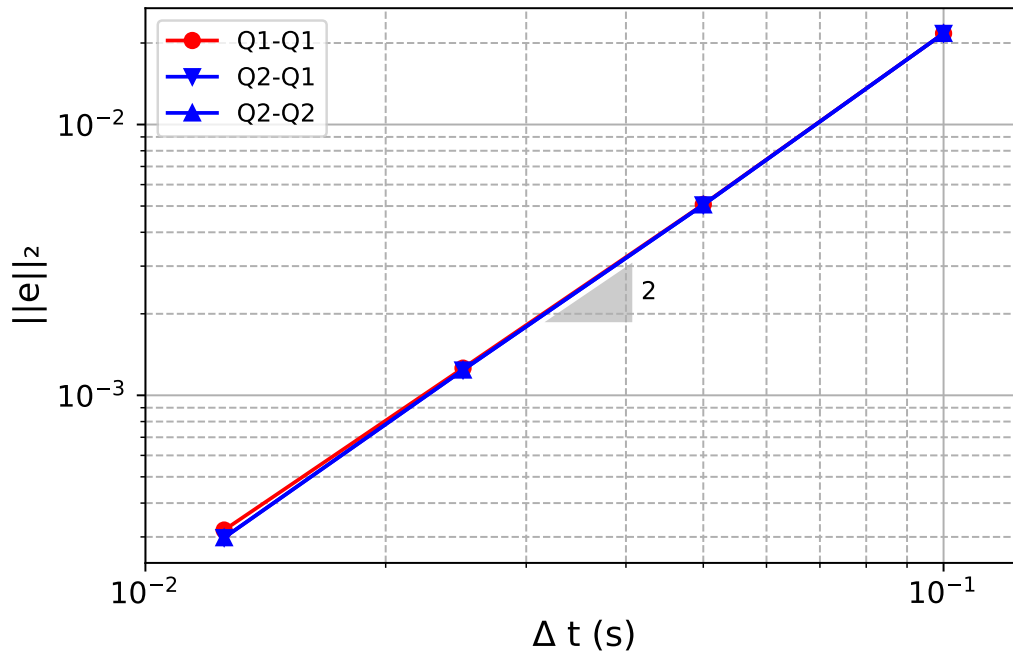


Figure 5.6 Case 3 analytical solution for (a) velocity, (b) pressure and (c) void fraction using model B with 4096 cells and Q1-Q1 elements at $t = 1$ s.



(a)



(b)

Figure 5.7 Case 3 velocity convergence plots for (a) BDF1 and (b) BDF2 using Model B with respect to mesh size.

In this case, the velocity field as well as the void fraction are unsteady and the velocity field is not divergence free. This leads to a nonzero mass source that should be accounted for. A very fine mesh size ($\Delta x = \Delta y = 0.015625m$) is used in this case so that spatial errors are negligible. This is important for the convergence analysis in time. The velocity, pressure and void fraction fields at $t = 1s$ are shown in Figure 5.6 for a timestep of $0.001s$ as to clearly and accurately represent the pressure field since the analytical solution is zero. The convergence plot is shown in Figure 5.7.

Discussion

The plots presented in Figures 5.2, 5.3, and 5.5 show that the velocity and pressure converge spatially to the correct order for all finite element orders investigated. This demonstrates the high-order capabilities of the proposed stabilized scheme for the VANS equations. Due to longer simulation times, no scheme higher than Q3-Q3 is investigated. However, a similar behavior is expected for higher-order schemes. Since Lagrange polynomials are used as an interpolation basis, we do not expect the present code to be well conditioned for very high-orders (> 6). In Figure 5.7 (a), we show that time convergence of our scheme is first-order for the different spatial schemes used. This is because time is discretized using the first order Backward Differentiation Formulation (BDF1). Similarly, in Figure 5.7 (b), we show second order convergence in time when using BDF2 as this represents a second order time discretization scheme. Thus, our code preserves the accuracy of the temporal discretization used. Higher order temporal schemes are also compatible with the code.

Spatial convergence for the transient case is not shown since exact convergence is not attained for the finer meshes. We attribute this discrepancy to the fact that a very small time step should be used in the study of spatial convergence of the transient case to reduce temporal errors. For the MMS solution, this leads to the presence of a very small time step.

Using MMS, we determined that our solver is globally mass conservative. The maximum global losses is of the same order of magnitude as the tolerance of the non-linear solver. Since the void fraction field in the MMS cases is always continuous, we always reach perfect mass conservation with respect to the non-linear solver. For steady flows, relative mass loss of the order of 10^{-17} could be obtained, which demonstrates the good mass conservation capabilities of this scheme. For the transient case, the global mass losses range between 10^{-6} and 10^{-8} . This error is dependent on the time discretization scheme as well as on the tolerance of the non-linear solver.

5.6 Simulation of Packed Bed for the Validation of the Stabilized VANS Scheme

After verifying our model using the method of manufactured solutions, we validate our model through the simulation of a packed bed and the prediction of the pressure drop inside it.

5.6.1 Simulation Setup

In order to realize this packed bed study, we perform two different simulations. The first simulation involves the discrete element method (DEM) which fills the bed with particles in order to create a non-uniform packing. The second simulation involves the VANS equations where we simulate a flow of fluid across the packing. A flow through a packed bed example on the documentation page of Lethe clearly represents the simulation setup with the different parameter files. All parameters necessary for the simulations can be found in Table 5.1.

Geometry Description

The simulation is carried out in a 3D lab-scale cylindrical packed bed using Q1-Q1, Q2-Q1 and Q2-Q2 elements. The geometry is generated using the `subdivided_cylinder` function of Deal.II. It has a total length of 200 *mm* and a radius of 25 *mm*. The bed is divided into 20 divisions across its half length. The width of the bed walls is neglected. A stopper is defined at a distance of 45 *mm* below the centroid of the bed to allow the suspension of particles and prevent their fall to the bottom of the bed. We used a non-uniform grid containing 3200 cells to describe the system. This is done to ensure better accuracy while respecting that the particle size should be at least one third smaller than the cell size in CFD simulations [104].

Discrete Element Method (DEM)

We perform the DEM simulations using Lethe-DEM [105,106]. For the purpose of validation, 200,000 particles having the same physical properties were considered for this simulation. All parameters for the DEM simulation are shown in Table 5.1. The particles have a diameter of 1 *mm* and a density of 2500 *kg/m*³. The particles are inserted randomly above the stopper where they fall under the influence of gravitational forces. We use the velocity Verlet method as the integration scheme for the motion of the particles. We used non-linear viscoelastic particle-particle and particle-wall contact force models. This is because a non-linear viscoelastic model presents a higher accuracy in calculating the collision forces [3]. The particles are allowed to settle on the stopper until their velocity dissipates. The DEM simulation is performed in parallel on 8 processors for 2 *s* with a time step of 2×10^{-5} *s*. We are left with a packed bed column with a height of 80 *mm*.

VANS-CFD Simulation

The gas chosen for this simulation is air. We define the various parameters of the VANS-CFD simulation in Table 5.1. The gas is introduced with a uniform velocity distribution at the inlet located at the bottom of the cylindrical bed. The simulation is carried out in parallel on 8 processors for 0.5 s with a time step of 2×10^{-3} s. For all cases, we ensure that steady state was reached at the end time. For the calculation of the fluid governing equations, we introduce a Dirichlet boundary condition for the velocity at the inlet of the bed. A slip boundary condition is applied to the walls of the cylinder. As an initial condition, the velocity is set to zero everywhere except at the inlet. We run the simulation for different inlet velocities which ranged between 0 m/s and 0.6 m/s with an increment of 0.05 m/s. This ensures that we remain below the minimum fluidization velocity (U_{mf}).

There exist various correlations to predict the minimum fluidization velocity. The choice is usually based on the particles' diameter and density. For a more detailed review of the different available correlations, we refer the reader to the article by Anantharaman et al. [107]. The minimum fluidization velocity (U_{mf}) was calculated based on the Wen-Yu correlation for Geldart D particles and is defined as [108]:

$$U_{mf} = \left[\left(33.7^2 + 0.0408 Ar \right)^{0.5} - 33.7 \right] \frac{\mu_f}{\rho_f d_p} \quad (5.45)$$

where Ar is the Archimedes number and is defined as:

$$Ar = \frac{g \rho_f (\rho_p - \rho_f) d_p^3}{\mu_f^2} \quad (5.46)$$

and ρ_p is the particles' density, g is the gravitational acceleration, and ϕ is the sphericity of the particle. $\phi = 1$ for spherical particles. In our case, $U_{mf} = 0.718$ m/s. For the purpose of determining U_{mf} , the void fraction ε_f of the bed is calculated as:

$$\varepsilon_f = \frac{(\pi r_b^2) H_b - n_p (\frac{4}{3} \pi r_p^3)}{(\pi r_b^2) H_b} \quad (5.47)$$

where n_p and r_p are the particles' number and radius respectively, and r_b and H_b are the bed's radius and height respectively. From the DEM simulation, the bed height was found to be 89.86 mm.

Table 5.1 Physical and numerical parameters for the packed bed simulation

<i>Simulation control</i>			
DEM end time (s)	2	VANS-CFD end time (s)	0.5
DEM time step (s)	2×10^{-5}	VANS-CFD time step (s)	2×10^{-3}
<i>Geometry</i>			
Bed Height (mm)	200	Bed Radius (mm)	25
Wall Thickness (mm)	0		
<i>Particles</i>			
Number	2×10^5	Diameter(m)	1×10^{-3}
Density(kg/m^3)	2500	Young Modulus (N/m^2)	1×10^6
Particle-particle poisson ratio	0.3	Particle-wall poisson ratio	0.3
Particle-particle restitution coefficient	0.2	Particle-wall restitution coefficient	0.2
Particle-particle friction coefficient	0.1	Particle-wall friction coefficient	0.1
Particle-particle rolling friction	0.2	Particle-wall rolling friction	0.3
<i>Gas phase</i>			
Viscosity ($Pa \cdot s$)	1×10^{-5}	Density (kg/m^3)	1
Inlet Velocity (m/s)	[0.05-0.6]	Void fraction smoothing factor L^2	5×10^{-6}
<i>Linear Solver</i>			
Method	GMRES	Max iterations	5000
Minimum residual	1×10^{-11}	Relative residual	10×10^{-3}
ILU preconditioner fill	1	ILU preconditioner absolute tolerance	1×10^{-14}
ILU preconditioner relative tolerance	1		
<i>Non-linear solver</i>			
Tolerance	1×10^{-9}	Max iterations	10

5.6.2 Results and Discussion

The particle packing result of the DEM simulation along with the meshed packed bed are shown in Figure 5.8. The particles take around 1.5 s to settle on the stopper. However, the simulation was run for 2 s in order to ensure that all particles become at rest. It is important that all particles possess a negligible velocity as the drag force is calculated using the relative velocity. If the particles had a non negligible velocity, the calculated drag would become incorrect resulting in an incorrect prediction of the pressure drop along the bed.

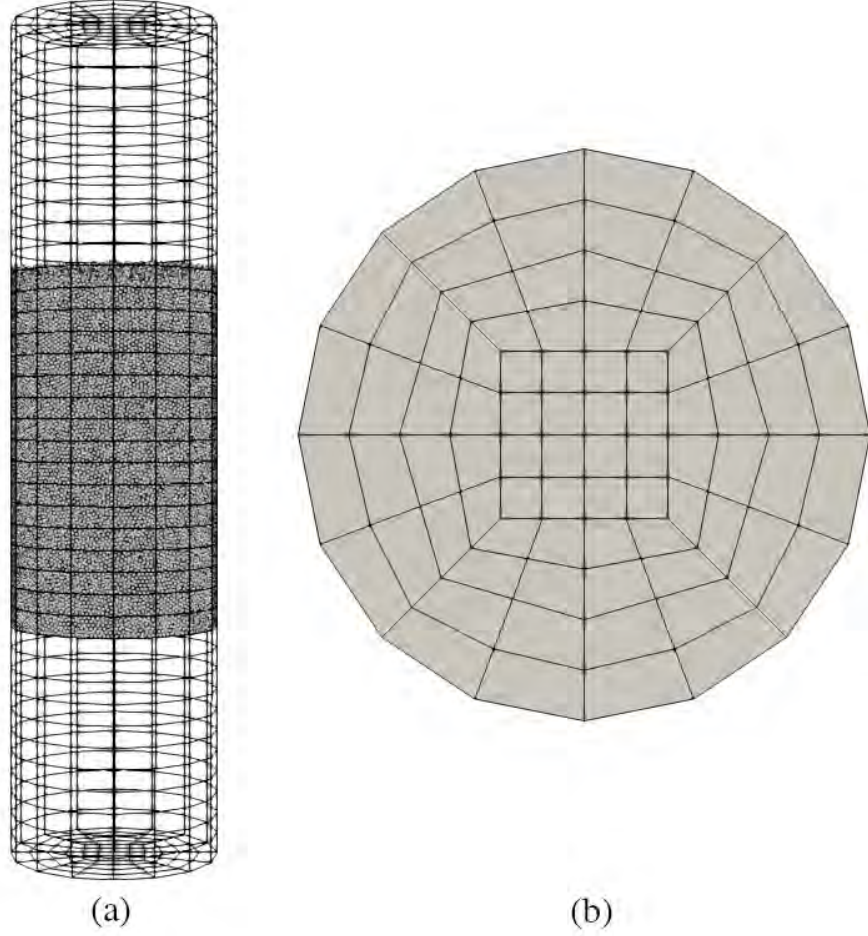


Figure 5.8 xy plane particle packing and mesh (a) and yz plane mesh (b) of packed bed

The velocity, pressure, and void fraction distributions are presented in Figure 5.9. The results shown are based on an inlet velocity $u_{in} = 0.5 \text{ m/s}$, and the Rong et al. drag model [100]. The void fraction shown in Figure 5.9 (a) appears to be spatially continuous. This is due to the smoothed $\mathcal{L}^2$ projection which overcomes the discontinuity of the Particle Centroid Method. This discontinuity is controlled using the smoothing length L . In this simulation, L^2 is taken to be equal to $5 d_p^2$. For the velocity distribution shown in Figure 5.9 (b), we can see some oscillations inside the packing region. This is explained by the non-uniform spacing between particles, resulting in higher velocities in regions with smaller spacing and vice versa. In Figure 5.9 (c), the pressure drops instantly inside the packing as expected. This is mainly due to friction inside the packing.

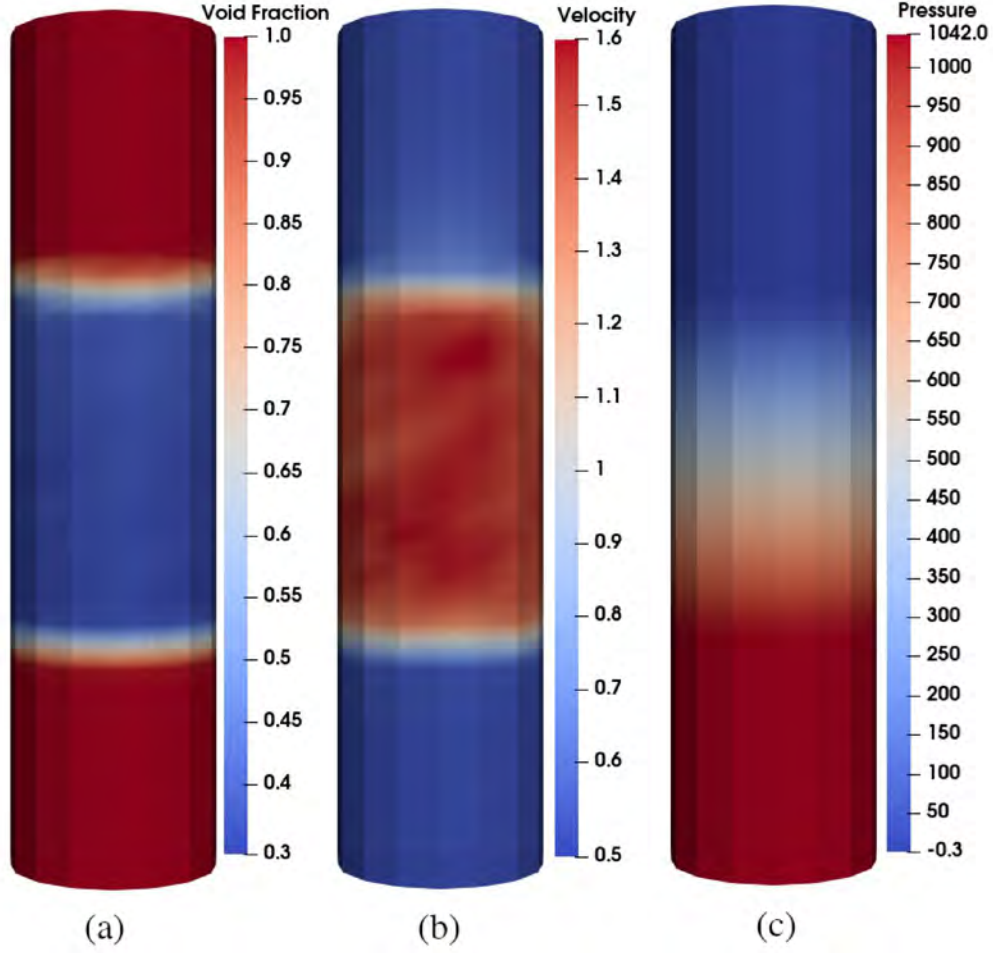


Figure 5.9 Solution of gas flow through packed bed using Q1-Q1 elements for (a) void fraction, (b) velocity and (c) pressure.

In order to validate our model, the results of our simulations are compared with the predicted Δp of the Ergun equation [95] as a function of Reynolds number. This equation is a correlation used to predict the pressure drop Δp across a packed bed of spherical particles and is denoted as:

$$\Delta p = \frac{150(1 - \varepsilon_f)^2 \mathbf{u}_f \mu_f H_b}{\varepsilon_f^3 d_p^2} + \frac{1.75(1 - \varepsilon_f) \rho_f \mathbf{u}_f H_b}{\varepsilon_f^3 d_p} \quad (5.48)$$

The Reynolds number used is the bed's Reynolds number:

$$Re = \frac{\rho_f \mathbf{u}_f D}{\mu_f} \quad (5.49)$$

where D is the bed's diameter.

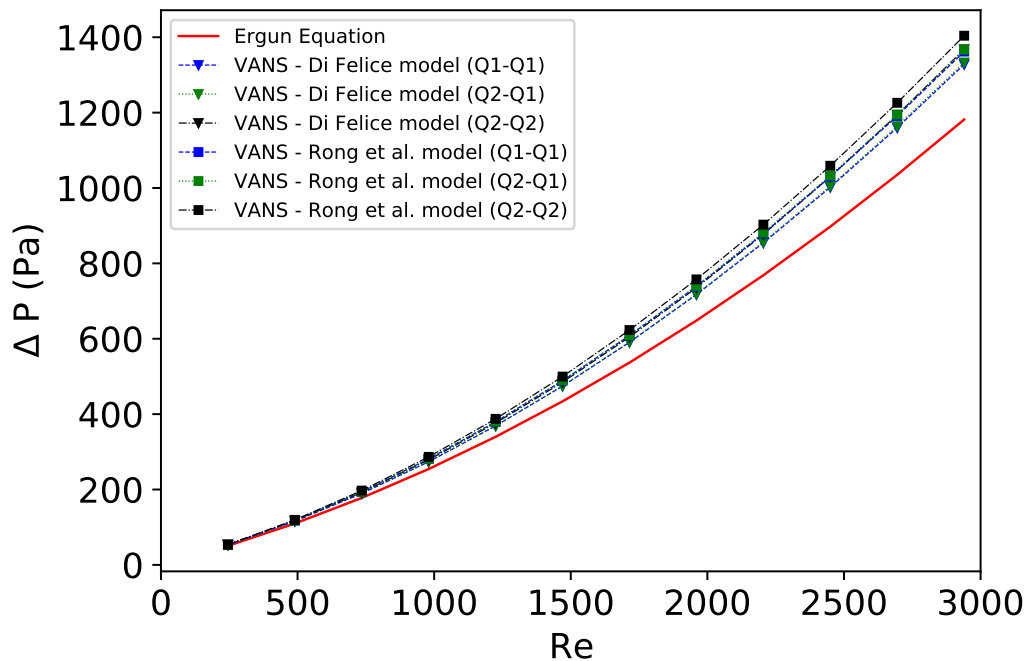


Figure 5.10 Comparison of model B pressure drop in packed bed as a function of inlet Reynolds number for different drag models and finite element orders.

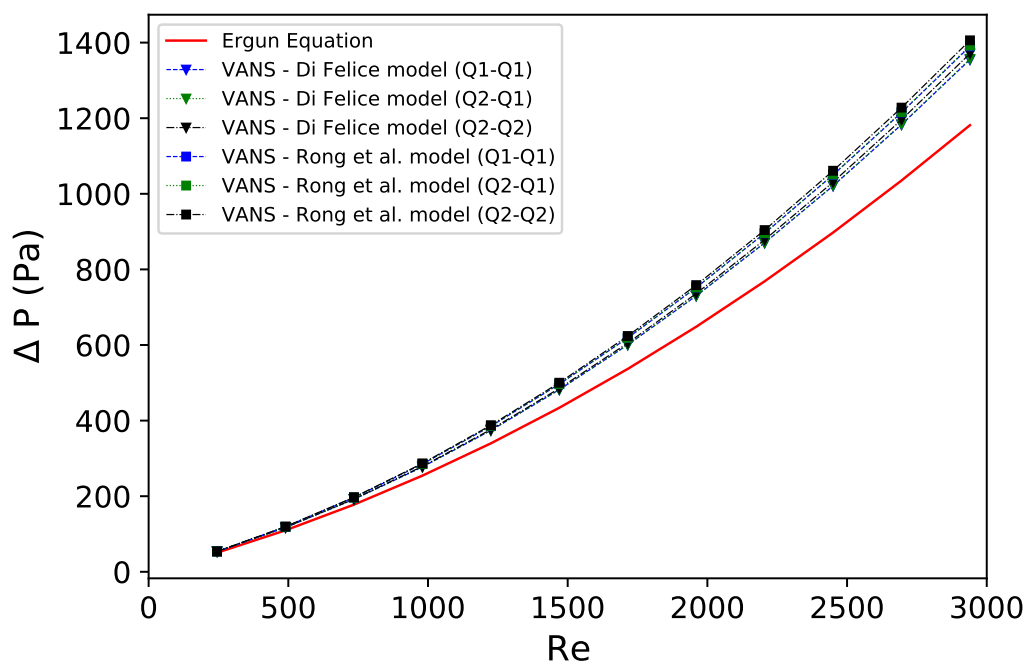


Figure 5.11 Comparison of model A pressure drop in packed bed as a function of inlet Reynolds number for different drag models and finite element orders.

For the Ergun equation, H_b is calculated in the same way as for the minimum fluidization velocity (U_{mf}). Similarly, in this case, $H_b = 89.86mm$. Figures 5.10 and 5.11 compare the pressure drop curves obtained from the simulations using Di Felice [98] and Rong et al [100] models for Q1-Q1, Q2-Q1 and Q2-Q2 elements using models B and A respectively with the predicted pressure drop obtained from the Ergun equation.

Using model B of the VANS equations, the two drag models show a good correlation with Eq. (5.48). They both slightly over predict the pressure drop compared to the Ergun equation for higher Re . However, it is important to note that the Ergun correlation being entirely empirical does not give precise pressure drop values and it might be that the pressure drop values obtained using the VANS solver are more precise than those obtained from the Ergun correlation. In both cases, the Rong et al. drag model shows more over prediction compared to the Difelice drag model. The β coefficient in the Rong et al model takes into account not only the particle's Reynolds number (Re_p) but also the bed's void fraction (ε_f). This can explain the over prediction of this model at higher Re values where the effects of the void fraction are amplified by the Reynold's number. Moreover, for the same drag model, using higher order elements leads to a higher over prediction of the pressure drop at higher Re values and does not change the predicted results at lower Re values. Using model A of the VANS equations, both drag models give similar results for the different element orders. As the order of the elements increased, the variation of the pressure drop remained negligible compared to the values obtained from Model B. However, the values of the pressure drop obtained using Model A were in general slightly greater than those obtained using Model B for the same element order. These results prove that the drag models' implementation in the VANS solver is correct. The local calculation of the drag in each element along with the volumetric integral of its value over all the elements successfully predicts the pressure drop in the packed bed. It also demonstrates that higher order elements are better suited for efficiently solving problems with a requirement for high accuracy, but for which the minimum mesh size is limited.

For the same packed bed simulation without bounding the void fraction, we determined the global mass source term and the maximum local mass source term at every inlet velocity for the Rong et al. [100] drag model using both models A and B of the VANS equations. The maximum local mass source term was determined by integrating the continuity equation over each element and choosing the value of the element with the maximum absolute value. The global mass source term was determined by summing up all element-wise integration of the continuity equation. The mass source terms are shown in absolute value scaled by the inlet velocity as in Figure 5.12.

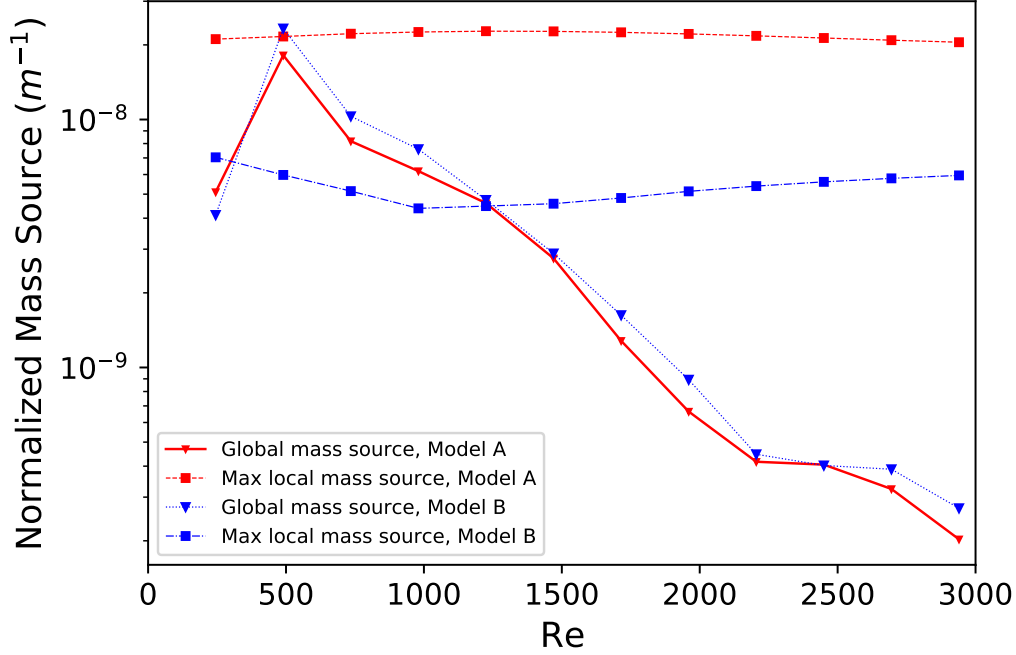


Figure 5.12 Comparison of local and global mass conservation of models A and B of the VANS equations using Rong drag model and Q1-Q1 elements.

Both models A and B show the same trend as well as similar values of the global mass source for different inlet velocities. Therefore, both our models are globally mass conservative achieving mass source term errors in the magnitude of 10^{-10} , which is the order of magnitude of the tolerance of the non-linear solver. Moreover, the two models show similar behavior for the maximum local mass conservation. As the inlet velocity increases, the local mass source for both models remains relatively constant in the magnitude of 10^{-9} for model B and 10^{-8} for model A. Even though Model B achieves better local mass conservation, the magnitude of the local error obtained for both models is relatively small. Therefore, it is safe to consider that without bounding the void fraction, both models are mass conservative. In this case, bounding the void fraction does not add any benefits to the simulation as the projected void fraction had a maximum value of 1.00001 and thus it didn't affect any aspect of the simulation. Some of the simulations were repeated while bounding the void fraction. The obtained results show diminished mass conservation in the magnitude of 10^{-6} . As we bound the void fraction, we slightly change the values of the void fraction at the extremities of the packing and as a consequence alter the mass preservative properties of the $\mathcal{L}^2$ projection. This explains the increase in the magnitude of the mass source term error.

5.7 Conclusion

This work presents a verified and validated stabilized finite element approach for the modeling of both forms A and B of the volume-averaged Navier Stokes equations which are used to model multi-phase flows. We were able to develop a parallel high-order finite element solver for these equations within Lethe, thus enhancing accuracy without requiring finer meshes. This is important as it helps circumvent one of the solid-fluid flow limitations concerning mesh size. We verified our solver using the method of manufactured solutions and showed that our model is consistent with the underlying discretization and globally mass conservative. The validation of the model through the prediction of the pressure drop in a packed bed simulation and its comparison with that of the Ergun correlation allowed us to confirm the validity of the drag models' implementation. In the presence of a discontinuous void fraction field, we controlled the stability of the simulation through our choice of the smoothing length L . This is often taken to be two or three times the particles' diameter. Finally, the methodology introduced here serves as a first step in developing a fully parallel high-order CFD-DEM solver by coupling the VANS solver presented in this paper with Lethe-DEM [105]. The rigorous verification and validation strategy deployed in this work can also be followed by other researchers who are developing solvers for the VANS equations, without regard to the numerical method used.

5.8 Acknowledgements

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CHAPTER 6 ARTICLE 2 : TOWARD HIGH-ORDER CFD-DEM: DEVELOPMENT AND VALIDATION

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Declaration: The author of this thesis has contributed to the literature review, code development, simulation and modelling, analysis of the results and the writing of the article.

Abstract: CFD-DEM is used to simulate solid-fluid systems. DEM models the motion of discrete particles while CFD models the fluid phase. Coupling both necessitates the calculation of the void fraction and the solid-fluid forces resulting in a computationally expensive method. Additionally, evaluating volume-averaged quantities locally restricts particle to cell size ratios limiting the accuracy of the CFD. To mitigate these limitations, we develop a unified finite element CFD-DEM solver which integrates the CFD and DEM solvers into a single software resulting in faster and cheaper coupling between the solvers. It supports dynamically load-balanced parallelization. This allows for more efficient simulations as load balancing ensures the even distribution of workloads among processors; thus, exploiting available resources efficiently. Our solver supports high order schemes; thus, allowing the use of larger elements enhancing the validity and stability of the void fraction schemes while achieving better accuracy. We verify and validate our CFD-DEM solver with a large array of test cases: particle sedimentation, a fluidized bed, the Rayleigh Taylor instability and a spouted bed.

6.1 Introduction

Multi-phase flows are prevalent in several industries such as food processing, oil and gas, pharmaceutical industries and many more [2, 3]. Understanding the underlying phenomena that control the behavior of such flows is important to develop state of the art equipment for solid-fluid contactors. Solid-fluid flows and particularly solid-gas flows, are characterized based on the number density of the particles. When this number is small, the flow is termed dilute solid-gas flow and the gas dominates the behavior of the flow. In this case, the solid particles exhibit negligible effects on the gas. When the number density is large, the flow is termed dense solid-gas flow. In this case, the movement of the solid phase becomes mainly controlled by particle-particle collisions. When this number density is bounded and thus lies

in between the two previously mentioned cases, the flow is referred to as dispersed flow where the solids constitute the dispersed phase and the fluid constitute the continuous phase. In this case, the flow is affected equally by both phases [1].

We encounter solid-gas flows in several technological applications such as pollutant control systems, combustion systems, and drying systems. Fluidized and spouted beds are among the common industrial applications which deal with solid-gas flows. Through the application of gas flow at the bottom of the bed, and when the gas flow is large enough to exert sufficient drag on the granular material allowing it to overcome gravity, particles fluidize. In the fluidized state, particles behave as a mixer allowing for a higher mass and heat transfer rates between the two phases resulting in a uniform temperature distribution [5]. This results in improved yields and efficiency in chemical and physical processes which employ such beds.

Fluidized and spouted beds differ in the way they operate. In fluidized beds, the fluid is introduced usually at the entire surface of the inlet while in spouted beds, the fluid enters through a small orifice of the base of the bed. This results in different fluidization behaviors. Contrary to a single fluidizing section in a fluidized bed, spouted beds can be divided into three sections. The spout which is the central core through which the fluid flows. The fountain, which contains the particles entrained by the spout, appears above the bed surface. The annulus is the surrounding annular region of the bed where the particles travel down from the fountain [4].

These beds are complex in their design, building, and operation when compared to other types of beds such as packed beds and stirred tank reactors and are more difficult to scale-up [6]. However, their advantages for the chemical industries make it vital to predict their behavior in order to accomplish design, scale-up, optimization, and troubleshooting of the processes involved [3]. Even though there exist several intrusive and non intrusive experimental techniques to investigate fluidized and spouted beds, their implementation is generally expensive and often infeasible for complex applications. Furthermore, the information that can be extracted from experiments is limited especially at the particle scale. Consequently, modelling can be used to understand the various phenomena occurring in different processes, enabling sensitivity analysis on different input parameters, and testing various configurations and operational conditions at a much cheaper cost [3].

Among the various modeling approaches, unresolved CFD-DEM is often used to study solid-fluid systems. It is an Eulerian-Lagrangian approach in which the flow field is divided into cells larger than the solid particles' size but sufficiently small to capture the flow field itself. Few commercial and open source CFD-DEM software exist to simulate solid-fluid flows using CFD-DEM. Usually, CFD and DEM software exist separately and are coupled through a

coupling interface. Commercial DEM software include EDEM [109], Rocky [110] and Asphex [111] while open source DEM software include LIGGGHTS [112] and Yade [113]. Commercial CFD software include COMSOL [114], Ansys Fluent [115], StarCCM+ [116] among others while open source CFD software include MFiX [50] and OpenFOAM [117]. Additionally, there exists several in-house codes used to publish studies related to solid-fluid flows [44, 104, 118]. To the best of our knowledge, MFiX, StarCCM+, and PFC [119] are the only unified CFD-DEM software meaning that both the CFD and DEM solvers are integrated into a single piece of software. However, such software do not support high order elements. Only Asphex [111] supports load balancing and can be integrated to CFD solvers using the CFDEM interface [120].

Unresolved CFD-DEM simulations are computationally expensive and possess some major limitations. The time step of integration is limiting as the DEM scheme is usually explicit and requires the particle time step to be very low (between 10^{-7} s to 10^{-4} s, depending on the size and the stiffness of the particles). Another limitation is the size of the mesh cells which should usually be at least three times the particle diameter in CFD-DEM simulations [3]. This is particularly important to ensure that certain void fraction calculation schemes are valid. In order to overcome this limitation, certain analytical schemes have been developed where the cell and particle intersections were determined analytically [76, 77]. However, these methods are computationally expensive as they involve the calculation of trigonometric functions at each time step [77, 121]. Other non-analytical approaches have been developed such as the divided particle volume methods (DPVM) [122, 123] which represents the particle as a porous cube. These methods added spatial smoothing which diffused the void fraction and thus, the presence of particles was weakly felt by the fluid [124]. Additionally, numerical strategies have been developed in order to increase the accuracy of the CFD simulation when coarser grids have to be used to ensure adequate calculation of the void fraction. These include the use of separate grids for CFD and for the void fraction where the void fraction grid is coarser than the CFD grid. Such studies included the use of two level grids [125–127] and three level grids [128, 129]. However, the mapping of information between grids has a non negligible computational cost that should be considered. The use of multiple grids is also challenging when the geometry of the simulation domain is complex.

More accuracy is required sometimes on the CFD side which is generally, at best, second-order accurate. Therefore, there is a trade off between accuracy and stability in such situations. As such, we propose high order schemes as an important factor in alleviating these challenges. They allow for better accuracy without decreasing the mesh size. Currently existing CFD-DEM software do not exploit high order schemes as they are more complicated and harder to implement than low order methods, and their computational memory requirement is much

greater. The importance of parallelization becomes evident when CFD-DEM can be run on multiple processors to achieve better computational efficiency. Parallelizing CFD-DEM simulations requires parallelizing the CFD, the DEM and the coupling between both models. Adding dynamic load balancing to the recipe allows us to benefit more from parallelization where the work loads are divided evenly among processors [105]. To the best of our knowledge, there is no CFD-DEM software that implements dynamic load balancing on all three components (CFD, DEM and coupling).

In this paper, we build a high-order FEM stabilized CFD-DEM solver within the open-source software Lethe [89] available at <https://github.com/lethe-cfd/lethe> which is based on the Deal.II framework [78]. This was achieved by coupling the Volume Averaged Navier-Stokes (VANS) solver [130] with the DEM model of Lethe [105]. The coupling is built in Lethe and does not require a separate coupling interface. The coupled solver includes all the advantages of the VANS solver [130]. It is a fully implicit solver that requires no stability condition on the fluid side. It is globally mass conservative and it accounts for the time variation of the void fraction in the continuity equation. Moreover, it supports both models A and B of the VANS equations. It enables fundamental comparison between the two models in CFD-DEM studies as results obtained from both models are analysed. Furthermore, and to the best of our knowledge, it represents one of the first unresolved CFD-DEM solvers with load balancing capabilities. This enables it to leverage available computing resources by assigning more processors to tasks with greater work loads leading to more efficient utilization of resources. Finally, it is the first high order CFD-DEM solver. As such, coarser meshes can be used without sacrificing accuracy on the CFD side.

The coupling is achieved through the void fraction as well as the particle-fluid forces. In order to verify and validate our unresolved CFD-DEM solver, we consider four test cases. We simulate a particle sedimentation case to determine the particle's terminal velocity. We model a fluidized bed and study the pressure drop and the bed height before and after fluidization. We simulate a heavy fluid on top of a lighter fluid to obtain the Rayleigh Taylor instability and determine its mixing width. Finally, we study a spouted bed and determine the time averaged particle velocity. The obtained results verify correct implementation of the solid-fluid forces, demonstrate global mass conservation, and show physically correct predictions of the hydrodynamics of the systems being studied.

6.2 Governing Equations and Coupling Strategy in CFD-DEM

In the CFD-DEM approach, the incompressible Newtonian fluid phase is modeled as a continuum. It is described by the volume averaged Navier Stokes (VANS) equations which take

into account the dependency of the fluid volume within a cell on the solid phase volume occupying it. In the present work, these equations are solved using the finite element method in an Eulerian description of matter. On the other hand, the dispersed solid particles are modeled as a discrete phase. The latter is described using the discrete element method [105]. Therefore, the CFD-DEM model represents an Eulerian-Lagrangian approach for solving multiphase flows.

6.2.1 Description of Fluid Phase

We model the fluid flow using either forms A or B of the volume averaged Navier Stokes equations. The continuity equation for an incompressible fluid is:

$$\rho_f \frac{\partial (\varepsilon_f)}{\partial t} + \rho_f \nabla \cdot (\varepsilon_f \mathbf{u}_f) = m' \quad (6.1)$$

where ρ_f is the fluid density, $\mathbf{u}_f$ is the fluid velocity, ε_f is the fluid's void fraction, and m' is the volumetric source of mass [46]. $m' = 0$ in the case of non reactive flows or when there is no source term added to the simulation. The momentum equation for model A of the incompressible VANS equations is:

$$\rho_f \left(\frac{\partial (\varepsilon_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}_f \otimes \mathbf{u}_f) \right) = -\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf_A} + \rho_f \varepsilon_f \mathbf{f} \quad (6.2)$$

while that of Model B is:

$$\rho_f \left(\frac{\partial (\varepsilon_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}_f \otimes \mathbf{u}_f) \right) = -\nabla p + \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf_B} + \rho_f \varepsilon_f \mathbf{f} \quad (6.3)$$

with

$$\boldsymbol{\tau}_f = \mu_f \left((\nabla \mathbf{u}_f) + (\nabla \mathbf{u}_f)^T \right) - \frac{2}{3} \mu_f (\nabla \cdot \mathbf{u}_f) \mathbf{I} \quad (6.4)$$

where p is the pressure, $\boldsymbol{\tau}_f$ the deviatoric stress tensor, $\mathbf{f}$ the external force (ex. gravity), and $\mathbf{F}_{pf}$ is the momentum transfer term between the solid and fluid phases and includes forces such as drag, virtual mass, Basset force, Saffman lift, and Magnus lift [90]. $\mathbf{I}$ is the identity or unit tensor.

The difference between the two models lies in the formulation of the momentum equation specifically in the derivation of the pressure and the stress tensor. In model A, the shear and pressure gradient forces are calculated and added to the fluid phase according to cell properties such as cell void fraction and cell pressure drop. However, in model B these forces

are calculated on individual particles and then lumped up with the drag force before being added to the fluid phase. Consequently, these solid-fluid interactions are defined explicitly in model B whereas, they are implicit in model A [44].

Finite Element Discretization

The weak form of the VANS equations for both the continuity and momentum equations include the streamline-upwind/Petrov-Galerkin (SUPG) stabilization, the pressure-stabilizing/Petrov-Galerkin (PSPG) stabilization, and the grad-div stabilization. These equations are:

$$\int_{\Omega} \left(\frac{\partial(\varepsilon_f)}{\partial t} + \varepsilon_f \nabla \cdot \mathbf{u} + \mathbf{u} \nabla \varepsilon_f \right) q d\Omega + \underbrace{\mathcal{SR} \cdot (\tau_u \nabla q)}_{PSPG} d\Omega_k = 0 \quad (6.5)$$

Form A:

$$\begin{aligned} & \int_{\Omega} \left(\varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} \right) \cdot \mathbf{v} d\Omega + \frac{1}{\rho_f} \left(\int_{\Omega} \left(\varepsilon_f \nu (\nabla^2 \mathbf{u}) + \nu \nabla \mathbf{u} \nabla \varepsilon_f \right) \cdot \mathbf{v} d\Omega \right. \\ & + \int_{\Omega} m' \mathbf{u} \cdot \mathbf{v} d\Omega - \int_{\Omega} \left(\varepsilon_f p \cdot \nabla \mathbf{v} + p \nabla \varepsilon_f \cdot \mathbf{v} \right) d\Omega + \int_{\Omega} \mathbf{F}_{pf_A} \cdot \mathbf{v} d\Omega \left. \right) - \int_{\Omega} \varepsilon_f \mathbf{f} \cdot \mathbf{v} d\Omega \\ & + \underbrace{\sum_K \int_{\Omega_k} \mathcal{SR} \cdot (\tau_u \mathbf{u} \cdot \nabla \mathbf{v}) d\Omega_k}_{SUPG} + \underbrace{\sum_K \int_{\Omega_k} \gamma \left(\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}) \right) (\nabla \cdot \mathbf{v}) d\Omega_k}_{grad-div} = 0 \end{aligned} \quad (6.6)$$

Form B:

$$\begin{aligned} & \int_{\Omega} \left(\varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \cdot \nabla \mathbf{u} \right) \cdot \mathbf{v} d\Omega + \frac{1}{\rho_f} \left(\int_{\Omega} \nu (\nabla \mathbf{u}) \nabla \mathbf{v} d\Omega \right. \\ & + \int_{\Omega} m' \mathbf{u} \cdot \mathbf{v} d\Omega - \int_{\Omega} p \nabla \cdot \mathbf{v} d\Omega + \int_{\Omega} \mathbf{F}_{pf_B} \cdot \mathbf{v} d\Omega \left. \right) - \int_{\Omega} \varepsilon_f \mathbf{f} \cdot \mathbf{v} d\Omega \\ & + \underbrace{\sum_K \int_{\Omega_k} \mathcal{SR} \cdot (\tau_u \mathbf{u} \cdot \nabla \mathbf{v}) d\Omega_k}_{SUPG} + \underbrace{\sum_K \int_{\Omega_k} \gamma \left(\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}) \right) (\nabla \cdot \mathbf{v}) d\Omega_k}_{grad-div} = 0 \end{aligned} \quad (6.7)$$

and

$$\mathcal{SR} = \varepsilon_f \frac{\partial \mathbf{u}}{\partial t} + \varepsilon_f \mathbf{u} \nabla \cdot \mathbf{u} + \frac{1}{\rho_f} \left(m' \mathbf{u} + \nabla p - \nu (\nabla^2 \mathbf{u}) + \mathbf{F}_{pf} \right) - \varepsilon_f \mathbf{f} \quad (6.8)$$

where $\mathcal{SR}$ is the strong residual associated with the PSPG and SUPG stabilizations. $\mathbf{q}$ and $\mathbf{v}$ are the pressure and velocity interpolation functions. Both the test functions and the interpolation functions are Lagrange polynomials of arbitrary order, but we limit ourselves to linear (Q1) and quadratic (Q2) tensor elements in this work. V_Ω is the volume of the domain Ω and γ is a parameter related to the augmented Lagrangian formulation [89]. The stabilization parameter τ_u is defined by Tezduyar [91] and is explained in detail in the Lethe paper [89]. For transient simulations, τ_u is defined as:

$$\tau_u = \left[\left(\frac{1}{\Delta t} \right)^2 + \left(\frac{2|\mathbf{u}|}{h_{conv}} \right)^2 + 9 \left(\frac{4\nu}{h_{diff}^2} \right)^2 \right]^{-1/2} \quad (6.9)$$

where Δt is the time step, h_{conv} and h_{diff} are the size of the element related to the convection transport and diffusion mechanism respectively [89]. The complete description, derivation and verification of the weak form of the VANS equations using the finite element method (FEM) along with the various stabilization techniques implemented is presented by El Geitani et al. [130].

All stabilization methods applied support both implicit stabilization where we use the velocity of the current time step in the stabilization formulation and explicit stabilization where we use the velocity at the previous time step. The last term in Eqs. (6.2) and (6.3) is not added in our solver as we don't solve for gravity in the fluid phase. The consequence of this is the addition of the buoyancy force on the solid phase and the redefinition of the pressure to include the hydrostatic pressure. It is important to note that this force is not explicitly added to the fluid phase of the VANS equations as it is implicit in the pressure.

The γ weight factor parameter for the grad-div stabilization implemented in the VANS equations [130] is calculated according to [92]:

$$\gamma = \nu + c^* \mathbf{u}_{f\Omega_e} \quad (6.10)$$

where c^* depends on the pressure behavior in element Ω_e . Since this information is rarely available, Olshanskii et al. [92] set c^* to a global constant of order 1. In our solver, we allow c^* to be a user defined value. The choice of c^* remains arbitrary in the literature and there is no clear consensus to the optimal value that should be used. Grad-div stabilization plays an important role not only in mass conservation but in the condition number of the linear systems arising when solving the VANS equations.

Order of the Scheme

$\mathbf{q}$ and $\mathbf{v}$ are functions used for the interpolation of the velocity and pressure within the cells. These functions can take many forms, but in the present work we use Lagrange polynomials. If the polynomial is of degree 1, then the underlying scheme is second-order accurate and it is denoted by Q1 in a tensor element (quadrilateral in 2D, hexahedron in 3D). If it is of degree 2, it results in a third-order scheme and it is denoted by Q2 in a tensor element. In general, a polynomial of degree n is denoted as Q_n and results in a $n + 1$ order scheme. However, it is important to note that in tensor elements, the order of the scheme applies to the edges of the element. The diagonal along the faces and the inside of the element are interpolated by a polynomial resulting from the tensor product of the polynomials at the edges of the element [131]. In 3D, the diagonal polynomial on the faces of the elements will be of degree $2n$ and within the elements they will be of degree $3n$. Thus, although the Q1 elements are formally second-order accurate in space, they possess high-order components along the faces and within the element and this greatly increases their accuracy when the velocity gradient is not aligned with the edges of the cells.

The velocity and the pressure can be interpolated with different functions. For example, a 2D problem having a scheme that is third order accurate in velocity and second order accurate in pressure can be expressed as a Q2-Q1 scheme. The polynomials interpolating the velocity and pressure at the sides of the element will be of degree 2 and 1 respectively. In our work, the polynomial interpolating the void fraction is always taken to be of degree 1 (Q1) since this keeps the void fraction bounded within the elements.

Void Fraction Calculation

In the literature, the derivative of the void fraction with respect to time in the continuity equation is usually set to zero as it introduces major instabilities to the pressure field. In our solver, we found that this quantity can be added to the equation if the density of the fluid is low (eg. for a gas). However, if the fluid is dense (eg. a liquid), this quantity causes the solution to diverge.

We calculate the void fraction in a cell by:

$$\varepsilon_f = \frac{v_{element} - v_{particles}}{v_{element}} \quad (6.11)$$

where $v_{element}$ is the volume of an element and $v_{particles}$ is the volume of all particles present within the element. In our solver, the latter is calculated by either the particle centroid method (PCM) due to its simplicity [49, 83] or by the satellite point method (SPM) [49]

which is more accurate than the PCM but more expensive. In the PCM method, if the centroid of the particle lies in a given cell, then the entire volume of the particle is considered to be in the cell. In the SPM method, each particle is divided into smaller sub-particles known as satellite particles each possessing its own volume. If the centroid of the satellite particle lies in a given cell, then the entire volume of the satellite particle will be considered to be in the cell.

In the context of the finite element method, the PCM and SPM are both calculated per element and then projected onto its nodes. The void fraction calculation using PCM and SPM is given by:

$$\varepsilon_{f_{pcm}} = 1 - \frac{\sum^{N_p} V_p}{V_{\Omega_e}} \quad (6.12)$$

$$\varepsilon_{f_{spm}} = 1 - \frac{\sum^{N_p} \sum^{N_{sp}} V_{sp}}{V_{\Omega_e}} \quad (6.13)$$

where V_p , V_{Ω_e} , V_{sp} , N_p and N_{sp} are respectively the particle volume, the element volume, the satellite point volume, the number of particles in an element and the number of satellite points in the particle that are also in the element. The full description of the void fraction scheme used and how it is implemented in the context of finite element is explained by El Geitani et al. [130].

6.2.2 Description of Solid Phase

Newton's second law describes the motion of the solid particles. There are two distinct particle motions in DEM simulations. The particles' translational movement is described by:

$$m_i \frac{\partial \mathbf{u}_{p,i}}{\partial t} = \sum_{j \in C_i} \mathbf{f}_{ij} + \sum_w \mathbf{f}_{w,i} + m_i \mathbf{g} + \mathbf{f}_{fp,i} \quad (6.14)$$

where m_i is the mass of particle i , $\mathbf{u}_{p,i}$ is the particle i 's velocity, $\mathbf{f}_{ij}$ are the interactions between particle i and particle j and C_i includes all particles in the contact list of particle i , $\mathbf{f}_{w,i}$ are the particle i and walls interactions and w loops over all walls in contact with particle i , $\mathbf{g}$ is the gravity and $\mathbf{f}_{fp,i}$ are the fluid and particle i interactions which represent the coupling forces between the two phases. The particles rotational movement is described

by:

$$I_i \frac{\partial \boldsymbol{\omega}_{p,i}}{\partial t} = \sum_{j \in C_i} \left(\mathbf{M}_{ij}^t + \mathbf{M}_{ij}^r \right) + \mathbf{M}_i^{ext} \quad (6.15)$$

where I_i is the moment of inertia of particle i , $\boldsymbol{\omega}_{p,i}$ is the angular velocity of particle i , $\mathbf{M}_{ij}^t$ and $\mathbf{M}_{ij}^r$ are respectively the tangential and rolling friction torques due to the contact between particle i and j , and $\mathbf{M}_i^{ext}$ denotes all other external torques. In our solver, we use the Rayleigh characteristic time in order to determine the critical time step required for stability of the DEM simulation. We calculate the critical time step of all particles and take the smallest as the Rayleigh time step. It is given by [132]:

$$\Delta t_{crit} = \min_{i \in N_p} \left(\frac{\pi r_i}{0.1631 \nu_i + 0.8766} \sqrt{\frac{\rho_i}{G_i}} \right) \quad (6.16)$$

where N_p is the total number of particles, ρ_i is the particle's density, G_i is the particle's shear modulus, ν_i is the particle's Poisson's ratio, and r_i is the particle's radius. It is common to use a DEM time step that is 20% of the Rayleigh time step. For simulations where particles reach high velocities, a time step smaller than the 20% Rayleigh time step might be required.

Particle-Particle and Particle-Wall Interactions

The soft sphere model is used to calculate contact forces using artificial overlaps and a set of imaginary springs and dashpots and torques resulting from particle collisions [39]. During collision, this overlap as well as the collision force change. The time step for such simulation should be small enough so that the contact between particles is processed in several time intervals [3]. We use a non-linear visco-elastic model to calculate the normal and tangential spring and damping constants [105]. The respective equations are presented in Table 6.1 where δ_n is the normal overlap, e is the coefficient of restitution, ν is Poisson's ratio, and i and j represent the particles in contact.

The contact force between two particles is calculated as a combination of normal and tangential contributions [105]:

$$\mathbf{f}_{ij} = \begin{cases} \mathbf{f}_{ij}^n = -(k_n \delta_n) \mathbf{n}_{ij} - (\eta_n \mathbf{v}_{rn}) \\ \mathbf{f}_{ij}^t = -(k_t \delta_t) - (\eta_t \mathbf{v}_{rt}) \end{cases} \quad (6.17)$$

where $\mathbf{v}_{rn}$ and $\mathbf{v}_{rt}$ are the normal and tangential components of the relative contact velocity. For additional details about DEM, we refer the reader to the Lethe-DEM paper [105].

Table 6.1 Normal and tangential spring and damping constants for the visco-elastic model.

Parameters	Equations
Normal spring constant	$k_n = \frac{4}{3}Y_e\sqrt{R_e\delta_n}$
Normal damping coefficient	$\eta_n = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_n m_e}$
Tangential spring constant	$k_t = 8G_e\sqrt{R_e\delta_n}$
Tangential damping coefficient	$\eta_t = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_t m_e}$
Effective mass	$\frac{1}{m_e} = \frac{1}{m_i} + \frac{1}{m_j}$
Effective radius	$\frac{1}{R_e} = \frac{1}{R_i} + \frac{1}{R_j}$
Effective shear modulus	$\frac{1}{G_e} = \frac{2(2-\nu_i)(1+\nu_i)}{Y_i} + \frac{2(2-\nu_j)(1+\nu_j)}{Y_j}$
Effective Young's modulus	$\frac{1}{Y_e} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}$
β	$\beta = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}}$
S_n	$S_n = 2Y_e\sqrt{R_e\delta_n}$
S_t	$S_t = 8G_e\sqrt{R_e\delta_n}$

To integrate Newton's equation of motion, we implement the Velocity Verlet scheme [133].

6.2.3 CFD-DEM Coupling

CFD and DEM are mainly coupled through the void fraction calculation and the fluid-particle interactions. In our code, the CFD and DEM both use the same mesh. This prevents the need to transfer solutions between meshes or localize the particle onto the CFD mesh and significantly reduces the computational cost. Additionally, our solver is fully parallelized. The parallelization of our solver is explained in detail in the Lethe [89] and Lethe-DEM [105] papers for the CFD and DEM components respectively. This parallelization supports adaptive mesh refinement, is flexible and scalable thanks to the method presented by Gassm  ller et al. [134] and implemented in the Deal.II library [78]. Every fluid-particle interaction is calculated using values interpolated at the particle's location by the FEM interpolation. The summation of individual fluid-particle forces over all particles in a cell results in the force applied on the fluid due to the particles. All forces are calculated only once per time step. The detailed algorithm is shown in the following section.

Coupling Scheme

The coupling strategy is given in detail in Figure 6.1. It couples the VANS solver [130] with Lethe-DEM [105]. The CFD and DEM solvers are coupled by introducing the DEM iterator within the CFD iterator. Initially, the void fraction is calculated, the VANS equations are solved for the fluid, the fluid-particle interactions are calculated and then the DEM iterator is called to solve Newton’s second equation of motion. In order to ensure temporal agreement between the CFD and DEM iterator, we restrict the choice of the time step to the CFD solver. The DEM time step is chosen implicitly by specifying a DEM coupling frequency given as:

$$f_{coupling} = \frac{\Delta t_{CFD}}{\Delta t_{DEM}} \quad (6.18)$$

where $f_{coupling}$ is the frequency at which the coupling occurs and Δt is the time step. As shown in the VANS article [130], our solver can achieve high order accuracy in both time and space. We can achieve second order or third-order accuracy in time using backward difference formulation (BDF2 or BDF3) and third order accuracy in space for the velocity field by using Q2-Q1 finite elements for velocity and pressure respectively. On the CFD side, our code is unconditionally stable since we use an implicit formulation in our evaluation of the VANS solution. On the DEM side, and in order to produce valid results, the DEM time step should be small enough to accurately capture particle-particle interactions. Since the fluid modeling is based on evaluating locally volume-averaged quantities, an element (Ω_e) volume should be at least one order of magnitude greater than the particle volume ($V_{\Omega_e} > 10V_p$) [135].

For the inter-phase coupling, and as we aim to solve dense solid-fluid systems, we assume 4 way coupling between the solid and fluid phases. In this case, the fluid affects the particles’ motion and the particles affect the fluid flow. In addition to this, particles motion is also affected by collisions between particles and between particles and walls where these interactions play an important role in characterizing the particles’ behavior [136].

Load Balancing

Our CFD-DEM coupled solver supports load balancing. Load balancing allows the distribution of all tasks among all available processors such that the overall computational time is optimized. Load balancing was possible thanks to the p4est [80] and Deal.II [78] finite element library. P4est allows for a user-specified weight function that returns a non-negative integer weight for each finite element. Thus, instead of partitioning the work into a uniform number of elements, it distributes it evenly by weight. This is important as sometimes

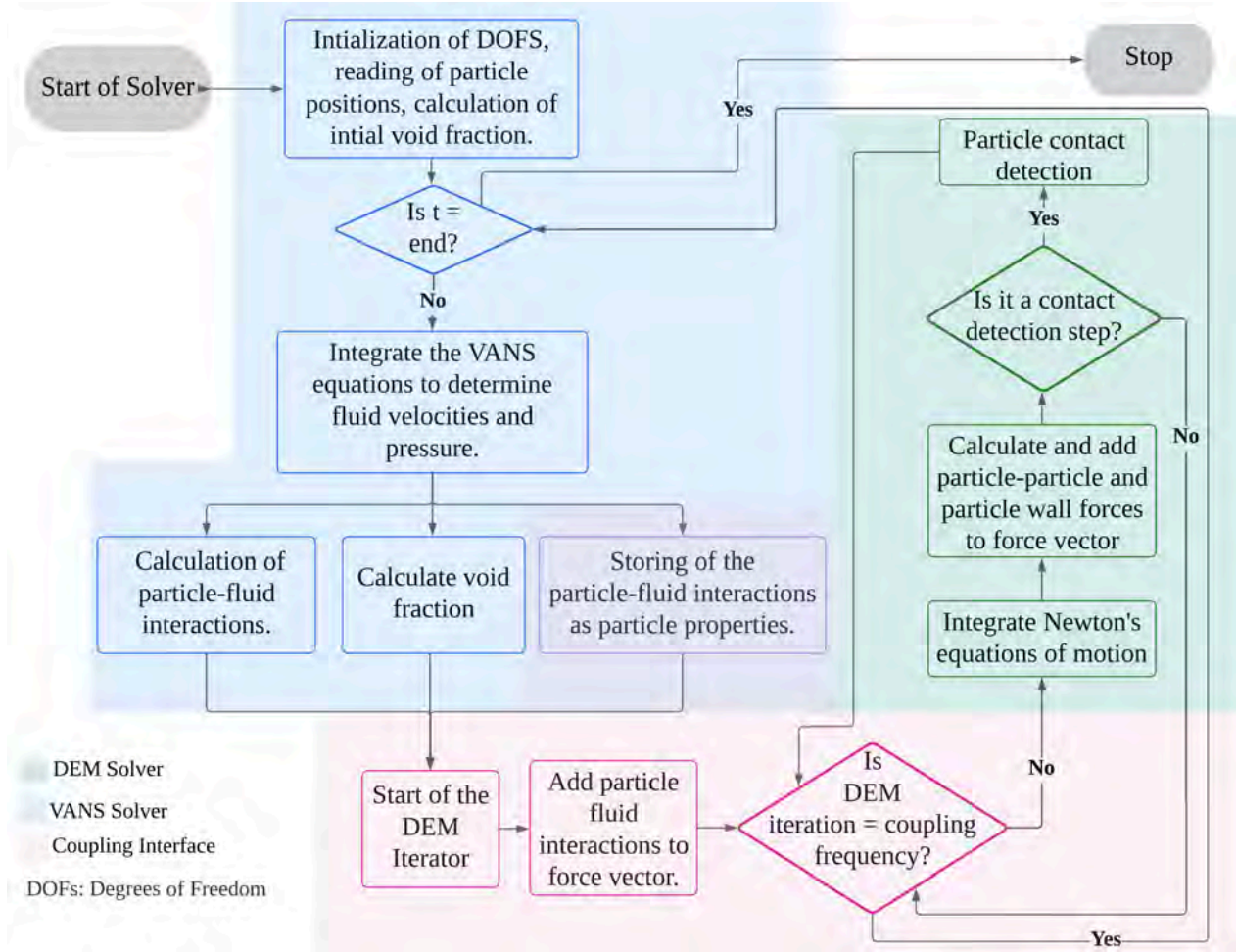


Figure 6.1 The CFD-DEM coupling scheme.

elements have varying mathematical unknowns to store and compute on [80]. This is true for CFD-DEM as the number of particles is not equal among elements. In the CFD-DEM solver of Lethe, each cell is assigned a weight based on its computational load. The sum of these weights is then distributed evenly among the available processors. In the absence of particles, the default cell weight is 1000. In CFD-DEM, we attribute a weight for a particle. The overall cell weight becomes the sum of the cell weight and all particles weights in the cell. Consequently, a cell with more particles will normally have a larger weight.

Asphex [111] also supports load balancing. However, due to the non unified nature of Asphex, load balancing is only performed on the DEM side. On the CFD side, load-balancing is performed by OpenFOAM. Even if both the CFD and DEM are separately load balanced, the information about the particles calculated by the DEM (position, velocity, angular velocity, etc.) must be sent from multiple cores to multiple cores using MPI since

the parallel decomposition of the DEM and the CFD do not coincide. In this case, the particle-fluid coupling, which includes the calculation of the solid-fluid forces and the void fraction, is not balanced. Nothing prevents all particles from ending up in a few cores of the CFD component of the code, which would be a significant bottleneck when calculating the coupling. This is where the Lethe CFD-DEM solver becomes attractive as it aims to overcome this particular limitation. In Lethe, load balancing ensures that communication between processors is performed only when particles moves between processors and not at each coupling step. This is not the case for non-unified solvers where communication is performed at each coupling step thus may result in more overhead as shown by the schematic of Figure 6.2.

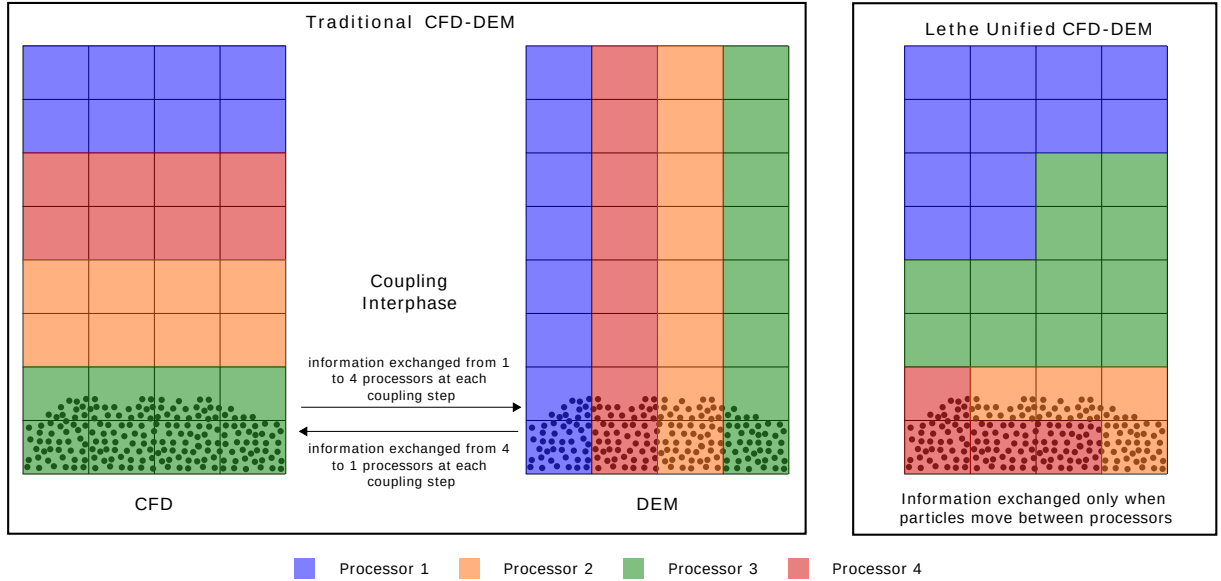


Figure 6.2 Representation of load balancing with 4 processors in a unified CFD-DEM solver and in a separately coupled CFD and DEM solvers

The application of load balancing in CFD-DEM software is relatively new. To our knowledge, our CFD-DEM solver demonstrates one of the first solvers with load balancing capabilities that take into account both physics in a unified software. Further studies must be performed in order to determine the optimum particle to cell weight ratios as this is affected by several factors. For example, a simulation where particle-particle contact forces are frequent usually requires a larger particle weight, whereas the same simulation with Q2-Q1 elements instead of Q1-Q1 elements will require a larger cell weight.

Particle-fluid Interactions

There exists several important forces that should be accounted for in the coupling process. These include the drag force, the buoyancy force, the pressure force, and the shear force. Since we are mainly interested in gas-solid flows in this work, we neglect virtual mass force, Basset force and lift force [83].

Drag Force

It is the force experienced due to the relative motion of the particle and fluid around it. We determine the drag force based on:

$$\mathbf{f}_D = \beta(\mathbf{u}_f - \mathbf{u}_{p,i}) \quad (6.19)$$

where $\mathbf{u}_{p,i}$ is the particle i velocity, and β is the inter-phase momentum exchange coefficient. According to Gidaspow, the interphase momentum exchange coefficient β differs between models A and B [46]:

$$\beta_B = \frac{\beta_A}{\varepsilon_f} \quad (6.20)$$

On the other hand, Zhou et al. [44] implement the same drag force for both models. In our derivation, we use the same drag force for both models. This is because only when considering the same drag force are the models A and B mathematically equivalent. When simulating a stationary solid phase, as the case of the packed bed which we simulated [130], we use the assumption of Eq. (6.20) as we only consider drag and buoyancy. Eqs. (6.37) and (6.39) demonstrate that the pressure gradient force should be applied back to the fluid phase only in model B. As such, not implementing this important force in the packed bed for model B necessitates the use of the momentum exchange coefficient as written in Eq. (6.20). This penalizes the pressure in model B by a factor of ε_f in order to compensate for the pressure gradient force resulting in a good pressure drop in the bed. This is not the case for model A as the pressure gradient force is already implicitly applied by the term $\varepsilon_f \nabla p$ of the momentum equation.

We calculate the drag force on a single particle as:

$$\mathbf{f}_D = \frac{1}{2} \rho_f C_D A_{ref} |\mathbf{u}_{f,p} - \mathbf{u}_{p,i}| (\mathbf{u}_{f,q} - \mathbf{u}_{p,avg}) \quad (6.21)$$

where $\mathbf{u}_{f,p}$ is the interpolated fluid velocity at the particle location calculated at the previous

time step, $\mathbf{u}_{f,q} = \mathbf{u}_f$ is the fluid velocity at the quadrature point, and $\mathbf{u}_{p,avg}$ is the average particles' velocity in the cell both calculated at the current time step. We use a Q_n interpolation that is homogeneous with the FEM scheme in order to interpolate the velocity at the particle location. A_{ref} is the particle reference area which is taken as the cross-section:

$$A_{ref} = \pi r_p^2 \quad (6.22)$$

where r_p is the particle radius and C_D is the drag coefficient. At the time of writing, our code supports Dallavalle [137], DiFelice [98], Rong [100], Koch and Hill [68], Beetstra [138], and Gidaspow [46] drag models. The inter-phase momentum exchange coefficient for Dallavalle model [137]:

$$\beta = \frac{1}{2} \rho_f \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 A_{ref} |\mathbf{u}_f - \mathbf{u}_{p,i}| \quad (6.23)$$

and Re_p is the particle Reynolds number and is expressed as:

$$Re_p = \frac{\rho_f \varepsilon_f |\mathbf{u}_f - \mathbf{u}_{p,i}| d_p}{\mu_f} \quad (6.24)$$

where μ_f is the fluid dynamic viscosity and d_p is the particle diameter. The inter-phase momentum exchange coefficient for the Di Felice model [98] is given:

$$\beta = \frac{1}{2} \rho_f \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 A_{ref} |\mathbf{u}_f - \mathbf{u}_{p,i}| \varepsilon_f \left[2 - \left[3.7 - 0.65 e^{\left(\frac{-(1.5 - \log_{10}(Re_p))^2}{2} \right)} \right] \right] \quad (6.25)$$

while that for the Rong et al. model is given as [100]:

$$\beta = \frac{1}{2} \rho_f \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 A_{ref} |\mathbf{u}_f - \mathbf{u}_{p,i}| \varepsilon_f^{2 - \left[2.65(\varepsilon_f + 1) - (5.3 - 3.5\varepsilon_f) \varepsilon_f^2 e^{\left(\frac{-(1.5 - \log_{10}(Re_p))^2}{2} \right)} \right]} \quad (6.26)$$

The Koch and Hill drag model is derived based on results obtained from lattice-Boltzmann simulations. It is calculated according to Eq. (6.19) where the momentum exchange coefficient

cient β is determined as [68]:

$$\beta = \frac{18\mu_f \varepsilon_f^2 \varepsilon_p}{d_p^2} \left(F_0(\varepsilon_p) + \frac{1}{2} F_3(\varepsilon_p) Re_p \right) \frac{V_{p,i}}{\varepsilon_p} \quad (6.27)$$

where $\varepsilon_p = 1 - \varepsilon_f$ is the particles void fraction, $V_{p,i}$ is the particle volume, and where

$$F_0(\varepsilon_p) = \begin{cases} \frac{1+3\sqrt{\frac{\varepsilon_p}{2}} + \frac{135}{64}\varepsilon_p \ln(\varepsilon_p) + 16.14\varepsilon_p}{1+0.681\varepsilon_p - 8.48\varepsilon_p^2 + 8.14\varepsilon_p^3} & \varepsilon_p < 0.4 \\ \frac{10\varepsilon_p}{\varepsilon_f^3} & \varepsilon_p \geq 0.4 \end{cases} \quad (6.28)$$

and

$$F_3(\varepsilon_p) = 0.0673 + 0.212\varepsilon_p + \frac{0.0232}{\varepsilon_f^5} \quad (6.29)$$

The Beetstra [138] drag model was obtained from lattice-Boltzmann simulations and the drag force for a single particle is expressed as:

$$\mathbf{f}_D = 3\pi\mu_f d_p \varepsilon_f \mathbf{u}_f F_i \quad (6.30)$$

where F_i is the normalized drag for a mono-dispersed system and is defined as:

$$F_i = \frac{10\varepsilon_p}{\varepsilon_f^2} + \varepsilon_f^2(1 + 1.5\varepsilon_p^{0.5}) + \frac{0.413Re}{24\varepsilon_f^2} \left[\frac{\varepsilon_f^{-1} + 3\varepsilon_p \varepsilon_f + 8.4Re_p^{-0.343}}{1 + 10^{3\varepsilon_p} Re_p^{-(1+4\varepsilon_p)/2}} \right] \quad (6.31)$$

The Gidaspow [46] drag model is a combination between the Ergun equation and Wen-Yu drag model. It is defined as:

$$\beta = \begin{cases} \frac{150(1-\varepsilon_f)^2 \mu_f}{\varepsilon_f d_p^2} + \frac{1.75(1-\varepsilon_f) \rho_f (\mathbf{u}_f - \mathbf{u}_{p,i})}{d_p} & \varepsilon_f < 0.8 \\ \frac{3}{4} C_D \frac{\varepsilon_f |\mathbf{u}_f - \mathbf{u}_{p,i}| \rho_f (1-\varepsilon_f)}{d_p} \varepsilon_f^{-2.65} & \varepsilon_f \geq 0.8 \end{cases} \quad (6.32)$$

where for the case of $\varepsilon_f \geq 0.8$, the drag coefficient C_D is determined as:

$$C_D = \begin{cases} \frac{24}{Re_p} \left(1 + 0.15(Re_p)^{0.687} \right) & Re_p < 1000 \\ 0.44 & Re_p \geq 1000 \end{cases} \quad (6.33)$$

For additional information about the different drag models available, we refer the reader to the article by Norouzi et al. [102] or by Bérard et al. [43].

Buoyancy Force

It is the force exerted by the fluid on the submerged particle that opposes its weight. It is given by the following equation [46]:

$$\mathbf{f}_B = -\rho_f V_{p,i} \mathbf{g} \quad (6.34)$$

The buoyancy force becomes important in fluidized and spouted beds when the ratio of particle to fluid densities is significant. The buoyancy force is only applied on the particles, as the pressure calculated using the VANS equations includes the hydro-static pressure.

Undisturbed Flow Forces

These forces are given by [43]:

$$\mathbf{f}_{\nabla p} = -V_p \left(\frac{\partial p}{\partial x} \right) = -V_{p,i} \nabla P \quad (6.35)$$

$$\mathbf{f}_{\nabla \cdot \tau} = -V_p \left(\frac{\partial \tau}{\partial x} \right) = -V_{p,i} \nabla \cdot \tau \quad (6.36)$$

where $\mathbf{f}_{\nabla p}$ and $\mathbf{f}_{\nabla \cdot \tau}$ are the pressure and shear forces respectively, and ∇P and $\nabla \cdot \tau$ are the gradient of the pressure and divergence of the stress tensor interpolated at the particle's location respectively. For Model A, these forces are implicitly added to the fluid since the void fraction multiplies the pressure and stress tensor gradients, and therefore should only be added explicitly to the particles. For Model B, it should be explicitly added for both solid and fluid phases.

All of the fluid-particle interactions are applied to both the solid and fluid phases to ensure that Newton's third law of motion is respected. The expression of the particle-fluid interactions for the VANS equations are $\mathbf{F}_{pf}$ for the force applied on the fluid phase and $\mathbf{f}_{fp}$ for the force applied on the solid phase. For model B, these forces become:

$$\mathbf{F}_{pf_B} = \frac{1}{V_{\Omega_e}} \sum_{N_p} \left(\mathbf{f}_{DB} + \mathbf{f}_{\nabla p} + \mathbf{f}_{\nabla \cdot \tau} \right) \quad (6.37)$$

$$\mathbf{f}_{fp_B,i} = \left(\mathbf{f}_{DB,i} + \mathbf{f}_{B,i} + \mathbf{f}_{\nabla p,i} + \mathbf{f}_{\nabla \cdot \tau,i} \right) \quad (6.38)$$

where V_{Ω_e} is the volume of the finite element Ω_e . The particle-fluid force of model A is given

by:

$$\mathbf{F}_{pf_A} = \frac{1}{V_{\Omega_e}} \sum_{N_p} \left(\mathbf{f}_{D_A} \right) \quad (6.39)$$

$$\mathbf{f}_{fp_A,i} = \left(\mathbf{f}_{D_A,i} + \mathbf{f}_{B,i} + \mathbf{f}_{\nabla p,i} + \mathbf{f}_{\nabla \cdot \tau,i} \right) \quad (6.40)$$

6.3 Verification and Validation of the CFD-DEM Model

In order to verify and validate our model, we simulate several test cases. The series of test cases include particle sedimentation, a fluidized bed, the Rayleigh Taylor instability and a spouted bed.

6.3.1 Particle Sedimentation Test Case

We simulate a dense particle initially at rest falling in a stagnant liquid and we measure the instantaneous velocity of the particle. We then compare the velocity obtained from the simulation with that calculated by numerically solving the following ordinary differential equation (ODE):

$$m_p \frac{\partial u}{\partial t} = \left(\mathbf{F}_D - V_p(\rho_p - \rho_f)\mathbf{g} \right) \quad (6.41)$$

where m_p is the particle mass and ρ_p is the particle density. After some time, the particle should reach a constant velocity known as the settling or terminal velocity. This occurs when the drag balances the gravitational force and buoyancy [46]. The settling velocity $\mathbf{v}_r$ is given as:

$$\mathbf{v}_r = \sqrt{\frac{V_p(\rho_p - \rho_f)\mathbf{g}}{\frac{1}{2}\rho_f C_D A_{ref}}} \quad (6.42)$$

where C_D is the drag coefficient given based on the drag model used. We use the DiFelice drag model.

Simulation Setup

The cylinder in which the particle will fall should be large enough so that its walls have no effect on the sedimentation of the particle. For this, we choose a cylinder with a radius 25 times greater than the particle's diameter (2 mm). The particle was inserted in the middle at a height of 0.08 from the center of the cylinder having the following coordinates (0.08,0,0).

The gravitational acceleration of 9.81 m/s^2 was applied in the x-direction. The DEM time step chosen was 3.28% of the Rayleigh time step. We chose a very coarse mesh as to avoid velocity fluctuations as the particle moves across cells. Only the drag and buoyancy forces were enabled for this simulation as to respect the ODE of Eq. (6.41). The physical properties chosen are typical values often used for water as a fluid and glass beads as the solids. We used Q1-Q1 second order finite elements in velocity and pressure. All simulation parameters are given in Table 6.2.

Table 6.2 Physical and numerical parameters for the particle sedimentation test case.

<i>Simulation control</i>			
End time (s)	0.5		
Coupling frequency	10^2	CFD time step (s)	10^{-3}
<i>Geometry</i>			
Bed Height (mm)	100	Bed Radius (mm)	50
Wall Thickness (mm)	0	Mesh Type	dealii::subdivided-cylinder
Mesh Refinement	1	Mesh Subdivisions in x	5
<i>Particles</i>			
Number	1	Diameter(m)	2×10^{-3}
Density(kg/m^3)	2500	Young Modulus (N/m^2)	1×10^6
Particle-particle poisson ratio	0.3	Particle-wall poisson ratio	0.3
Particle-particle restitution coefficient	0.2	Particle-wall restitution coefficient	0.2
Particle-particle friction coefficient	0.1	Particle-wall friction coefficient	0.1
Particle-particle rolling friction	0.2	Particle-wall rolling friction	0.3
<i>Gas phase</i>			
Viscosity ($\text{Pa} \cdot \text{s}$)	1.005×10^{-6}	Density (kg/m^3)	997
Inlet Velocity (m/s)	0	Void fraction smoothing factor L^2	0
<i>Linear Solver</i>			
Method	GMRES	Max iterations	5000
Minimum residual	1×10^{-11}	Relative residual	10×10^{-3}
ILU preconditioner fill	1	ILU preconditioner absolute tolerance	1×10^{-14}
ILU preconditioner relative tolerance	1		
<i>Non-linear solver</i>			
Tolerance	1×10^{-9}	Max iterations	10

Results and Discussion

We show the instantaneous velocity of the particle in Figure 6.3. Based on the obtained results, the velocity of the particle follows the analytical solution until it reaches the correct value of the settling velocity $\mathbf{v}_r = 0.2328\text{m/s}$.

This simple test case allows the validation of our drag and buoyancy implementation.

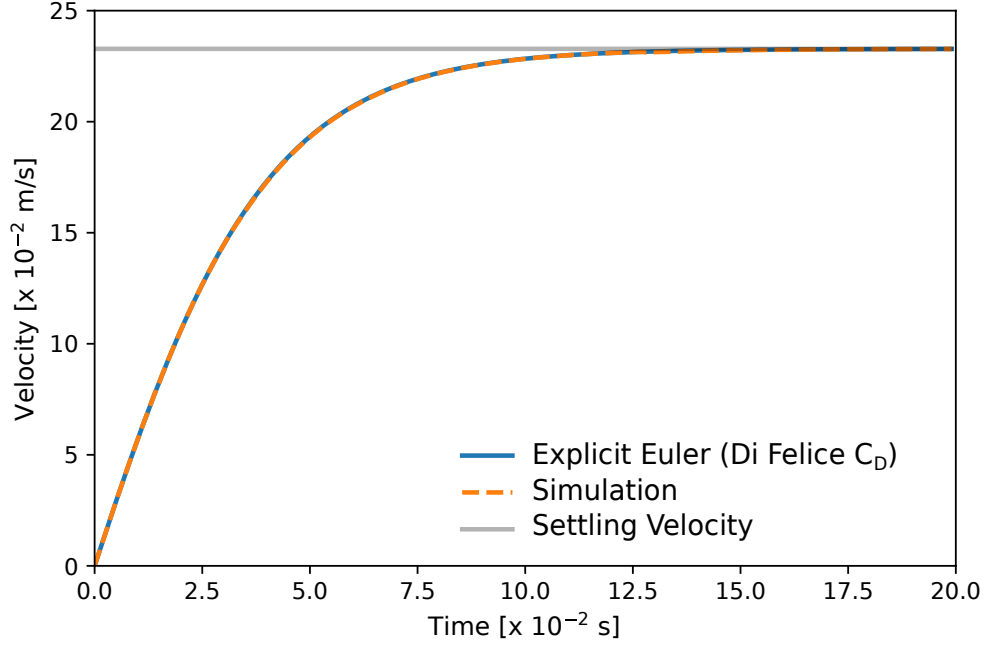


Figure 6.3 Instantaneous velocity of particle during sedimentation.

6.3.2 Fluidized Bed Test Case

We study the pressure drop as a function of inlet velocity in a fluidized bed. We compare the measured pressure drop with that obtained from the Ergun equation. The Ergun equation is a correlation that predicts the pressure drop in a packed bed and is given by [95]:

$$\Delta p = \frac{150(1 - \varepsilon_f)^2 \mathbf{u}_f \mu_f H_b}{\varepsilon_f^3 d_p^2} + \frac{1.75(1 - \varepsilon_f) \rho_f \mathbf{u}_f^2 H_b}{\varepsilon_f^3 d_p} \quad (6.43)$$

where H_b is the bed's height. After fluidization, the pressure drop becomes constant and proportional to particle weight held by the fluid and is given as:

$$\Delta p = \frac{N_p V_p (\rho_p - \rho_f) g}{A_b} \quad (6.44)$$

where N_p is the total number of particles in the bed and A_b is the bed's cross sectional area. In a fluidized bed, the pressure drop is only the contribution of the drag and buoyancy forces. We simulate the fluidized bed test case using both Q1-Q1 and Q2-Q1 elements to demonstrate the high order capabilities of our CFD-DEM solver. For the discretization in time, we use the first order backward difference scheme (BDF1).

Simulation Setup

We first use the DEM solver to fill a cylindrical bed with 200,000 spherical particles with a diameter of $500 \mu m$ belonging to the Geldart B group. The gravitational acceleration of $9.81 m/s^2$ was applied in the x-direction. The DEM time step chosen was 10.38% of the Rayleigh time step. The particles are packed at a distance of $0.04 m$ above the inlet to allow the fluid flow to develop before entering the packing. This also eliminates any effects the void fraction might have at the inlet. The DEM simulation had a final time of $1 s$ to allow the particles to settle and for their kinetic energy to dissipate. Air flow is then introduced at the bottom of the bed at varying inlet velocities from $0.02 m/s$ to $0.28 m/s$ with increments of $0.02 m/s$. An additional velocity of $0.15 m/s$ was added as it represents the value close to the minimum fluidization, thus it allows us to better understand the behavior at minimum fluidization. The simulation was run once using the PCM and once using the SPM with 7 satellite particles for void fraction calculation. We choose a smoothing length for the void fraction equivalent to $4 d_p^2$. We study the fluidization curve of the bed obtained using the Di Felice [98] drag model. The simulation parameters are given in Table 6.3.

Table 6.3 Physical and numerical parameters for the fluidized bed test case.

<i>Simulation control</i>			
End time (s)	5	Time discretization scheme	BDF1
Coupling frequency	10^2	CFD time step (s)	10^{-3}
<i>Geometry</i>			
Bed Height (mm)	400	Bed Radius (mm)	10
Wall Thickness (mm)	0	Mesh Type	dealii::subdivided-cylinder
Mesh Refinement	2	Mesh Subdivisions in x	40
<i>Particles</i>			
Number	2×10^5	Diameter(m)	5×10^{-4}
Density(kg/m^3)	1000	Young Modulus (N/m^2)	1×10^6
Particle-particle poisson ratio	0.3	Particle-wall poisson ratio	0.3
Particle-particle restitution coefficient	0.9	Particle-wall restitution coefficient	0.9
Particle-particle friction coefficient	0.1	Particle-wall friction coefficient	0.1
Particle-particle rolling friction	0.1	Particle-wall rolling friction	0.1
<i>Gas phase</i>			
Viscosity ($Pa \cdot s$)	1×10^{-5}	Density (kg/m^3)	1
Inlet Velocity (m/s)	[0.02-0.28]	Void fraction smoothing factor L^2	1.25×10^{-6}
<i>Linear Solver</i>			
Method	GMRES	Max iterations	5000
Minimum residual	10^{-10}	Relative residual	10×10^{-3}
ILU preconditioner fill	1	ILU preconditioner absolute tolerance	10^{-14}
ILU preconditioner relative tolerance	1-1.1	max krylov vectors	1000 2000
<i>Non-linear solver</i>			
Tolerance	1×10^{-9}	Max iterations	10

There exists various correlations to predict the minimum fluidization velocity. Based on the particles diameter and density, we compare the simulation results with different correlations. We used Ergun [95], Wen-Yu [108], and Noda et al. [139] correlations for the minimum fluidization velocity. For a more detailed review on the different available correlations, we refer the reader to the article by Anantharaman et al. [107]. The Ergun minimum fluidization Re_{mf} is defined as:

$$Re_{mf} = \left(\left(\frac{42.86(1 - \varepsilon_{mf})}{\phi} \right)^2 + 0.571\varepsilon_{mf}^3\phi Ar \right)^{0.5} - \left(\frac{42.86(1 - \varepsilon_{mf})}{\phi} \right) \quad (6.45)$$

where ε_{mf} is the void fraction at minimum fluidization, ϕ is the sphericity of the particles ($\phi = 1$ for spherical particles), and Ar is the Archimedes number and is defined as:

$$Ar = \frac{g\rho_f(\rho_p - \rho_f)d_p^3}{\mu_f^2} \quad (6.46)$$

The Wen-Yu minimum fluidization Re_{mf} is defined as:

$$Re_{mf} = \left(33.7^2 + 0.0408Ar \right)^{0.5} - 33.7 \quad (6.47)$$

The Noda et al. minimum fluidization Re_{mf} is defined as:

$$Re_{mf} = \left(19.29^2 + 0.0276Ar \right)^{0.5} - 19.29 \quad (6.48)$$

The minimum fluidization velocity (U_{mf}) is obtained from Re_{mf} by:

$$Re_{mf} = \frac{\rho_f U_{mf} d_p}{\mu_f} \quad (6.49)$$

For this case, we found the minimum fluidization velocity using Eq. (6.45) to be $U_{mf} = 0.137$ m/s, Eq. (6.47) to be $U_{mf} = 0.135$ m/s, and Eq. (6.48) to be $U_{mf} = 0.147$ m/s. The fluidization pressure drop is calculated using Eq. (6.44) to be $\Delta p_{fluidization} = 408.34$ Pa. Grad-div stabilization was particularly interesting in this case when solving model B of the VANS equations where stability was dependant on the choice of c^* . Model A showed an enhanced stability with an optimal choice of c^* taken to be the size of the element for all cases. This was not the case for model B, where the solver was unstable for some cases.

Hence, the choice of $c^* = 1$.

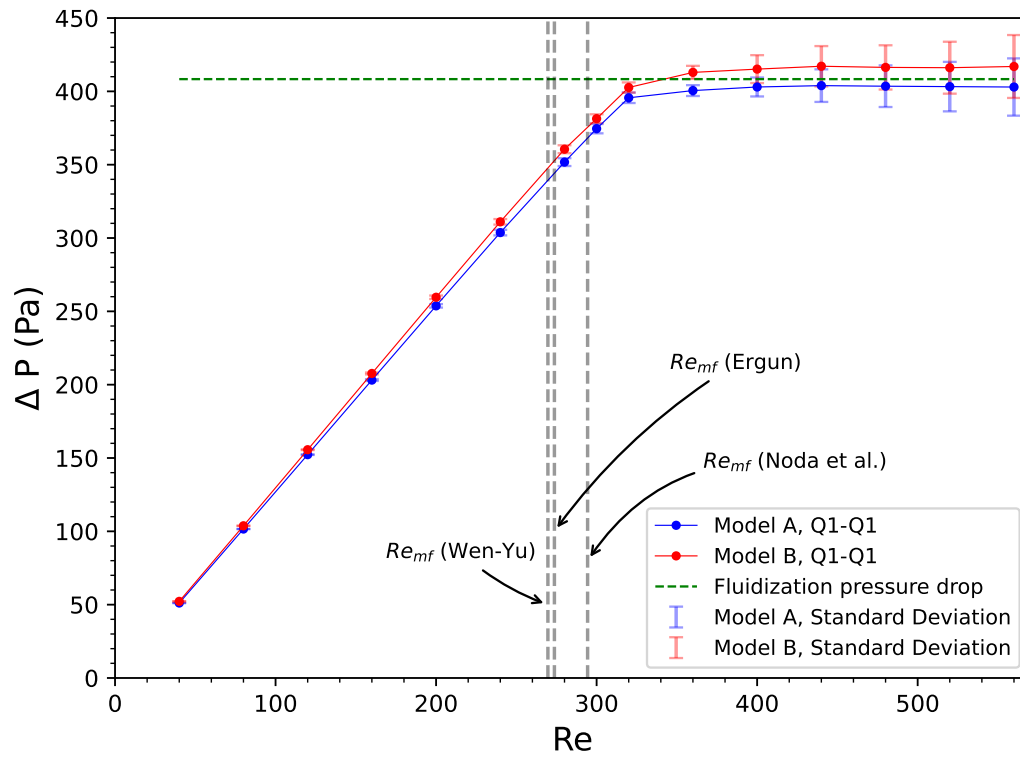
Results and Discussion

We calculate the pressure drop instantaneously, and we average it over 0.5 s after the pressure stabilizes. Figure 6.4 shows the pressure drop as a function of the different inlet velocities for both models A and B of the VANS equations for different finite element orders using the SPM void fraction scheme.

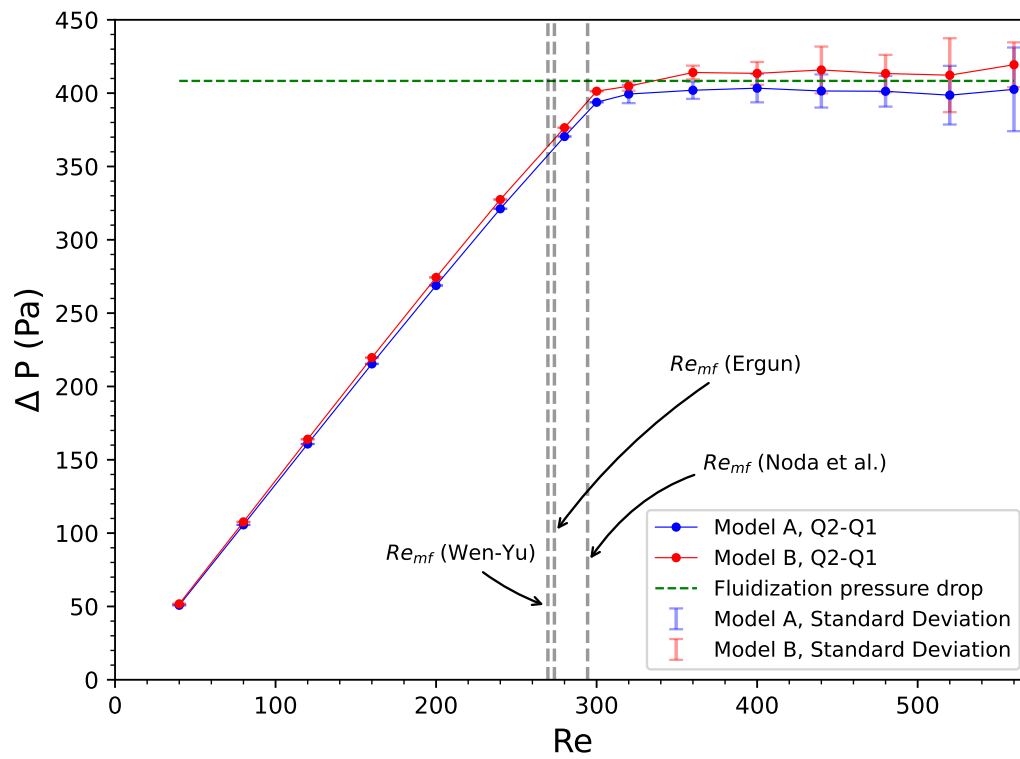
As the results for pressure drop did not differ between using the PCM and SPM void fraction schemes, only results obtained using SPM are presented. The convergence of model B with Q2-Q1 elements was difficult as the system of model B is already stiff and using high order elements exacerbates the stiffness of the system. The use of SPM instead of PCM for void fraction calculation did not help in the convergence of Q2-Q1 model B simulations. The stiffness of model B comes from explicitly adding the pressure and shear forces to the fluid. For model B with Q2-Q1 elements, few simulations with inlet velocities above minimum fluidization were not converging to the tolerance of 10^{-9} for longer simulation times. Model A is considerably more stable than model B in CFD-DEM simulations as convergence was obtained easily for the different elements orders. The bars shown represent the standard deviation over a period of 0.5 s.

For both finite element orders, it can be seen that models A and B result in a relatively close pressure drop in the bed. Model B results in a slightly larger standard deviation and that can be attributed to its instantaneous pressure drop fluctuating to larger magnitudes than that of model A. The fluctuations in pressure drop for both models is slightly higher for second order elements. Since higher order elements capture better the turbulence in the flow, we expect to observe higher fluctuations in the pressure drop.

Figure 6.5 presents the instantaneous bed height for both models using Q1-Q1 elements and an inlet velocity of 0.28 m/s. The height of both models is highly oscillatory explained by the slug flow behavior of the fluidized bed where large bubbles form at the inlet of the bed and break at the outlet of the packing region. Models A and B do not lead to the same instantaneous physical behavior. This is in part due to the chaotic behavior of a fluidized bed. The time averaged height of both models is relatively close and as such, the beds behavior is statistically similar. We notice that the two void fraction schemes lead to different bed fluctuations at the same time-step as shown in Figure 6.5, although the average height barely changes between SPM and PCM schemes. The change was more noticeable in model B where the average height is around 0.075 for PCM and 0.0725 for SPM compared to model A where the average height was 0.075 for PCM and 0.076 for SPM.

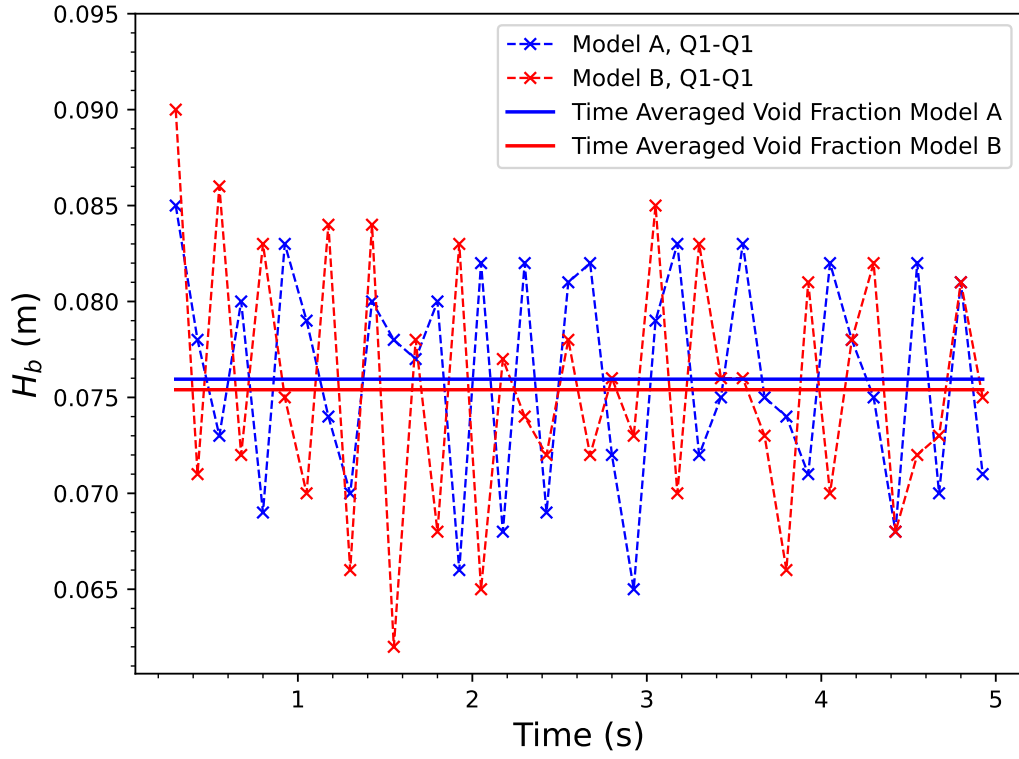


(a) pressure drop using Q1-Q1 elements

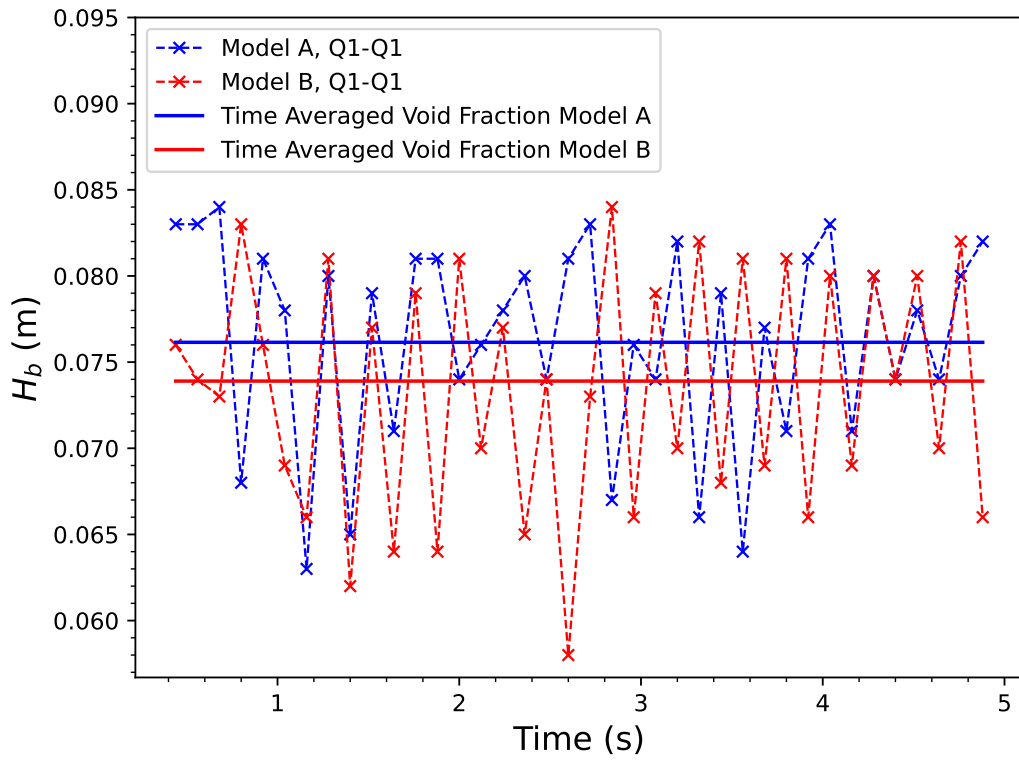


(b) pressure drop using Q2-Q1 elements

Figure 6.4 Pressure drop in fluidized bed as a function of inlet Re number using SPM.



(a) Height fluctuation using PCM



(b) Height fluctuation using SPM

Figure 6.5 Instantaneous bed height fluctuation for inlet velocity of 0.28 m/s (cont.)

For Q1-Q1 elements, we compare the time averaged height in the bed for both models as shown in Figure 6.6. The bed height was averaged over a period of 1 s. Differences between average heights using PCM and SPM are minor so only SPM results are presented.

The time averaged height is relatively close in both models for the different inlet velocities. The variation at each inlet velocity over 3 s is shown as the standard deviation which represents the magnitude of fluctuation of the bed height over this period. Model B results in fluctuations that are more pronounced when compared to those of model A as demonstrated by the standard deviation in Figure 6.6. Therefore, model A and B, though mathematically equivalent are physically different when considering the instantaneous behavior of the fluidized bed. This is caused by the different treatment of the pressure force on the fluid.

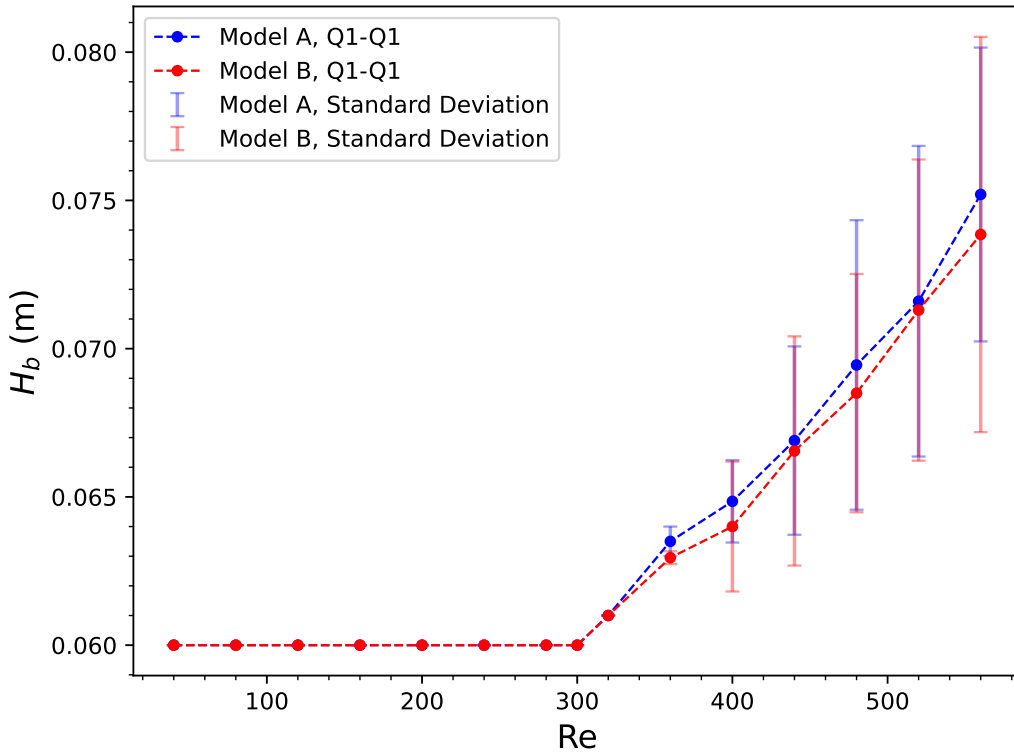


Figure 6.6 Average bed height as a function of inlet Re number using Q1-Q1 elements using SPM.

6.3.3 The Rayleigh-Taylor Instability Test Case

We study the evolution of the Rayleigh-Taylor instability as a function of different fluid and particle densities. This is a well known case in which a heavy fluid is located above a light fluid. The difference in densities makes this case an inherently unstable problem. The fluids

start mixing together under the effect of gravity. Initially, an exponential instability growth period occurs after which the mixing layer is described according to the following [140]:

$$h = \alpha A g t^2 \quad (6.50)$$

where h is the width of the mixing layer, g is the gravitational acceleration, t is the time and A is the Atwood number and is defined as:

$$A = \frac{\rho_{hf} - \rho_{lf}}{\rho_{hf} + \rho_{lf}} \quad (6.51)$$

where $\rho_{hf} = \varepsilon_f \rho_f + (1 - \varepsilon_f) \rho_p$ is the density of the heavy fluid since the heavy fluid is a mixture of fluid and particles and $\rho_{lf} = \rho_f$ is the density of the light fluid. The constant α varies slightly with the Atwood number. It is believed to be insensitive to initial conditions [141]. Therefore, we start all our simulations with the same initial conditions. According to Snider, it lies between 0.05 and 0.07 [140]. A historical survey by Dimonte et al. [141] for α obtained from experiments and numerical simulations found that α can have values between 0.03 and 0.08 [141]. It is important to note that Eq. (6.50) is only valid after the initial exponential growth period. We expect to obtain slightly larger values of α in our simulations as we are working in 3D where single modes grow faster than in 2D [141].

Simulation Setup

Similar to the fluidized bed test case setup, we insert the particles using the DEM solver before starting the CFD-DEM simulation. Particles of the same diameter and density were non-uniformly and randomly inserted in the upper section (initial height of particles is 0.05 m) of a 3 dimensional rectangular bed. The gravitational acceleration of 9.81 m/s^2 was applied in the y -direction. No initial perturbation is placed on the interface of the two fluids; however, small perturbations occur as a result of the random distribution of particles.

We use the Dallavalle drag model [137] as we want a drag force independent of the void fraction. We solve model A of the VANS equations. We apply slip boundary conditions on the side walls of the beds as to eliminate boundary effects. We apply no slip boundary conditions on the top and bottom walls to prevent fluid re-circulation. Three test cases were simulated with varying Atwood numbers. The ratio of the DEM time step chosen to the Rayleigh time step for each case as well as all parameters are presented in Table 6.4. Our choice of densities result in a close range of Atwood numbers, therefore, we expect that the difference in the instabilities and the mixing length will be relatively small.

Table 6.4 Parameters for the setup of the Rayleigh-Taylor Instability.

Particle radius (m)	0.0001	0.0001	0.0001
Particle density (kg/m^3)	3	5	10
Fluid density (kg/m^3)	1	1	1
Initial particle volume fraction	0.088	0.088	0.088
gravity (m/s)	0,-9.8,0	0,-9.8,0	0,-9.8,0
Number x,y,z mesh size	$18 \times 150 \times 18$	$18 \times 150 \times 18$	$18 \times 150 \times 18$
Bed x,y,z size (m)	$0.01 \times 0.15 \times 0.01$	$0.01 \times 0.15 \times 0.01$	$0.01 \times 0.15 \times 0.01$
Atwood Number	0.0817	0.151	0.286
Number of Particles	837925	837925	837925
CFD time step (s)	5×10^{-4}	5×10^{-4}	5×10^{-4}
CFD-DEM coupling frequency	500	500	500
$\Delta t_{DEM}/\Delta t_{crit}$ (%)	58.04	44.95	31.78

Results and Discussion

We measure the mixing width as the height of the bed starting from the first position where we have the diluted region of particles and ending with the last denser layer having less particles than the initial particle packing. This ensure we capture the complete mixing width. Figure 6.7 shows the plot of the growth rate of the mixing layer as a function of time.

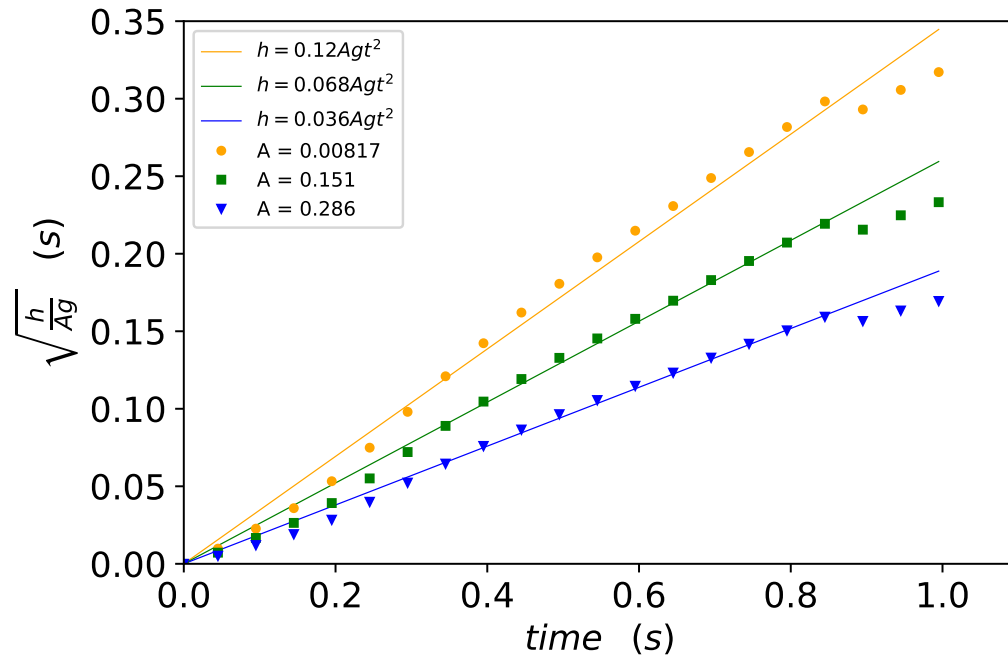


Figure 6.7 Growth rate of the mixing layer as a function of time.

The measurement of the mixing layer agrees well with the correlation of the mixing layer. The initial 0.2 s do not agree with the correlation as they represent the initial exponential instability growth where correlation (6.50) is not valid. Additionally, the sudden drop observed at around time 0.9 s is attributed to a big bubble of the light fluid reaching the top of the bed. As such, the packing at the top of the bed is disturbed, and not enough particles remain to feed the instability which eventually leads to the breaking of the mixing layer, thus rendering correlation (6.50) invalid after 0.9 s . We observe this behavior in Figure 6.8 which shows snapshots depicting the growth of the Rayleigh-Taylor instability at different times in the simulation for $A = 0.286$. In Figure 6.8, the fluid is not shown and only the particles' are presented along with their velocities.

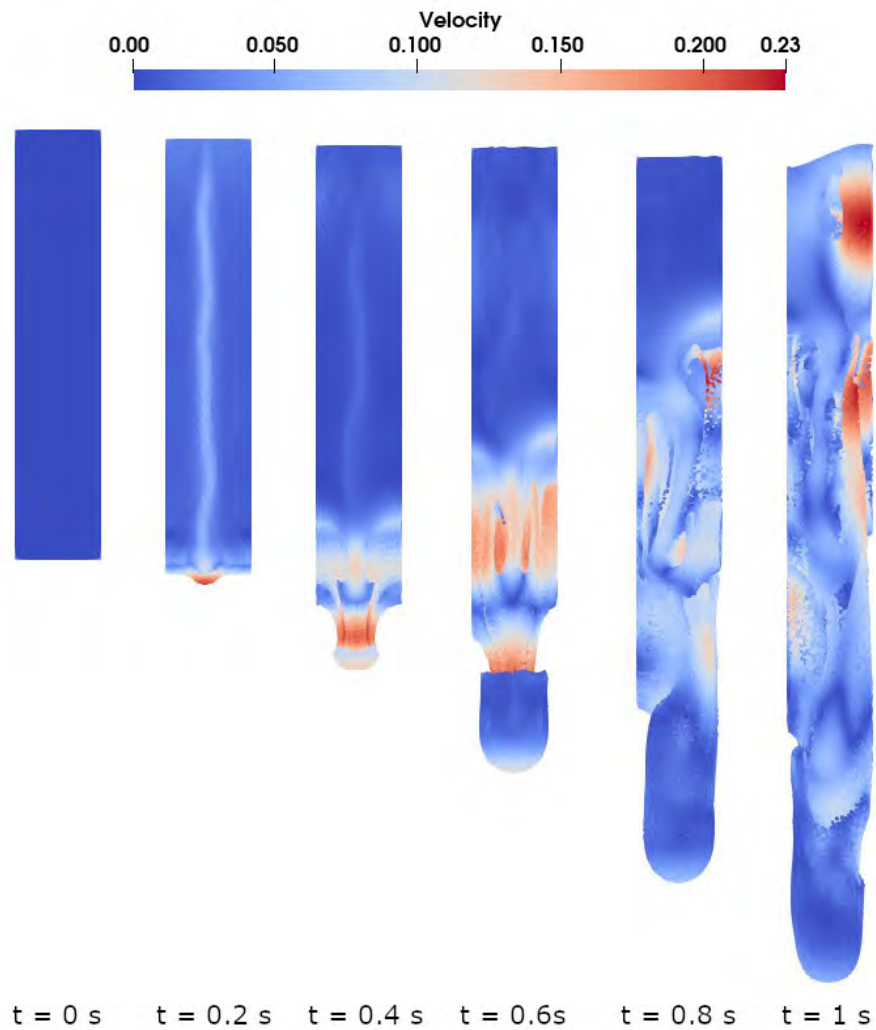


Figure 6.8 Side view of the 3D growing Rayleigh-Taylor instability plumes showing the particles' positions and velocity at different simulation times.

The bubble at $t = 1 \text{ s}$ is responsible for the sudden turn over in the curves observed at the end of the mixing layer growth of Figure 6.7. From an angle, we show the 3D plumes for $A = 0.286$ at $t = 0.45 \text{ s}$ in Figure 6.9.

The instability is formed as a major single central mushroom-shaped plume surrounded by minor plumes. The instability remains symmetrical until $t = 0.5 \text{ s}$ after which it breaks down. The symmetrical plumes created demonstrate the mass conservation property of our solver. This is clear from the formation of the plumes where the light fluid moves upward to allow space for the heavy fluid moving downwards.

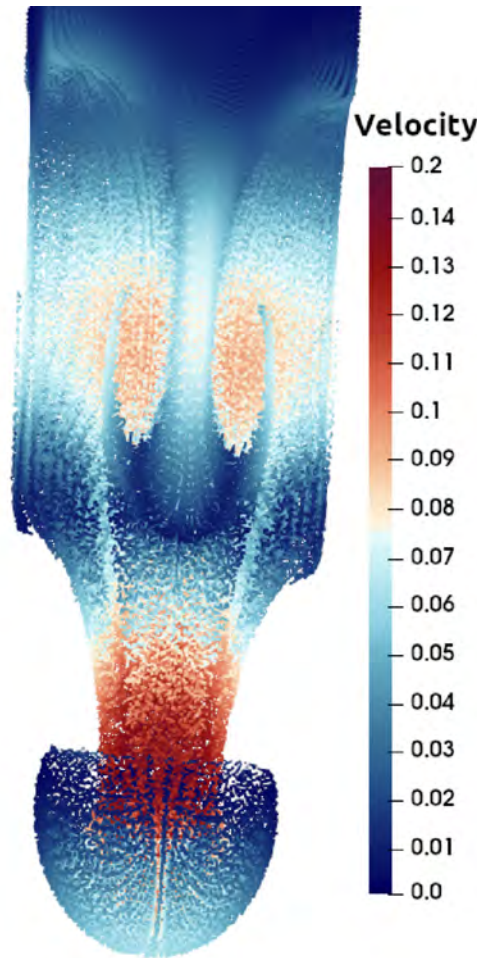


Figure 6.9 Angle view of the 3D growing Rayleigh-Taylor instability plumes for $A=0.286$ and $t=0.45 \text{ s}$.

Additionally, the circular shape of the mushroom inwards at its extremity is only achieved due to the highly accurate Q_n interpolation of the particles' properties and position within a cell.

6.3.4 Spouted Bed Test Case

We simulate a rectangular spouted bed. We calculate the time averaged particles velocities at different positions in the bed and compare the data obtained with experimental results obtained using particle image velocimetry [142].

Simulation Setup

The bed size, geometry, solid and fluid properties are extracted from the experiment of Yue et al. [142]. Figure 6.10 shows the schematic geometry of the simulation.

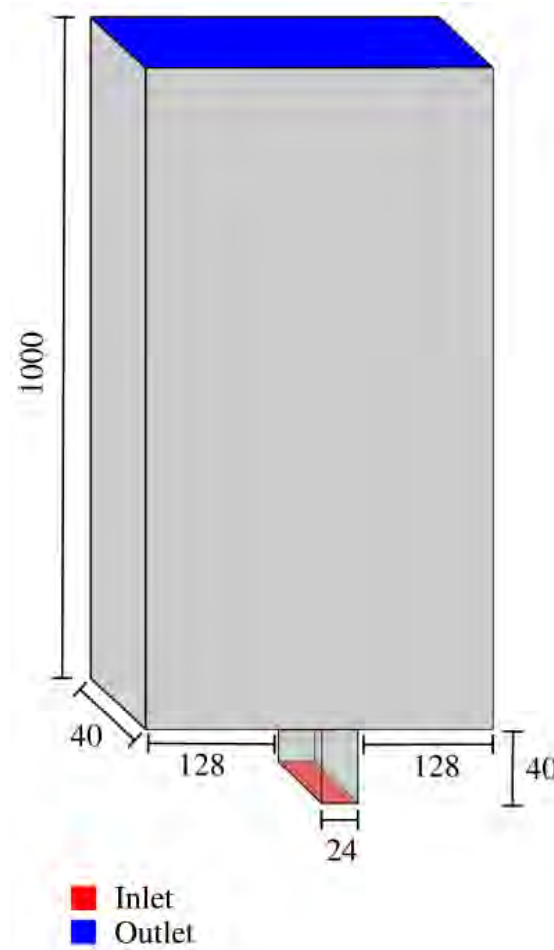


Figure 6.10 Scheme of the spouted bed geometry (unit: mm).

The authors did not specify the number of particles used but they specified the static bed height to be 200 mm. Based on the given geometry, and in order to obtain a similar static bed height, we use 175800 particles with the same properties as those used by Yue et al. [142].

The particles used in this test case belong to the Geldart D group. In order to obtain better distribution of the flow and stability of the solver, we add to the geometry a small channel at the bottom of the bed through which we introduce the gas. The geometry and mesh were generated using the open source software GMSH [143]. For this case, we solve model A of the VANS equations. The gravitational acceleration of 9.81 m/s^2 was applied in the y-direction. The DEM time step used was 4.02% of the Rayleigh time step. The study is performed using Q1-Q1 for both PCM and SPM with 7 satellite particles and Q2-Q1 elements using only PCM to calculate the void fraction, a smoothing length of $L^2 = 5d_p^2$ for the void fraction, and a grad-div stabilization parameter (c^*) equal to the element size. For the Q2-Q1 simulation, convergence was difficult for (c^*) the size of the element, so the value of (c^*) 10 times the element size was chosen as it made the Q2-Q1 simulations robust. We increment the spout inlet velocity gradually from 0 m/s at $t = 0 \text{ s}$ until it reached its maximum value of 20.8 m/s at $t = 0.05 \text{ s}$. This ensure a smooth transition of the bed from rest to the fluidized regime and prevents an initial shock from occurring due to the sudden introduction of a high velocity at $t = 0 \text{ s}$. Table 6.5 presents the physical and numerical parameters for this test case.

We perform the simulations for four particle-particle and particle-wall friction coefficients (0.3, 0.2, 0.1, and 0.05) and determine that a value of 0.3 for both allowed for the most realistic behavior of the spouted bed that is comparable to the behavior obtained from the experiments. The coefficient of rolling friction had some effect on the behavior of the bed and using a value of 0 led to the closest results with the experiments, thus it was neglected by assuming no rolling friction of particles. We apply slip boundary condition for all walls of the bed and the channel except the channel's base (inlet) and the bed's top wall (outlet). At the inlet, we apply a Dirichlet boundary condition with the value of the inlet velocity in the y-direction. For the outlet, we apply a zero traction boundary condition when the fluid is leaving the domain and we penalize the flow when the fluid is inbound. This prevents flow re-entry when there is turbulent structures or vortices leaving the domain. The outlet boundary condition imposed is:

$$\int_{\Gamma_o} (\nu \nabla \mathbf{u} \cdot \mathbf{n} - p \mathbf{I} \cdot \mathbf{n} - \beta (\mathbf{u} \cdot \mathbf{n})_- \mathbf{u}) \cdot \mathbf{v} d\Gamma = 0 \quad (6.52)$$

where β is a constant, p is the pressure, $\mathbf{I}$ is the identity matrix, $(\mathbf{u} \cdot \mathbf{n})_-$ is $\min(0, \mathbf{u} \cdot \mathbf{n})$ $\mathbf{v}$ is the velocity test function and Γ_o is the outlet boundary. For further details, we refer the reader to the work of Arndt et al. [144]. In order to prevent the particles from falling into

the channel, we define a floating wall which is an imaginary wall only felt by the particles at the top of the channel at the intersection between the channel and the bed base.

Table 6.5 Physical and numerical parameters for the setup of the spouted bed test case.

<i>Simulation control</i>			
End time (s)	20	Time discretization scheme	BDF2
Coupling frequency	100	CFD time step (s)	5×10^{-4}
<i>Geometry</i>			
Bed Height (mm)	1000	Bed Width (mm)	280
Bed Depth (mm)	40	Wall Thickness (mm)	0
Channel Height (mm)	40	Channel Width (mm)	24
Channel Depth (mm)	40		
<i>Mesh</i>			
Mesh Type	gmsb		
Bed Subdivisions in x-y-z	36-100-4	Channel Subdivisions in x-y-z	2-5-4
<i>Particles</i>			
Number	175800	Diameter(m)	25×10^{-4}
Density(kg/m^3)	2500	Young Modulus (N/m^2)	1×10^7
Particle-particle poisson ratio	0.25	Particle-wall poisson ratio	0.25
Particle-particle restitution coefficient	0.9	Particle-wall restitution coefficient	0.9
Particle-particle friction coefficient	0.3	Particle-wall friction coefficient	0.3
Particle-particle rolling friction	0	Particle-wall rolling friction	0
<i>Gas phase</i>			
Viscosity ($Pa \cdot s$)	1.81×10^{-5}	Density (kg/m^3)	1
Inlet Velocity (m/s)	20.8		
<i>Linear Solver</i>			
Method	GMRES/AMG	Max iterations	1000/100
Minimum residual	10^{-8}	Relative residual	10^{-2}
ILU preconditioner fill	1	ILU preconditioner absolute tolerance	10^{-10}
ILU preconditioner relative tolerance	1	max krylov vectors	200
<i>Non-linear solver</i>			
Tolerance	1×10^{-9}	Max iterations	25

Results and Discussion

For both Q1-Q1 and Q2-Q1 simulations, we measure the time averaged particle velocity profile in the direction of the flow at different heights (y-axis) of the bed and we compare the values with the experimental results of Yue et al. [142]. The results obtained using both the PCM and SPM void fraction schemes are presented. The heights in Figures 6.11 and 6.12 are normalized by the static bed height. Figure 6.11 shows the average particles velocity magnitude at different heights in the spouted bed along the bed's width for the

Q1-Q1 simulation using the PCM and SPM void fraction schemes.

The spout is centralized at $x = 0 \text{ m}$ and the velocities obtained from the simulation agrees well with the experimental velocities. It is important to note that the experimental velocities were measured using Particle Image Velocimetry (PIV) which already involves errors in measurement. Around the central spout, we observe re-circulation zones at $x \in [0.05, 0.1] \text{ m}$ & $x \in [-0.1, -0.05] \text{ m}$. The calculated re-circulation velocity magnitude is smaller than that measured in the experiments. This could be due to errors in the PIV measurements as the zones are not symmetric in the experiments contrary to what they

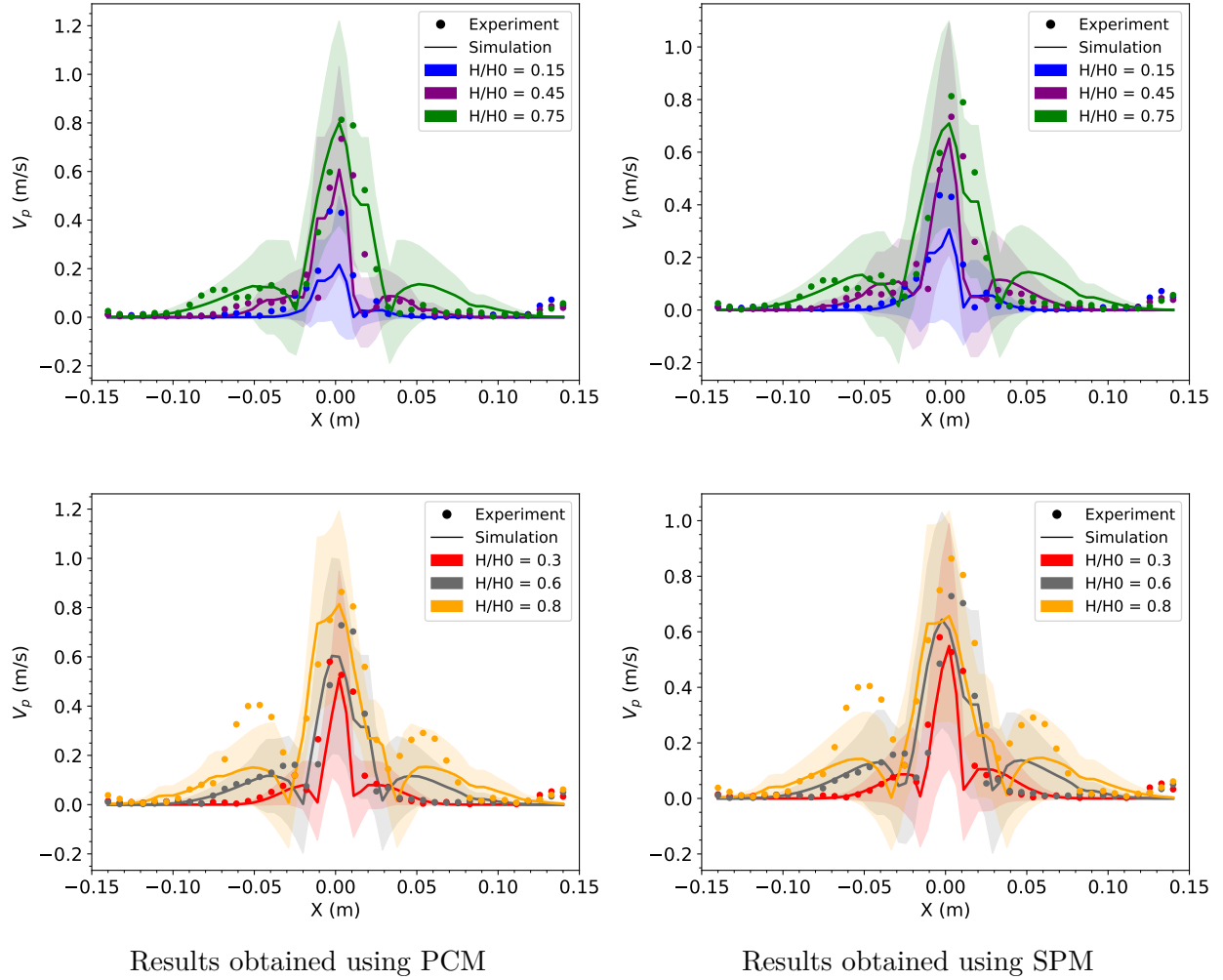


Figure 6.11 Distribution of particle velocity magnitude in vectors along the X direction at different height levels for Q1-Q1 simulation.

should be. Additionally, we calculate the particles average velocity magnitude by averaging over the finite elements cells which is different than the averaging procedure performed in the

experiments. However, the general trend of the results follows well that of the experiments. We average over the last 15 s out of the 20 s of the simulation to ensure that the averaging is performed only when the pseudo steady state has been reached. We show the standard deviation of our curves as a zone of the same color. This standard deviation represents the fluctuation of particles velocity at this location with respect to time. All experimental velocities lie in the respective standard deviation zones except for the re-circulation velocities at $H/H_0 = 0.8$. This demonstrates that despite all possible measurement and averaging errors, the simulation gives good results comparable to the experimental results of the bed.

The difference between results obtained using PCM and SPM are minimal. The main difference lies in the spout region where the PCM scheme leads to higher average particle velocities compared to the SPM scheme. This might be explained by the strong temporal discontinuity of the PCM scheme which can lead to high gradients in the void fraction profile resulting in high velocity gradients as well. Even though the SPM is also discontinuous in time, the effect of this discontinuity is reduced due to the refinement of the particles.

To investigate and better understand the effect of high order methods, we simulate the same case using Q2-Q1 elements. This is done only using the PCM void fraction scheme, as the effect of the void fraction scheme was described using Q1-Q1 elements and the aim is to determine the effect of high order schemes on the behavior of the spouted bed. The results are shown in Figure 6.12

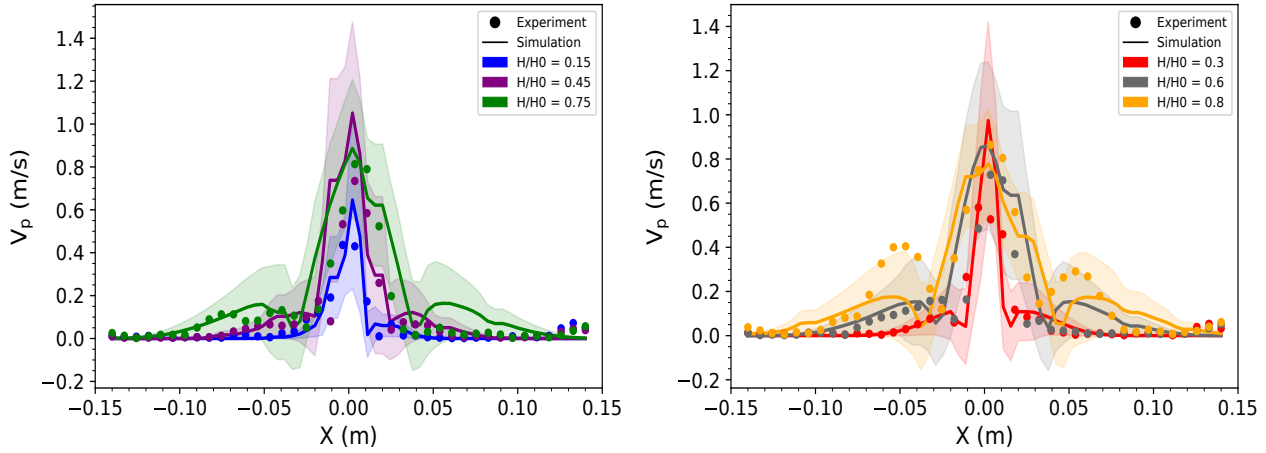


Figure 6.12 Distribution of particle velocity magnitude in vectors along the X direction at different height levels for Q2-Q1 simulation using PCM.

The differences between Q1-Q1 and Q2-Q1 simulations results are mainly localized in the

spout region at low values of the reference height. The four smallest heights from 0.15 till 0.6 have a much higher average particle velocity in Q2-Q1 simulations compared to the Q1-Q1 simulation while the two largest heights of 0.75 and 0.8 have a relatively similar velocity profile in both simulations. This can be attributed to the fact that the Q2 interpolation captures more adequately the fluid jet in the spout region because it induces less numerical dissipation. The Q2-Q1 scheme also has a richer interpolation space and can capture a velocity profile that abruptly changes in space. The Q2-Q1 results are thus in much better agreement with the experimental results in this region. In general, the oscillation of the curves in time are more prominent in the Q1-Q1 than in the Q2-Q1 results. This explains the overall thinner standard deviation zones in Figure 6.12 compared to Figure 6.11. However, around $x = 0$ m and for the heights closer to the inlet, the standard deviation is high. This is caused by the high velocity and turbulent structures in this region leading to strong oscillations with time. Finally, the experimental particles velocities in the re-circulation zones for height 0.8 lies within the standard deviation zone calculated from the simulation. Thus, this zone is also better captured in the Q2-Q1 simulation.

In general, certain studies which included CFD-DEM simulations of spouted beds produced results which were similar to the results obtained by our Q1-Q1 simulation while others did not. Jajcevic et al. [68] obtained results which agreed well with their experiments for a single spout where the higher bed height possessed the larger solid velocities while Gryczka et al. [145] obtained results which did not agree with their experiments where the simulated solid velocities were much smaller than the experimentally measured velocities. Zhao et al. [146] and Duarte et al. [147] both obtained results which were tending to an inverted trend than our Q1-Q1 results. They obtained the largest particle velocities at the smallest heights and the lowest particle velocities with the largest heights. The results of Duarte et al. [147] did not agree well with experimental results of He et al. [148] against which they were comparing.

Effect of load balancing on computational time

Our CFD-DEM solver supports load balancing; however, there are many parameters that should be accounted for to ensure enhanced computational efficiency such as the ratio of solid particle to fluid cell weight and the frequency of load balancing. Among these parameters, we focus on studying the ratio of solid particle to fluid cell weight. For the purpose of this study and to reduce the computational cost of the simulation, we simulated the spouted bed test case with a coarser mesh of 18-70-4 for the bed and 2-3-4 for the channel in x-y-z and with half the number of particles (87,900 particles) using Q1-Q1 elements for different particle to

fluid cell weight ratios at six different numbers of processors. The simulation was run for 1 s of real time and a time step of 0.001 s using the dynamic load balancing approach which automatically detects the load balancing steps from the distribution of particles and cells among the processors [105]. All other parameters were kept the same as given in Table 6.5. The result is shown in Figure 6.13.

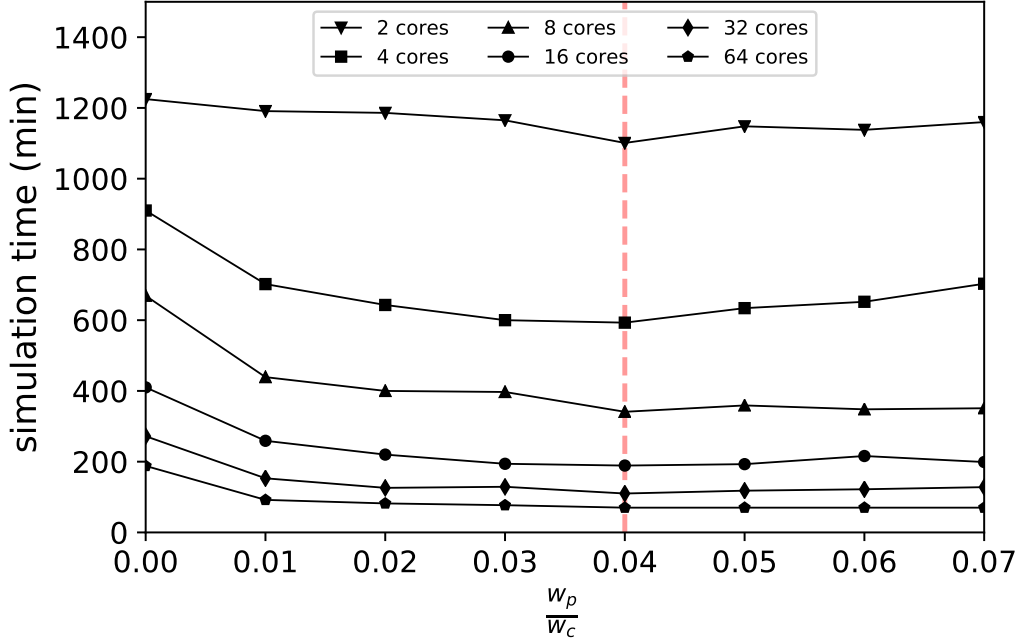


Figure 6.13 Overall simulation time as a function of the the particle to cell weight ratio for different number of processors.

For all simulations, a particle to cell weight ratio of 0.04 is the optimum ratio. However, the difference in speed between two neighboring ratios of 0.04 is negligible as it only adds few minutes to the simulation. As such, knowing the neighborhood of the optimal weight ratio to use is sufficient as it can affect drastically the speed especially for simulations with a lower number of processors. Moreover, looking at the trend of simulation time as a function of weight ratios, we observe that the bigger the number of processors used, the less effect the change in weight ratios has on the overall simulation time.

We plot the speedup of the simulation as a function of the number of processors in a logarithmic scale as shown in Figure 6.14. Overall, the CFD-DEM solver scales well. For a lower number of processors, our solver scales better than for an increased number of processors. This is because at lower number of processors, the matrix assembly of the CFD solver is the most consuming part and can take up to 70 % of a time step. The higher the number of

processors, the faster the matrix assembly gets as the matrices on each processor become smaller. However, increasing the number of processors beyond a certain value, in this case 16, leads to a decrease in the scaling. This is due to the DEM solver that becomes slower.

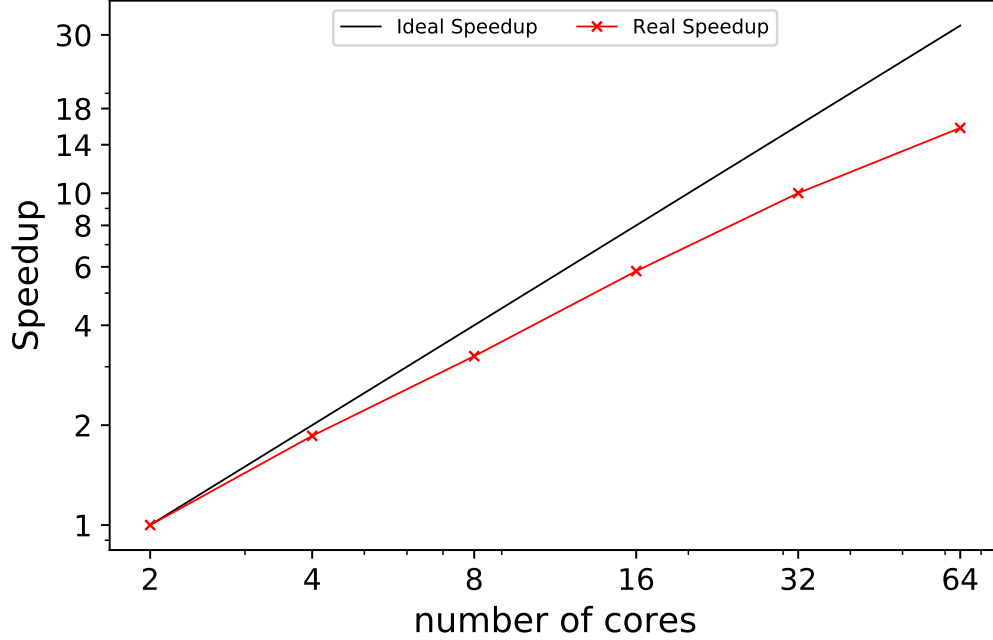


Figure 6.14 Simulation speedup as a function of processors in logarithmic scale

Our DEM solver uses the notion of ghost particles which are particles seen by the current processor but owned by another neighboring processor. As the number of processors increase, the number of ghost particles increase as well as a single particle is owned by one processor but can be seen as a ghost particle by more and more processors. This leads to an increase of the computational cost as the DEM solver has to perform more calculations related to the ghost particles. For 2 processors, an average of 43950 particles exists in a single processor. This value approximately decreases by a factor of 2 everytime we double the number of processors. At 16 processors, this value is around 5493 particles per processor. Additional decrease in this value leads to a decrease in the scalability of the DEM solver for which quasi-ideal scaling could be obtained at 20,000 particles per core [105].

6.4 Conclusion

This work presents a verified and validated stabilized finite element approach for the modeling of multi-phase flows using unresolved CFD-DEM. Our unified coupled solver is robust,

parallel and supports both models A and B of the VANS equations. It supports high order finite elements which allows for more accurate results using bigger mesh sizes thus respecting the requirement for large enough mesh sizes without compromising accuracy. Also, it is among the first CFD-DEM software to support load balancing. This helps improve the computational efficiency of our solver as available resources can be exploited more effectively by balancing work loads among processors. Moreover, the DEM and CFD portions of the code run on the same mesh which results in cheaper communication and coupling between them. Furthermore, our formulation is locally and globally conservative.

Our solver can simulate solid-fluid flows for different applications. We validate the code with different test cases. In the fluidized bed test case, we show that even though model A and B are mathematically equivalent, they result in different instantaneous physical behavior of fluidized beds. Model A is more stable and results in less stiffness of the system being solved. From the Rayleigh Taylor instability, we prove mass conservation of our solver as well as accurate interpolation of the particle-fluid forces. The spouted bed test case allows us to compare the particles velocity at different bed heights with experimental data. In this case, the use of high-order schemes leads to time-averaged particle velocity profiles which are in better agreement with experimental results, especially in the spout region. We can thus conclude that our results are realistic and our formulation is validated. We think that the use of higher-order schemes is a promising way to simulate complex solid-fluid flows using CFD-DEM since it allows for a richer and more accurate description of the flow field while maintaining an adequate particle to cell size ratio.

6.5 Acknowledgements

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CHAPTER 7 ARTICLE 3 : QUADRATURE-CENTERED AVERAGING SCHEME FOR ACCURATE AND CONTINUOUS VOID FRACTION CALCULATION IN COMPUTATIONAL FLUID DYNAMICS-DISCRETE ELEMENT METHOD SIMULATIONS

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Declaration: The author of this thesis has contributed to the literature review, code development, simulation and modelling, analysis of the results and the writing of the article.

Abstract: We propose a novel method to calculate the local void fraction in solid-fluid Euler-Lagrange models in an attempt to better predict the behavior of multi-phase flows in complex CFD-DEM simulations. This method is efficient, continuous in both time and space and valid in structured and unstructured meshes. Cheap and common methods such as the particle centroid method (PCM) are commonly used to determine the void fraction. When particles are partially located in a cell, their volume contribution is not evaluated accurately, leading to inaccurate prediction of the void fraction and, consequently, inaccurate simulations. This also affects the stability of the simulation and introduces constraints on the elements size as well as the time step for the coupling between CFD and DEM. There are several analytical approaches that accurately determine the void fraction but these methods might not be always feasible due to their high computational cost as well as their inability to properly function on unstructured meshes. The proposed method aims at resolving these problems. We demonstrate the capacity of this method using its implementation in Lethe, an open-source CFD-DEM software.

7.1 Introduction

Fluidized and spouted beds are often encountered in pharmaceutical, food processing, oil and gas industries in addition to many others [2, 3]. They are often used in drying systems, pollutant control systems, and combustion systems [5]. Due to their design and operation complexity, these beds are difficult to build and scale up [6]. Therefore, investigating the dynamics of such beds becomes vital to understand the underlying phenomena governing the different processes and allowing to test different configurations and operational conditions [3]. Computational fluid dynamics-discrete element method (CFD-DEM) proved to be an

effective method in capturing the macro- and micro-scale characteristics of two phase flows that provide information specifically at the particle scale [124]. In CFD-DEM, the coupling between the solid and the fluid phase is accomplished through the incorporation of the void fraction field defined as the fraction of fluid volume in an averaging volume and the solid-fluid interactions into the Volume Averaged Navier-Stokes (VANS) equations. These equations are presented as the continuity equation (Eq. 7.1) and the momentum equation (Eq. 7.2 for model A of the VANS equations) :

$$\rho_f \frac{\partial (\varepsilon_f)}{\partial t} + \rho_f \nabla \cdot (\varepsilon_f \mathbf{u}_f) = 0 \quad (7.1)$$

where ρ_f is the fluid's density, $\mathbf{u}_f$ is the fluid's velocity and ε_f is the fluid's void fraction.

$$\rho_f \left(\frac{\partial (\varepsilon_f \mathbf{u}_f)}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}_f \otimes \mathbf{u}_f) \right) = -\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot (\boldsymbol{\tau}_f) + \mathbf{F}_{pf}^A + \rho_f \varepsilon_f \mathbf{f} \quad (7.2)$$

with

$$\boldsymbol{\tau}_f = \mu_f \left((\nabla \mathbf{u}_f) + (\nabla \mathbf{u}_f)^T \right) - \frac{2}{3} \mu_f (\nabla \cdot \mathbf{u}_f) \mathbf{I} \quad (7.3)$$

where p is the pressure, $\boldsymbol{\tau}_f$ the deviatoric stress tensor, $\mathbf{f}$ the external force, and $\mathbf{F}_{pf}$ is the momentum transfer term between the solid and fluid phases and includes forces such as drag, virtual mass, Basset force, Saffman lift, and Magnus lift [90]. $\mathbf{I}$ is the identity or unit tensor. These equations are the result of rigorous local averaging of local variables over averaging volumes that are large compared to the particle spacing and small compared to the complete system, to translate the Navier-Stokes equations for the fluid and the Newtonian equations of motion for the particles into continuum momentum balances for both the fluid and particles [149]. Theoretically, these averaging volumes do not need to coincide with the cells of the mesh. Yet, the majority of void fraction schemes use this assumption.

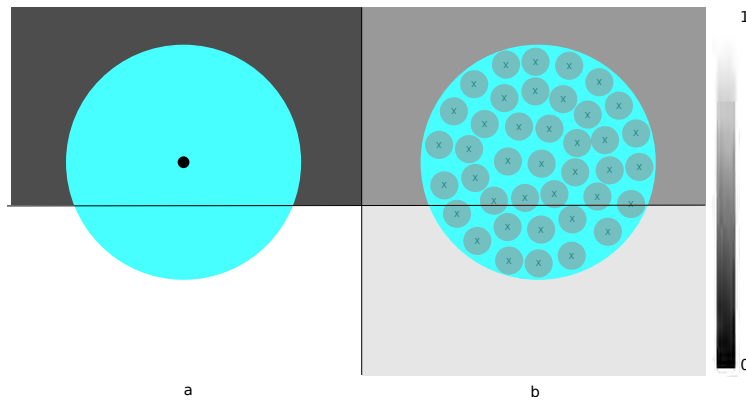


Figure 7.1 Representation of the particle volume fraction map for (a) PCM and (b) SPM.

The accuracy of the void fraction calculation directly influences the stability as well as the quality of the CFD-DEM simulation [150]. As such, several attempts have been made to accurately and efficiently predict the void fraction in CFD-DEM simulations. There exists various approaches for the calculation of the void fraction in a fluid cell, some of which are analytical methods while the others are approximation methods such as the particle centered method (PCM) and its derivatives such as the satellite point method (SPM) [54] which are presented in Figure 7.1 .

In the context of the finite element method, the PCM and SPM are both calculated per element and then projected onto its nodes. The void fraction calculation using PCM and SPM is given by:

$$\varepsilon_{f_{pcm}} = 1 - \frac{\sum^{N_p} V_p}{V_\Omega} \quad (7.4)$$

$$\varepsilon_{f_{spm}} = 1 - \frac{\sum^{N_p} \sum^{N_{sp}} V_{sp}}{V_\Omega} \quad (7.5)$$

where V_p , V_Ω , V_{sp} , N_p and N_{sp} are respectively the particle volume, the element volume, the satellite point volume, the number of particles in an element and the number of satellite points in the particle that are also in the element. After finding the void fraction value in each element, we apply an $\mathcal{L}^2$ projection by solving the minimization problem of the following equation:

$$\min_{\varepsilon \in \mathbb{R}} \frac{1}{2} \sum_i \left(\sum_j \varepsilon_j \varphi_j - \varepsilon_{f_i} \right)^2 \quad (7.6)$$

where ε_j and φ_j are the projected void fraction and the finite element shape function on each node j respectively and ε_{f_i} is the void fraction in each cell calculated previously. Thus, the $\mathcal{L}^2$ projection results in assembling and solving the following finite element system:

$$\int_\Omega \varphi_i \varepsilon_j \varphi_j d\Omega = \int_\Omega \varepsilon_{f_i} \varphi_i d\Omega \quad (7.7)$$

where φ_i is the void fraction test function. To the right hand side of Eq. 7.7, we add a

smoothing term which allows to smooth the void fraction field and reduce high void fraction gradients resulting from discontinuities in the void fraction. It is represented as:

$$\iint_{\Omega} L^2 \nabla \varphi_i \nabla \varphi_j \varepsilon_j d\Omega \quad (7.8)$$

where L is the smoothing length specified by the user. The PCM is computationally inexpensive since it only searches for the centroid of the particles. If the centroid lies within a given cell, then the entire body of the particle is considered to be in this cell. However, this method leads to large errors when the centroid of the particle lies near a cell boundary [124] leading to discontinuities in time and space and resulting in significant instabilities in the simulation and unrealistic flow behaviors. Peng et al. [150] found that the PCM can achieve similar numerical stability and prediction accuracy as the analytical approach when the cell is beyond 3.82 times the particle diameter. Nonetheless, using such big cell sizes limits the accuracy in solving the fluid phase as capturing the meso-scale flow structures becomes difficult. This is because, by default, most methods assume the cell to be the averaging volume for the VANS equations where in fact, it does not have to be. As such, a smaller cell size may satisfy the assumptions of CFD-DEM governing equations [150] rendering them valid if the methods implemented use an averaging volume independent from the cell size. In the SPM, each particle is divided into sub-particles and then the centroid of each sub-particle is treated similarly to the PCM method. A modified PCM method was developed by Peng et al. [124] where the particles are meshed into cells and the volume of the cells where added to the CFD cell in which their center is located. The SPM and the modified PCM suffers from the same limitations as the PCM. They are still discontinuous in space and time but the effect of this discontinuity is mitigated in space due to the refinement of the particle.

On the other hand, the analytical methods use geometrical-based approaches to determine the intersection between the particle and the cell and thus determine the exact volume of the particle that lies in that cell [150]. In the literature, there exist several approaches for analytically determining the void fraction: void fraction calculation in one dimensional classical soil mechanics problem [74], two dimensional problem of dense gas-solid [75], and three dimensional problems using structured meshes [76] as well as two and three dimensional solutions using unstructured meshes [77]. However, even though the analytical method is accurate and does not suffer from the same limitations of the PCM method, it is computationally very expensive as it involves the calculation of trigonometric functions at every CFD time step [77, 121]. For example, since the discrete particle method (DPM) using the analytical method is computationally expensive, the authors used a look-up table which helped save only 2-5 % of CPU time [77]. This look-up table consists of pre-computing and storing the

trigonometric analytical solutions of a particle intersection allowing the interpolation of the particles volume instead of calculating it at each CFD time step and thus speeding up calculations [77]. Additionally, analytical methods are difficult to implement in unstructured meshes which are required to simulate complex geometries [150].

In an attempt to reduce the computational cost of the analytical methods and to generalize its implementation to a wider range of geometries, several non analytical approaches were developed where approximate schemes instead of geometrical functions were used to relate the particle to the cell [150]. The divided particle volume methods (DPVM) [49, 122, 123] represents the particle as a porous cube. This method adds small amounts of spatial smoothing in comparison to the analytical approach. To reduce the smoothing effect, the corrected cube DPVM was developed [49, 123]. In these methods, spatial smoothing diffused the void fraction and thus, the presence of particles was weakly felt by the fluid [124]. Other applicable approaches included: grouping the fluid cell with its neighboring cells and calculating the void fraction for the group using the PCM method [151], using a single volume-averaging sphere per CFD cell in which the void fraction was calculated and then mapped onto the CFD mesh [152], implementing the statistical kernel method using a Gaussian distribution with a standard deviation of $1 d_p$ [49, 153, 154], using cubes to subdivide particles which resulted in errors because cubes cannot smoothly represent curved boundaries [155–157], and the use of a larger square grid as the averaging volume to calculate the void fraction before mapping it onto an arbitrary shaped CFD grid with a smaller cell size [121]. Another method used less often in CFD-DEM is coarse graining (CG) where neighboring particles are clumped together to form a single grain. This leads to better continuity and significant computational cost reduction but nonetheless introduces some inaccuracies in the numerical results [158, 159]. In essence, CG is similar to SPM in the way particles are clustered. However, the difference between these methods is that SPM is a refining strategy where the refined particles are only used for void fraction calculation while CG is a coarsening strategy where the particles of the same cluster are linked by the forces they feel and the movements they undergo. Since these methods, in general use the cell as the averaging volume, they are limited by the type and the size of the mesh used and the results obtained are usually highly mesh dependent.

Most of these approaches were developed in the context of the finite volume method (FVM). In an attempt to overcome the limitations concerning computational efficiency, accuracy, and stability which many methods suffer from, we aim at decoupling the averaging volume from the computational cell size. We therefore develop a new analytical void fraction scheme in the context of the finite element method and implement it in the open source CFD-DEM software Lethe [89, 105, 130, 160]. The scheme calculates the void fraction in a volume-averaging sphere centered at the quadrature point which is where we are interested

in determining the void fraction. Our developed scheme is analytical since it involves the calculation of intersections between particles and volume-averaging spheres and it is cheaper than current analytical methods since sphere-sphere intersections are much simpler to evaluate than sphere-polyhedron intersections. We demonstrate the space and time continuity of our scheme as well as its computational efficiency using a particle sedimentation case. We then prove the superiority of the QCM scheme over the other discussed methods through the study of the Boycott effect in the sedimentation of a group of particles in water. We later demonstrate its accuracy in predicting fluidization patterns as well as its mass conservation properties by simulating bubble formation in a flat spouted bed and comparing with experimental results as well as other void fraction schemes.

7.2 Description of the Method

We implement a new void fraction scheme that leverages the finite element method and which is available within the open-source software Lethe at <https://github.com/lethe-cfd/lethe>.

In finite elements, equations are assembled through the integration over every cell by summing over the weak form of the residual calculated at quadrature points which are defined using quadrature rules (e.g. Gauss-Legendre quadrature). The number of quadrature points is determined by the equation and the degree of the polynomial we seek to integrate. For example, Gauss-Legendre quadrature in 1D can integrate polynomials of order $2n_q - 1$ using n_q quadrature points. The method we propose in this work involves constructing a volume-averaging sphere around each quadrature point and then calculating the void fraction inside of it. We call our new void fraction method the quadrature centered method (QCM) as it is based on calculating the void fraction directly at every quadrature point. It is important to note that our scheme is applicable when an analytical formulation is available for the calculation of intersection between the particles and the volume-averaging spheres. In the present work, we limit our discussion to spherical particles for which the sphere-sphere intersections are easy to calculate.

Figure 7.2 schematically demonstrates the volume-averaging spheres used for a given mesh. Instead of calculating the void fraction in a cell using the particle centered method (PCM) or the satellite point method (SPM) and then projecting it onto the quadrature points through $\mathcal{L}^2$ projection, we evaluate it directly at the quadrature point. This makes the quadrature points of the same element feel different void fraction values depending on the number of particles neighboring the quadrature point instead of feeling the same element value of the void fraction. Moreover, the volume-averaging spheres can exceed their mother cell bound-

aries and as such, can feel particles from neighboring cells. Since the calculation for the sphere-sphere intersections are exact, this renders the scheme not only continuous in space but also in time. Thus, it results in better stability of the solver and is not limited by the size of the CFD cell as is the case with other methods such as the PCM. Furthermore, the intersection between two spheres (particle and volume-averaging sphere) is easier to calculate than the intersection between a sphere and a polyhedron (particle and cell) which makes the determination of the void fraction analytically more computationally efficient. Additionally, this method can be implemented on any finite element mesh whether structured or unstructured since we use volume-averaging spheres that are not bounded by the CFD cell. As such, implementing this method in unstructured meshes as well as in meshes with different cell sizes requires no modifications. The approach can thus work with tensor elements (quadrilaterals in 2D, hexahedron in 3D) or with simplex elements (triangles or tetrahedron). This method could also be extended to the finite volume approach by calculating the void fraction using the QCM at the centroid of the finite volume cells resulting in a method similar to that implemented by Kuang et al. [152]. The only consequence would be the absence of intrinsic variations of the void fraction within the cells as occurs in FEM.

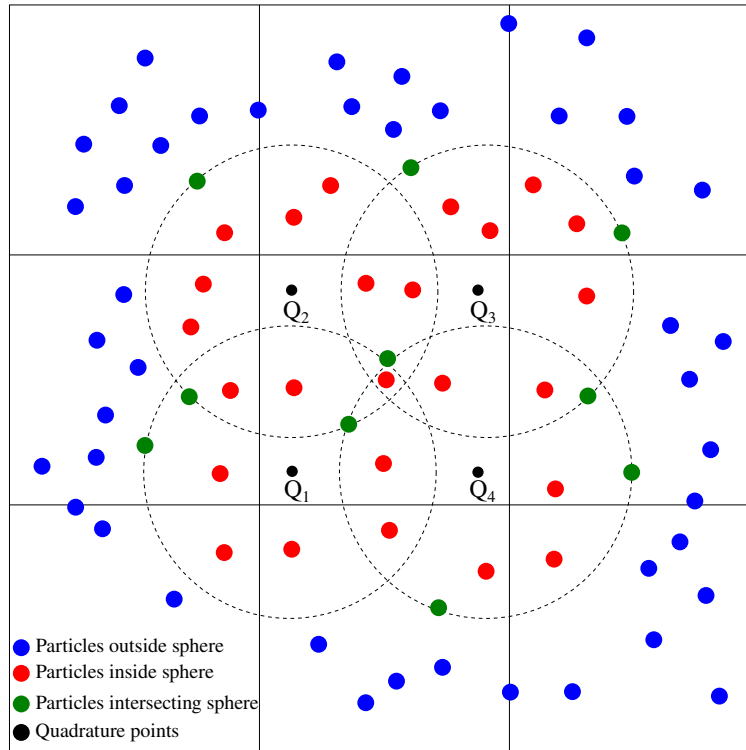


Figure 7.2 Volume-averaging spheres used in the calculation of the void fraction in computational cells for a 4 point quadrature rule.

We determine the distance d between the center of the particle and the quadrature point in order to locate the particle with respect to the volume averaging sphere and we calculate the solid fraction of particles in the sphere accordingly. Figure 7.3 shows the three possible cases between a particle and the sphere where R_s is the radius of the volume-averaging sphere and r_p is the radius of the particle.

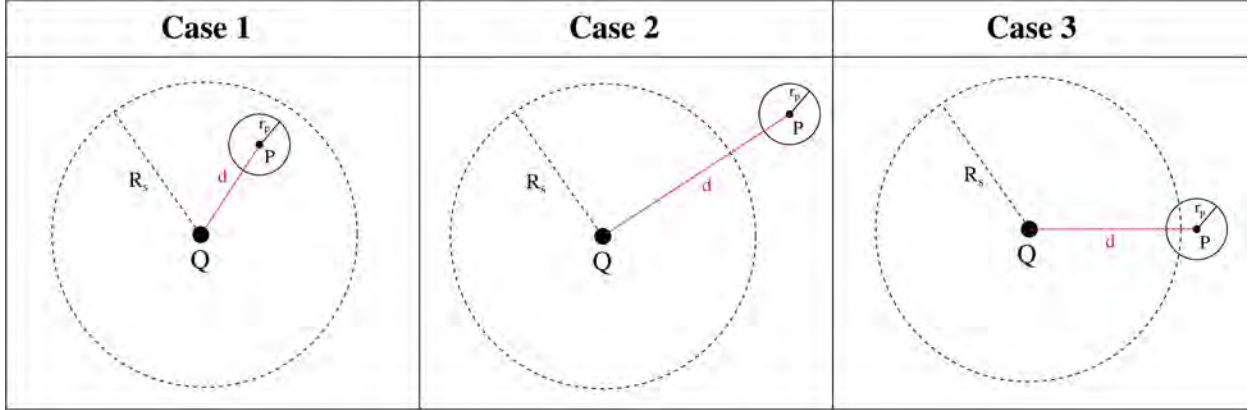


Figure 7.3 Volume-averaging sphere and particle intersection.

The void fraction at a quadrature point is calculated as follows:

$$\varepsilon_f = 1 - \frac{\sum_j V_{s,j}}{V_{sphere}} \quad (7.9)$$

where $V_{s,j}$ represents the solid volume of the j^{th} particle in the volume-averaging sphere and V_{sphere} represents the volume of a single volume-averaging sphere. The choice of the sphere's volume can be adapted to the simulation requirements but for a general case, we aim to take it by respecting the following:

$$\frac{h_\Omega}{2} \leq R_s \leq h_\Omega \quad (7.10)$$

where h_Ω is the size of element Ω . This ensures that no particle inside the cell is missed by the spheres and that the volume of the spheres do not lie outside the neighboring cells of the current cell. To ensure adequate parallel efficiency, the parallel solver only generally keep one layer of ghost cells. Consequently, we wish to ensure that we only need to loop over the first layer of neighboring cells to detect the neighboring particles.

In our implementation, unless otherwise specified, we take the radius to be the maximum usable ($R_s = h_\Omega$) to ensure better spatial distribution. Whether in 2D or in 3D, three cases

exist to determine the particles volume in a volume-averaging sphere as shown if Figure 7.2.

Case 1: particle j completely inside the volume-averaging sphere applicable when $d \leq R_s - r_p$. The volume of the particle (V_p) is entirely added to the volume of solids in sphere (V_s).

$$V_{s,j} = \frac{\pi d_p^D}{2D} \quad (7.11)$$

where d_p is the particle's diameter and D is the dimension of the problem.

Case 2: particle j completely outside the volume-averaging sphere applicable when $d \geq R_s + r_p$. We do nothing in this case as the particle does not contribute to the solids volume inside the sphere.

Case 3: particle j is partially inside the volume-averaging sphere applicable when $R_s - r_p < d < R_s + r_p$. In this case, we calculate the intersection between the sphere and the particle and we add to the solids volume, the volume of the portion of the particle that lies inside the sphere. In order to do so, we use the definition of a spherical cap to calculate the volume of intersection between the particle and the sphere. This volume of intersection is determined as the sum of the volume of the two spherical caps A and B shown in Figure 7.4 that make up the intersection between the particle and the sphere.

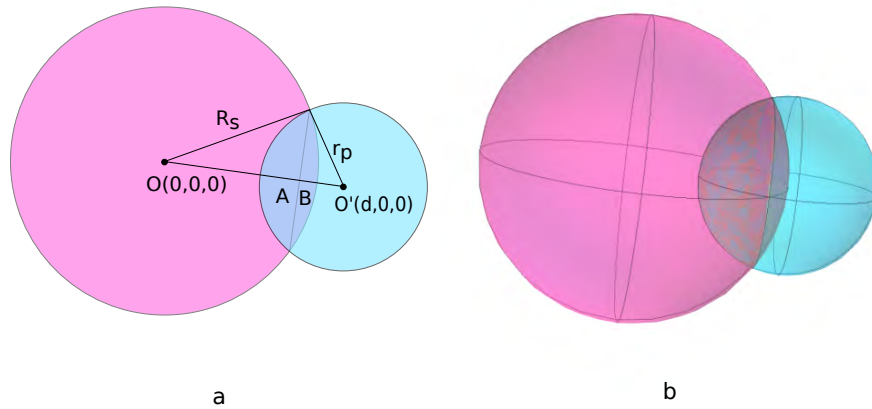


Figure 7.4 Intersection between two spheres in a) 2D and b) 3D

It is defined as:

$$V_{s,j} = \begin{cases} r_p^2 \cos^{-1} \left(\frac{d^2 + r_p^2 - R_s^2}{2dr_p} \right) + R_s^2 \cos^{-1} \left(\frac{d^2 - r_p^2 + R_s^2}{2dR_s} \right) - \frac{1}{2}\sqrt{C}, & \text{in 2D} \\ \frac{\pi(R_s + r_p - d)^2(d^2 + 2dr_p - 3r_p^2 + 2dR_s + 6r_pR_s - 3R_s^2)}{12d}, & \text{in 3D} \end{cases} \quad (7.12)$$

where C is:

$$C = (-d + r_p + R_s)(d + r_p - R_s)(d - r_p + R_s)(d + r_p + R_s) \quad (7.13)$$

Additionally, since there exist more than one sphere per cell and a particle can be felt by more than one sphere, we normalize our void fraction to ensure mass conservation. For the volume-averaging spheres, we multiply its volume by the weight of its respective quadrature point and then divide it by the sum of the weights of all quadrature points in the given cell. This ensures that the sum of all spheres' volumes in a cell is equal to the volume of the cell while also accounting for the fact that not all quadrature points contribute equally to a cell's volume. For the particle volume in sphere, we divide by the total particle contribution in all spheres in which it is felt and then multiply by the the particle volume. The normalization thus becomes:

$$\bar{V}_{sphere} = \frac{V_{sphere}w_q}{\sum_i w_i} \quad (7.14)$$

$$\bar{V}_s = \frac{\sum_j (V_{s,j}V_p)}{V_{contribution}} \quad (7.15)$$

where w_q is the weight of the quadrature point which represents the center of the current sphere, w_i is the weight of the i^{th} quadrature point in the cell and $V_{contribution}$ is the total of all the particle volume contribution in the system.

This method is valid at the boundaries. Even though the volume-averaging spheres of boundary cells might exceed the domain, the fact that we normalize the spheres volumes by the cell volume and the solids volume in the sphere by its total contribution makes the error due to the region out of the computational domain negligible. This ensures temporal and spatial continuity at the boundaries as well as mass conservation.

7.3 Particle Sedimentation

In order to demonstrate the spatial and temporal continuity of the quadrature centered method void fraction scheme, we simulate a test case of particle sedimentation in water

using the CFD-DEM solver in Lethe [160]. We compare this method with two different void fraction schemes: the particle centered method and the satellite point method. Only these methods are evaluated as they represent well-known methods frequently used and which are relatively simple to implement in a software parallelized using distributed memory parallelization (MPI).

7.3.1 Simulation Setup

We simulate the particle sedimentation in a rectangular bed large enough so that the particle does not feel the walls. The mesh was chosen to have a non negligible void fraction ($\varepsilon_f < 0.97$) while being large enough to fit at least three particles so that the PCM is valid. We did not use smoothing for the void fraction as we want to showcase the behaviors of the methods without interference of artificial smoothing. The particle was placed at the top of the bed and allowed to fall due to gravity. Only drag and buoyancy forces were enabled for this simulation. The physical and numerical parameters for the simulation are presented in Table 7.1.

Table 7.1 Physical and numerical parameters for the particle sedimentation test case.

<i>Simulation control</i>			
End time (s)	0.25		
Coupling frequency	10^2	CFD time step (s)	10^{-3}
<i>Geometry</i>			
Bed Height (mm)	200	Bed Width and Length (mm)	100
Wall Thickness (mm)	0	Mesh Type	dealii::subdivided-hyper-rectangle
Mesh Refinement	0	Mesh Subdivisions in x-y-z	5-24-5
<i>Particles</i>			
Number	1	Diameter(m)	5×10^{-3}
Density(kg/m^3)	2500	Young Modulus (N/m^2)	1×10^6
Particle-particle poisson ratio	0.3	Particle-wall poisson ratio	0.3
Particle-particle restitution coefficient	0.2	Particle-wall restitution coefficient	0.2
Particle-particle friction coefficient	0.1	Particle-wall friction coefficient	0.1
Particle-particle rolling friction	0.2	Particle-wall rolling friction	0.3
<i>Liquid phase</i>			
Viscosity ($Pa \cdot s$)	1.002×10^{-3}	Density (kg/m^3)	997
Inlet Velocity (m/s)	0	Void fraction smoothing factor L^2	0
<i>Linear Solver</i>			
Method	GMRES	Max iterations	5000
Minimum residual	1×10^{-10}	Relative residual	10×10^{-3}
ILU preconditioner fill	1	ILU preconditioner absolute tolerance	1×10^{-12}
ILU preconditioner relative tolerance	1		
<i>Non-linear solver</i>			
Tolerance	1×10^{-9}	Max iterations	10

We perform the simulation using the three previously mentioned void fraction schemes and

the Difelice drag model [98]. We perform the SPM for two different numbers of pseudo-particles (7 and 56). We track the sedimenting particle velocity and compare it between the different methods implemented.

7.3.2 Results and Discussion

The instantaneous particle velocity is shown in Figure 7.5 for the Difelice drag model [98]. The velocity profile of the particle follows the analytical solution until reaching the correct value of the settling velocity $v_r = 0.4276\text{m/s}$ which occurs when the drag balances the gravitational force and buoyancy [46]. v_r is calculated as:

$$\mathbf{v}_r = \sqrt{\frac{V_p(\rho_p - \rho_f)\mathbf{g}}{\frac{1}{2}\rho_f C_D A_{ref}}} \quad (7.16)$$

where V_p is the volume of the particle, ρ_p and ρ_f are the particle and fluid densities respectively, $\mathbf{g}$ is the gravitational acceleration, A_{ref} is the particle's cross-sectional area and C_D is the drag coefficient given based on the drag model used.

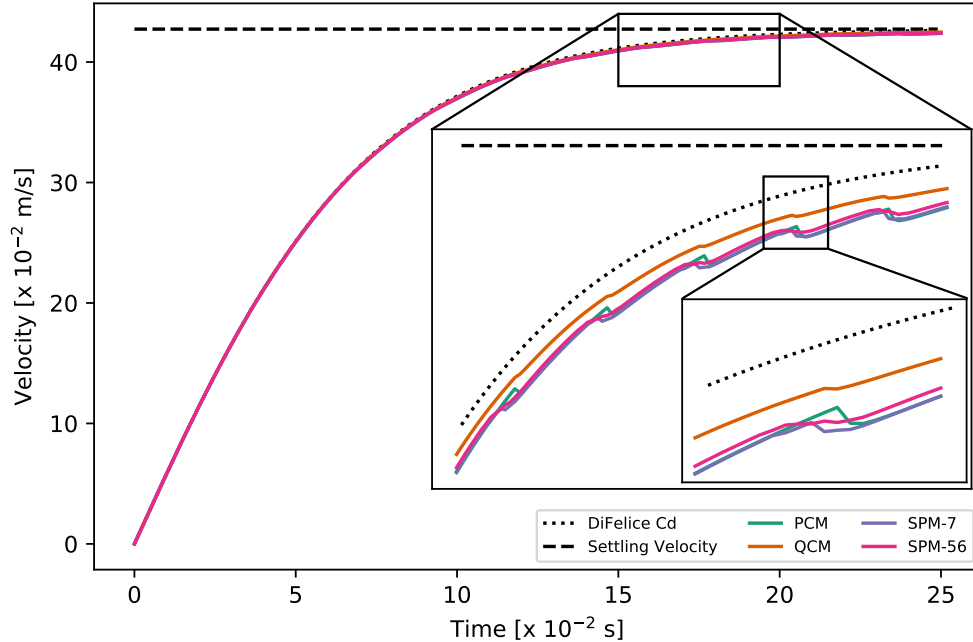


Figure 7.5 Instantaneous particle velocity during sedimentation for the different void fraction schemes.

The QCM leads to a slightly higher velocity values than the PCM and SPM methods which is closer to the expected derived value as it is not as sensitive to the size of the cells. The PCM is discontinuous as the void fraction completely migrates from the first cell to its neighbor as soon as the particle's center passes between cells. We observe the same phenomenon with the SPM of 7 pseudo-particles. When we increase the number of pseudo-particles to 56, the discontinuity is reduced. The void fraction still diffuses largely among neighboring cells for the PCM and SPM methods as all quadrature points of the current cell feel the same void fraction. The QCM method leads to a continuous void fraction as its void fraction profile does not jump between elements in two consecutive CFD time steps but transitions progressively with time. This is because no new quadrature points from neighboring cells actually see the particle or start losing sight of the particle until it has moved sufficiently. This leads to a more realistic representation of the void fraction not only in time but also in space as the void fraction is not as diffused as the other methods.

Effect of the CFD Time Step

Additionally, we study the dependence of the void fraction scheme on the CFD time step for a simulation time of 0.2 s. For this, we rerun the simulation with smaller cells (mesh subdivision in x-y-z is 14-24-14). This allows to have a non negligible void fraction ($\varepsilon_f < 0.96$) in the element resulting in more influence on the velocity and as such, the effect of the CFD time step would be clear.

However, it is expected that the simulation will slightly under-predict the particle velocity due to the large particle to cell size ratio. The case was simulated for CFD time steps of 10^{-3} s, 10^{-4} s, 10^{-5} s and 10^{-6} s. Figure 7.6 demonstrates the particle's velocity profile for the different cases. Only PCM and QCM are studied as the SPM is considered as a smoother PCM method. Therefore, it suffers from the same limitations of the PCM but due to its smoother nature, its instability is often delayed compared to the PCM. A decrease in the CFD time step results in an increase in the instability and discontinuity of the PCM method. Below a certain time step, the PCM simulations become unrealistic. This is due to the term $\frac{\partial \varepsilon_f}{\partial t}$ of the VANS equations [130] which tends towards infinity as the CFD time step tends to 0. Since the PCM is discontinuous, this term becomes far too large below a certain value of the time step. On the other hand, the QCM method does not result in under-prediction of the particle velocity for all CFD time steps and it is invariant to the changes in the time step. Its stability is not affected and as such it is shown to be continuous with time. This is important especially in simulations where more temporal accuracy is desired. The continuity in time of the QCM scheme ensure that the CFD-DEM solver is well posed for all values of

Δt as demonstrated by this test case. This is one of the main results of this work.

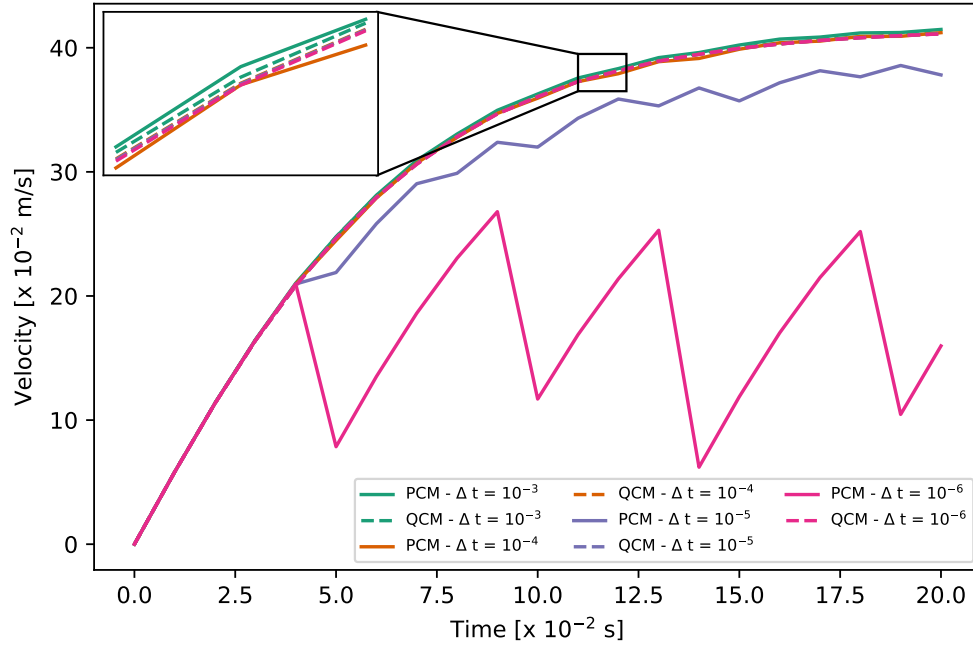


Figure 7.6 Effect of the CFD time step on the void fraction schemes.

Effect of the Cell to Particle Size Ratio

We study the dependence of the void fraction schemes on the spatial discretization as well. We begin with a mesh subdivided in x-y-z into 2-4-2 subdivisions. In order to have a non-negligible void fraction with such large cells, we increase the size of the particles to 0.01 m . We then refine the mesh three times simulating the particle sedimentation at each refinement. Similarly to the previous section, only PCM and QCM were compared. In QCM, R_s is a user defined constant and as such, we want to determine the influence of this choice on the overall performance of the method. Therefore, we consider two cases: the first case takes $R_s = h_\Omega$ while the second case takes $R_s = 2 d_p$. The results obtained from both cases are shown in Figures 7.7 and 7.8 respectively. When R_s depends on the size of the mesh elements, the QCM behaves somewhat similarly to the PCM as the mesh is refined. This is because the volume of the sphere around a quadrature point becomes smaller with every refinement. This leads to very high solid to fluid volume fractions in the sphere which results in unrealistically small values of the void fraction. This is the same in the case of the PCM. The last two refinements with the smallest cell sizes lie below the minimum cell size for which the governing equations are valid and for which the PCM is stable and accurate [150]. Thus, the bad prediction of the velocity. However, even the though the velocity values obtained

by the QCM are not valid at smaller meshes, they still represent a continuous scheme unlike the PCM where the velocity values oscillate nonphysically. This issue can be circumvented by defining a constant sphere radius. We took $R_s = 2 d_p$.

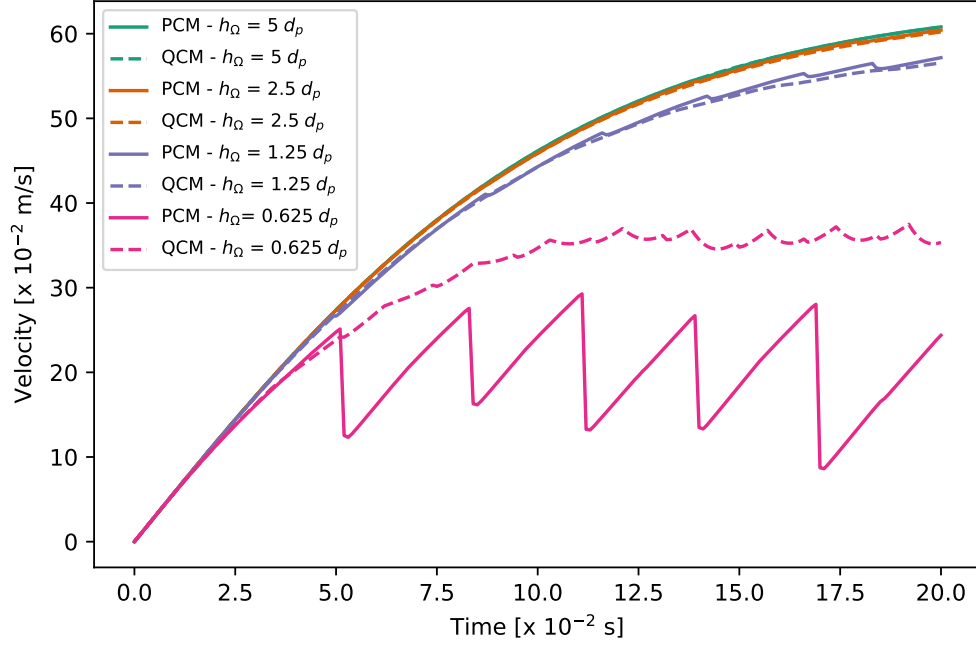


Figure 7.7 Effect of the element size on the void fraction schemes using QCM with $R_s = h_\Omega$.

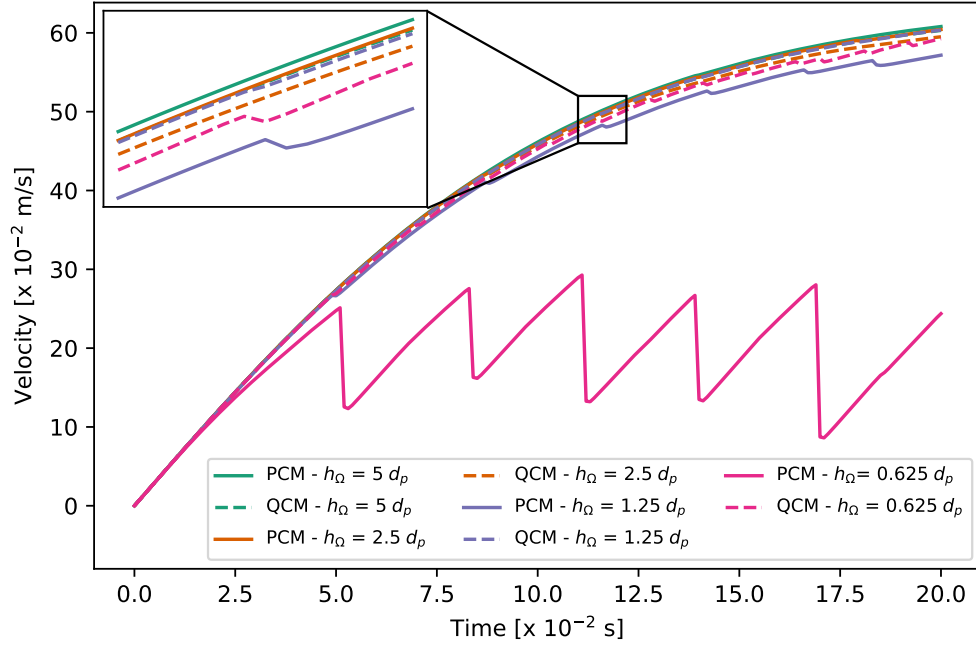


Figure 7.8 Effect of the element size on the void fraction schemes using QCM with $R_s = 2 d_p$.

By defining a fixed radius R_s , the size of the virtual sphere becomes independent of the mesh. This ensures that no matter the size of elements, the void fraction is always calculated using a volume large enough for the VANS equations to be valid. This allows us to use a much finer mesh than normally allowed in CFD-DEM for most void fraction schemes going all the way to meshes smaller than the particle size as shown in Figure 7.8 for the case of $h_\Omega = 0.625d_p$. As such, we achieve higher accuracy on the fluid phase by capturing better the fluid flow without sacrificing the validity and stability of the void fraction scheme used. The initial mesh as well as the last two refinements do not satisfy the condition of Eq. (7.10) as $R_s = 0.4h_\Omega$ for the initial mesh, $R_s = 3.2h_\Omega$ for the last refinement and $R_s = 1.6h_\Omega$ for the previous refinement. Nonetheless, the QCM works well. This is because in the case of a single sedimenting particle, even though the sphere might exceed the neighboring cells, there are no other particles in the system to be detected. Therefore, the method does not miss any particle in the system. This is not true for dense solid-fluid systems. Additionally, for the initial mesh, where the sphere used is too small compared to the cell size, a discontinuity is noticed in the zoomed portion of the Figure 7.8. In this case, parts of the particle are not captured by the small spheres which can lead to mass losses and discontinuities as the particle moves between spheres.

Numerical Efficiency

We determine the computational efficiency for the different methods as we increase the number of particles. In order to fit a large number of particles without changing the size of the geometry, we decrease the diameter of the particles from 5 *mm* to 2 *mm*. For the purpose of obtaining results faster, we increase the CFD time step from 10^{-3} s to 10^{-2} s as well as the coupling frequency from 100 to 500 to ensure a small enough DEM time step. Figure 7.9 presents the average computational time of each method per CFD time step as a function of the number of particles N .

The numerical efficiency of SPM decreases drastically as the number of pseudo-particles increases. At low number of particles N , the difference in computational time between the methods is not important. This slight difference becomes significant when the number of particles increases. For $N < 150$, the QCM is the most expensive. For $150 < N < 2000$, the QCM becomes cheaper than the SPM with 56 pseudo-particles. However, as the problem becomes larger and for $N > 2000$, the QCM becomes more efficient than the SPM method even when only 7 pseudo-particles are used.

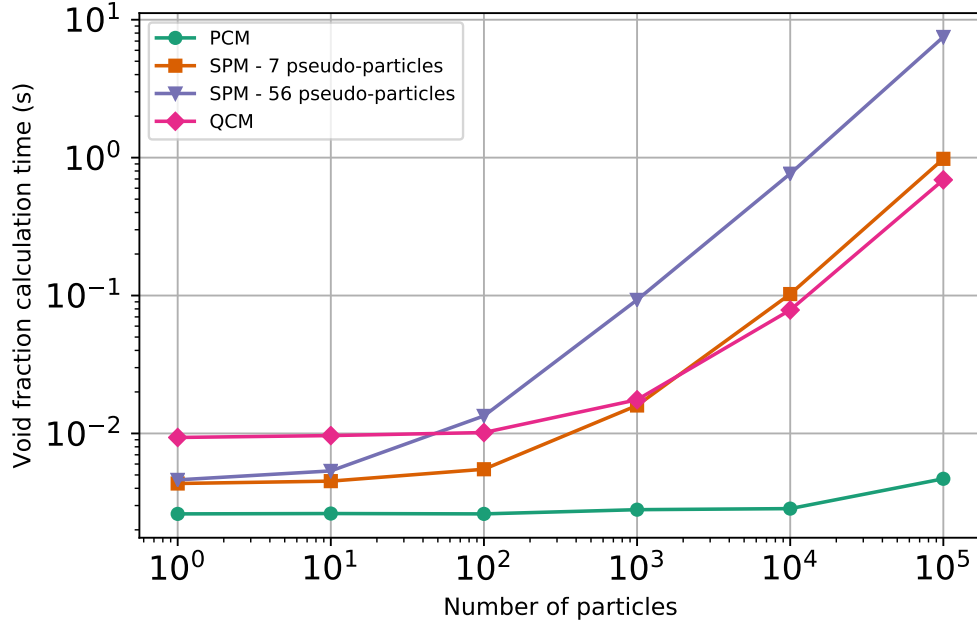


Figure 7.9 Average time required to calculate the void fraction in a CFD time step as a function of the number of particles.

The PCM remains the most computationally efficient method as it is the simplest to implement. In addition to its spatial and temporal continuity, the QCM shows that for large problems, its computational cost is relatively good and comparable to other non-analytical methods. Overall, the added cost of the QCM did not increase the simulation run time significantly ($< 10\%$).

7.4 Boycott Effect

We compare the PCM, SPM with 7 pseudo particles, and QCM performances to determine their effect on the stability of a dense liquid-solid system and their accuracy is solving such systems.

7.4.1 Simulation Setup

The setup of the simulation is similar to that of the previous particle sedimentation case described in Table 6.2. The new bed height is 400 *mm* while the bed length and width were kept the same at 100 *mm*. The mesh subdivisions in x-y-z are 20-60-20 and were determined so that the PCM is valid. For QCM, we choose R_s as to obtain a volume averaging sphere with the same volume as the element (Ω) in which its center is located, so that $R_s = \sqrt[3]{\frac{3V_\Omega}{4\pi}}$.

100,000 particles with a diameter of 0.002 m and density of 2500 kg/m^3 were inserted at the top of the bed and were allowed to fall under the force of gravity. The simulation was run for 4 s with a CFD time step of 10^{-3} s and a coupling frequency of 50. More solid-fluid forces were enabled for this simulation compared to the single particle sedimentation. These are drag, buoyancy, shear and pressure forces. The Difelice [98] drag model was used to calculate the drag force. Initially, the smoothing length was set to 0 for all the void fraction schemes. Three different inclination angles α of the bed relative to the vertical were studied, $\alpha = 0^\circ, 5^\circ, 10^\circ$. The inclination of the bed was simulated by changing the direction of the gravity vector. It is given as $\vec{g} = (0, -9.81, 0)$ for $\alpha = 0^\circ$, $\vec{g} = (-0.855, -9.773, 0)$ for $\alpha = 5^\circ$ and $\vec{g} = (-1.703, -9.66, 0)$ for $\alpha = 10^\circ$.

7.4.2 Results and Discussion

The simulation using the SPM void fraction scheme was unstable. We smoothed the void fraction field by using smoothing lengths $L^2 = 2d_p^2, 4d_p^2, 6d_p^2$ but the SPM method remained unstable and the linear solver failed to converge after few iterations for the different smoothing lengths used. For the PCM, the linear solver was also struggling to converge when no smoothing was implemented. Therefore, we reran the simulation with smoothing lengths $L^2 = 2d_p^2, 4d_p^2$. The PCM worked for all inclination angles when $L^2 = 4d_p^2$. However; increasing the smoothing length adds more artificial diffusion to the void fraction scheme. Table 7.2 summarizes the conditions under which the different void fraction schemes work for a dense solid-liquid simulation where the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ of the continuity equation is enabled.

Table 7.2 Stability condition for the various void fraction schemes: unstable (red) and stable (green).

	$(\partial\varepsilon_f/\partial t)$ enabled				$(\partial\varepsilon_f/\partial t)$ disabled			
Method	Smoothing Length (L^2)				Smoothing Length (L^2)			
PCM	0	$2d_p^2$	$4d_p^2$	$6d_p^2$	0	$2d_p^2$	$4d_p^2$	$6d_p^2$
SPM	0	$2d_p^2$	$4d_p^2$	$6d_p^2$	0	$2d_p^2$	$4d_p^2$	$6d_p^2$
QCM	0	$2d_p^2$	$4d_p^2$	$6d_p^2$	0	$2d_p^2$	$4d_p^2$	$6d_p^2$

The failure of the linear solver is due to the first term $(\rho_f \frac{\partial(\varepsilon_f)}{\partial t})$ of the continuity equation (Eq. 7.1) which is very stiff when the void fraction is discontinuous and as $\Delta t_{CFD} \rightarrow 0$. This leads to the presence of a singular matrix that prevents the convergence of the linear solver. In this case, $\Delta t_{CFD} = 10^{-3}$ which is a normal value for a CFD simulation. Normally, when the fluid used is a gas, this term does not affect the stability of the simulation due to the very small density of gases in general which significantly reduce the effect of this term,

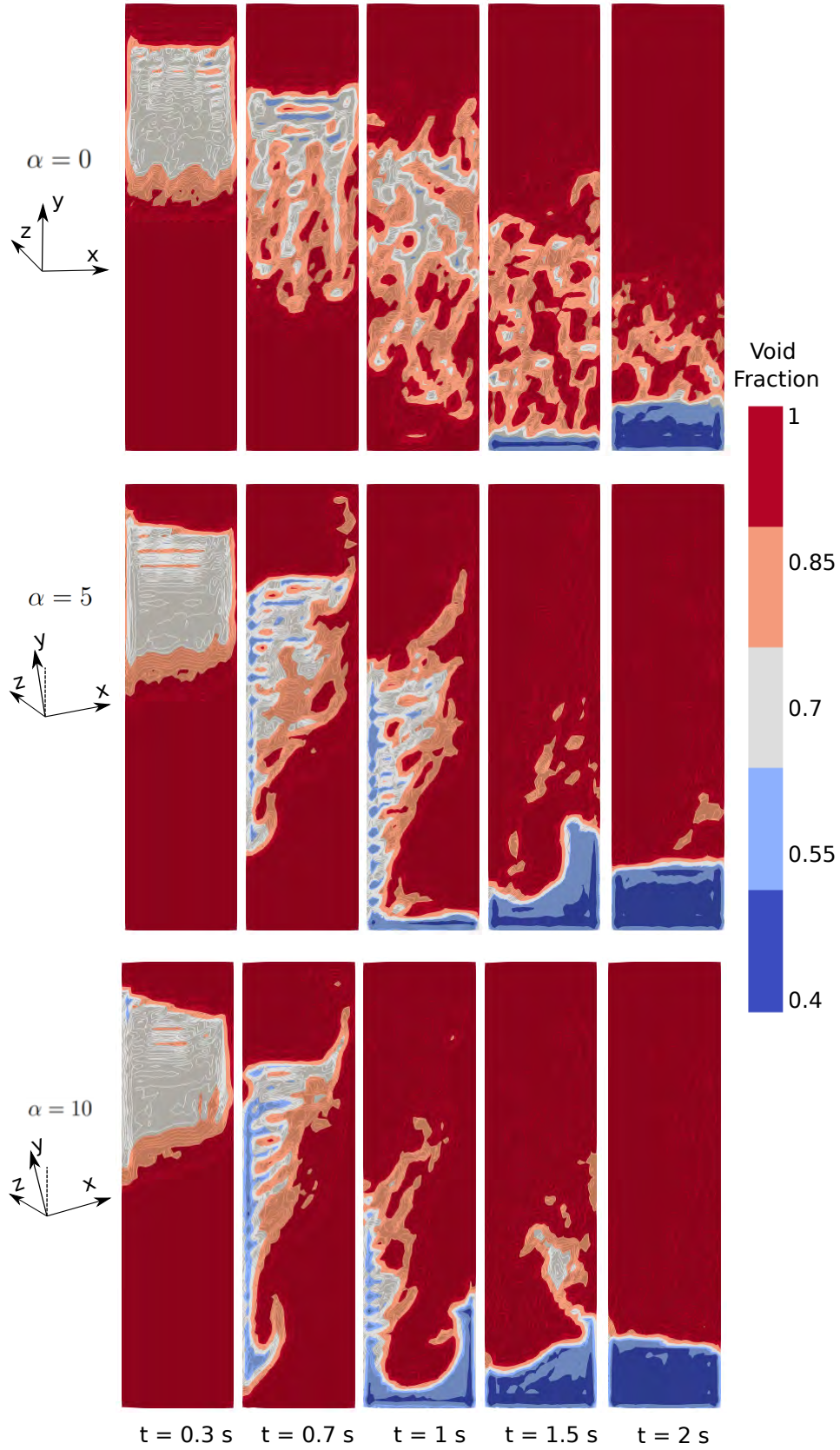


Figure 7.10 2D snapshots of the void fraction profile during the sedimentation of the particles in water at different inclination angles for the QCM scheme.

however; using a liquid as the fluid makes this term more dominant. The stiffness of this term is aggravated by the small CFD time step used and the temporal discontinuity of the void fraction scheme implemented. The QCM worked well with no smoothing for the different inclination angles where the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ was well-posed due to the time continuity of the QCM scheme.

Figure 7.10 shows time snapshots of a 2D slice of the void fraction profile during the sedimentation process at different inclination angles for the QCM void fraction scheme. As the bed becomes more inclined, the particles sedimentation becomes faster and the particles reach the bottom of the bed in a shorter time compared to the non inclined bed. This is because the particles gain momentum due to being hindered by the upward motion of the fluid. This upward motion of the fluid is a response to mass conservation represented by the continuity equation. As the particles are subjected to gravitational forces, they fall downwards. This requires the fluid to move upwards to give space for the particles falling. The void fraction during the sedimentation process is highly fluctuating as particles are falling fast.

The QCM was able to simulate the sedimentation with no difficulty on the linear and non linear solvers leading to fast convergence of the simulation. For PCM, some stiffness was noticed even with the smoothing of the void fraction where some iterations were taking longer to converge. The larger the inclination angle of the bed was, the longer the simulation with PCM took to converge at each time step. This is due to the increased particles velocity as we increase the angle α , where now particles are travelling more per time step leading to a larger temporal discontinuity in the void fraction field which makes the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ more unstable. The simulation took twice as much time for PCM as for QCM when $\alpha > 0$ to reach the end time of 4 s. Using a smoothing length larger than $L^2 = 4d_p^2$ could help reduce the stiffness of the system being solved as it helps reduce the discontinuity of the void fraction scheme. The SPM failed since the first few iterations at simulating this case when the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ of the continuity equation was enabled as it resulted in a singular matrix which prevented the linear solver from converging. Even though the SPM is less discontinuous than the PCM, the refinement of each particle (in this case 7 pseudo particles) makes the discontinuities more frequent than with the PCM which explains the rapid explosion of the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$.

Usually, in CFD-DEM simulations involving a liquid as the fluid, the first term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ of the continuity equation (Eq. 7.1) is neglected as it is unstable and highly discontinuous. As the CFD time step decreases, this term is very large for the slightest discontinuity in time of the void fraction. The density of a liquid being much larger than that of a gas increases the effect of this term resulting in unstable systems. However, neglecting this term solely

on a numerical basis without any physical explanation is not justifiable as we are no longer solving the volume averaged Navier-Stokes equations. In order to prove this, we monitored the y-velocity and the y-position of the center of mass of our system in time for the different void fraction schemes used. For this, we rerun the simulation using the different void fraction schemes for the stable cases with the least smoothing requirement as shown in Table 7.2. The results obtained are shown in Figure 7.11 for the y-position and Figure 7.12 for the y-velocity of the center of mass.

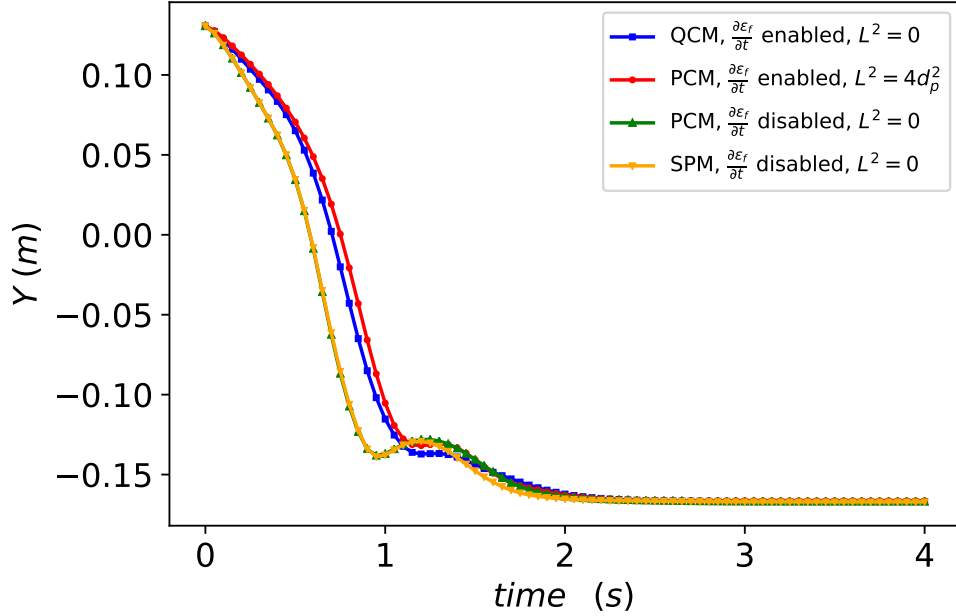


Figure 7.11 The y-position of the center of mass of the cluster of particles as a function of time.

As the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ is neglected, the particles fall faster. This is demonstrated by the center of mass position and velocity where at the same simulation time, the simulations with the disabled term resulted in faster sedimentation due to larger particles velocities. This becomes more obvious when comparing the two PCM simulations in Figures 7.11 and 7.12. We explain this by the concept of mass conservation. As the particles move downwards, the term $\rho_f \frac{\partial(\varepsilon_f)}{\partial t}$ enhances the upward movement of the fluid to give space for the particles to sediment. This upward movement slows down the particles that are in the way of the fluid. When this term is neglected, fluid is less affected by the difference in void fraction below and at the particles locations resulting in less upward movement of the fluid and as a result faster particles.

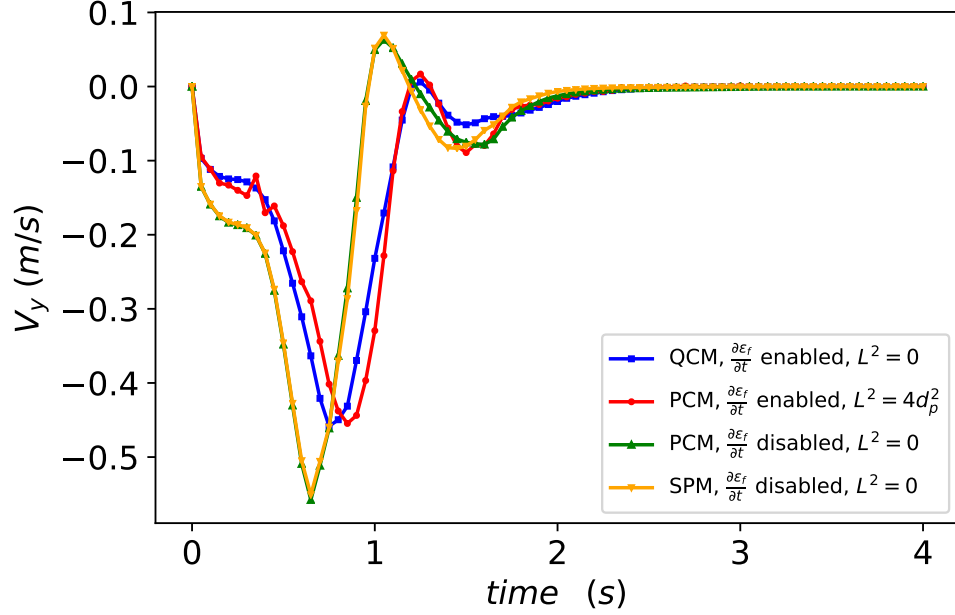


Figure 7.12 The y-velocity of the center of mass of the cluster of particles as a function of time.

7.5 Flat Bubbling Spouted Bed

We aim at validating our void fraction scheme by studying its effect on fluidization. For this purpose, we simulate using the CFD-DEM solver in Lethe [160] the same flat bubbling spouted bed as Wu et al. [77] and we compare with their simulations results as well as the experimental results and the simulation results by Bokkers et al. [161]. It is important to note that Wu et al. [77] and Bokkers et al. [161] used the hard sphere model in their simulations for the DEM. However, our solver uses the soft sphere model. Therefore, it is expected that there will be discrepancies in the results but the aim is not to compare the DEM models. For more information about these two models, we refer the reader to the book by Norouzi et al. [3]. In this section, we compare the shape and size of the bubble formed as well as the height of the bed of particles 0.2 s after initial gas injection. We also look at the profile of the void fraction obtained from the different schemes.

7.5.1 Simulation Setup

The geometry as well as the physical properties of the particles are taken from Wu et al. [77]. The mesh was chosen by taking the cell size to be slightly greater than $3 d_p$ so that the CFD-DEM simulation for the various void fraction schemes is valid [3]. We did not use smoothing

of the void fraction in this case to show the exact behavior of each method. The physical and numerical parameters for this simulation are found in Table 7.3.

Table 7.3 Physical and numerical parameters for the spouted bed test case.

<i>Simulation control</i>			
End time (s)	0.2		
Coupling frequency	10^2	CFD time step (s)	10^{-4}
<i>Geometry</i>			
Bed Dimensions (m)	0.15 x 0.45 x 0.015	Wall Thickness (mm)	0
Mesh Type	GMSH	Mesh Subdivisions in x-y-z	15-45-1
Spout Width (m)	0.01	Spout Mesh Subdivisions in x-y-z	1-10-1
<i>Particles</i>			
Number	31050	Diameter(m)	25×10^{-3}
Density(kg/m^3)	2526	Young Modulus (N/m^2)	1×10^6
Particle-particle poisson ratio	0.25	Particle-wall poisson ratio	0.25
Particle-particle restitution coefficient	0.97	Particle-wall restitution coefficient	0.33
Particle-particle friction coefficient	0.2	Particle-wall friction coefficient	0.1
Particle-particle rolling friction	0.4	Particle-wall rolling friction	0.1
<i>Gas phase</i>			
Viscosity ($Pa \cdot s$)	1.81×10^{-5}	Density (kg/m^3)	1
Inlet Spout Velocity (m/s)	20	Inlet Background Velocity (m/s)	1.25
Void fraction smoothing factor L^2	0	Grad-div parameter (c^*)	0.005
<i>Linear Solver</i>			
Method	GMRES	Max iterations	1000
Minimum residual	1×10^{-10}	Relative residual	10×10^{-2}
ILU preconditioner fill	2	ILU preconditioner absolute tolerance	1×10^{-12}
ILU preconditioner relative tolerance	1		
<i>Non-linear solver</i>			
Tolerance	1×10^{-8}	Max iterations	10

For this simulation, we enable buoyancy, shear stress, pressure and drag forces. The Gidaspow model [46] was used to calculate the drag. This drag model is not the best model to be used in this study as it features a discontinuity in the calculation of the drag force at the void fraction value of $\varepsilon_f = 0.8$. Since this value of the void fraction is present in our bed, other drag models would be more appropriate. However, since we are comparing with a study in which the Gidaspow [46] model was implemented, we use it solely for comparison purposes. For more details on the description of the particle-fluid forces, we refer the reader to the Lethe CFD-DEM article [160]. We also choose R_s as to obtain a volume averaging sphere with the same volume as the element (Ω) in which its center is located, so that $R_s = \sqrt[3]{\frac{3V_\Omega}{4\pi}}$.

7.5.2 Results and Discussion

The formation of the bubble at the base of the flat bubbling spouted bed after 0.2 s using the Gidaspow drag model [46] is shown in Figure 7.13 for the various void fraction schemes used.

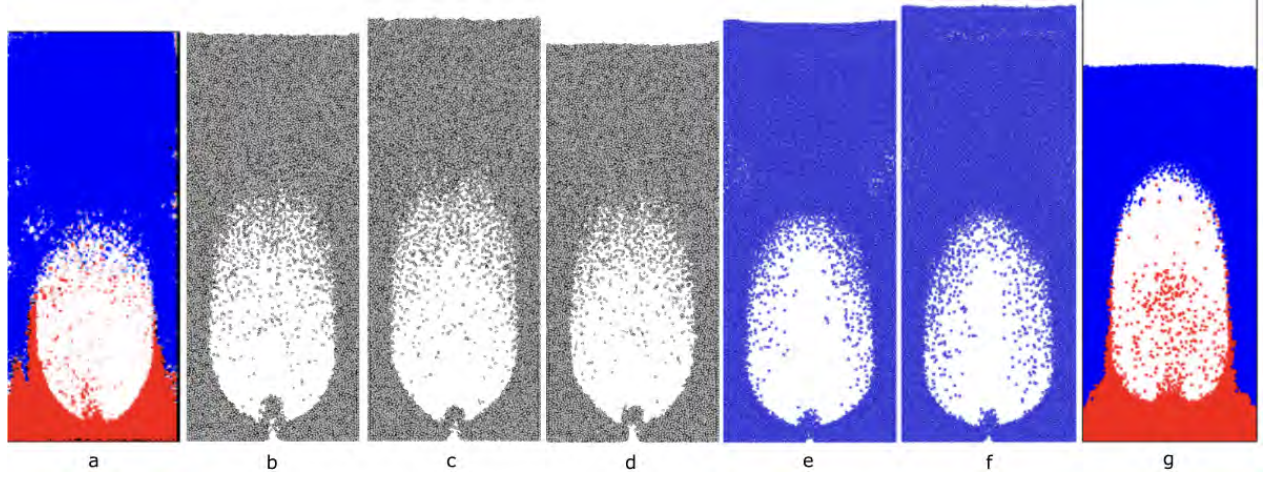


Figure 7.13 Particle distribution in a flat fluidized bed 0.2 s after central gas injection. (a) Experimental result by Bokkers et al [161]; (b) QCM; (c) PCM; (d) SPM; (e) DPM using analytical method [77]; (f) DPM using point approximate method (PAM) approach [77], and (g) DPM [161].

Comparing between our three simulations, we notice that for the same simulation conditions, the QCM and SPM result in more accurate predictions than the PCM when compared with the experimental results. The PCM result in a larger bed height (about 5% increase) while the SPM under-predicts the bed height by 1.2 % compared to the QCM which predicts the bed height correctly. The PCM leads to few pockets of gas in the portion of the bed above the top of the bubble. This is also noticeable in the DPM using the point approximate method (PAM) approach. Additionally, in all three methods we implemented, the shape and size of the bubble we obtain lies in between the results obtained by Bokkers et al. [161] and Wu et al. [77]. For the simulations performed by Wu et al. [77], the analytical approach (Figure 7.13 (e)) results in accurate bed height prediction and bubble formation contrary to the point approximate method where the bed height was over-predicted (Figure 7.13 (f)). Additionally, the simulation by Bokkers et al. [161] (Figure 7.13 (g)) leads to an over-prediction of the bubble size but to an under-prediction of the bed height. We find this unrealistic since generally a bigger bubble occupies a larger volume which should lead to a larger bed height to compensate for the volume occupied by the bubble. Even though Wu et al. [77] and Bokkers et al. [161] both use the hard sphere model and the Gidaspow drag

correlation [46] in their simulations, their results are contradictory. The shape and size of the bubble as well as the bed height are completely different. The simulations by Wu et al. [77] results in particles falling down around the bubble contrary to the experimental results. This might be caused by the mesh size. Bokkers et al. [161] used a mesh with 675 elements while Wu et al. [77] used 5.6 times more cells (3780 elements). This leads to different values of the void fraction within a given cell which influences the value of the drag force in this cell. Additionally, the choice of solid-fluid forces applied can drastically change the results. Wu et al. [77] and Bokkers et al. [161] did not explicitly give details on all the solid-fluid forces they accounted for and as such, we cannot reproduce their simulations accurately.

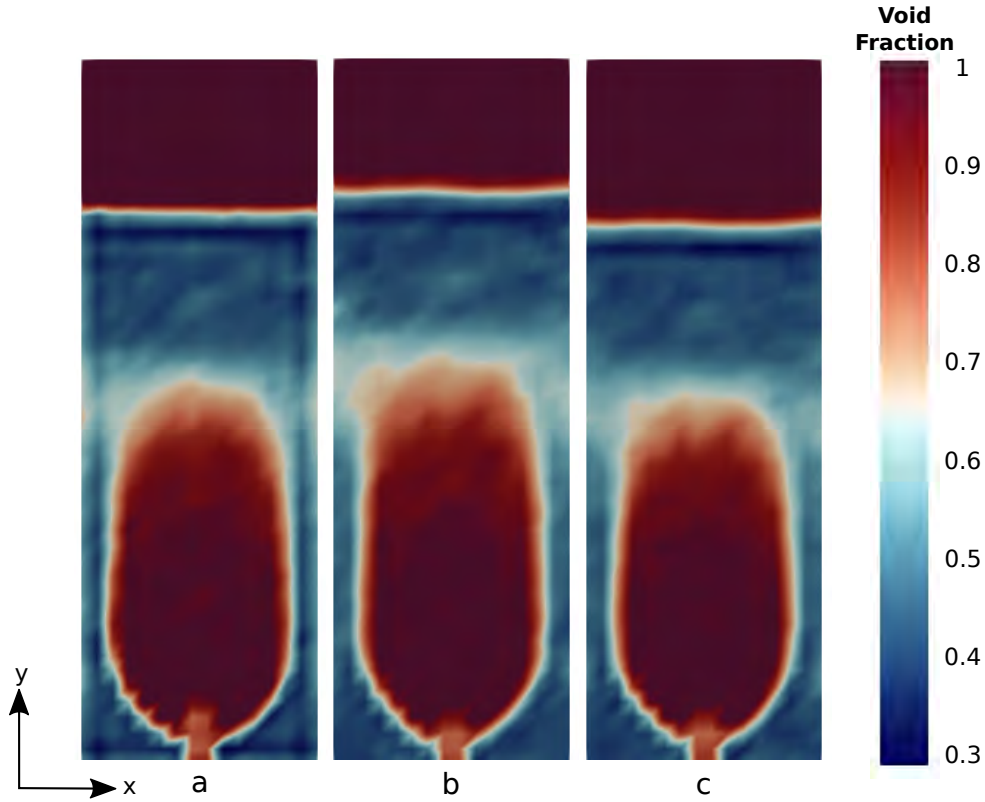


Figure 7.14 2D slice showing the void fraction ε_f profile in a flat fluidized bed 0.2 s after central gas injection. (a) QCM; (b) PCM; and (c) SPM.

In our simulation, we use the same mesh as the one used by Bokkers et al. [161] except for the inlet channel where we used a more refined mesh. Using the QCM method, we obtain results comparable to those of the experiment as well as to the results from the simulation of the DPM using the analytical method. QCM, SPM and DPM using the analytical method show good bubble size even though the DPM bubble is more compact. In our simulations, particles fall down through the bubble as also seen experimentally and in the simulation by Bokkers et

al. [161]. Moreover, the height of the bed in the simulations of both the QCM and the DPM using the analytical approach is similar to the experimental bed height. Additionally, the particle spout seen at the base of the bubble is reproduced in all simulations even though the QCM leads to a slightly more pronounced spout than the other simulations. The occurrence of this particle spout is dependent on the grid resolution of the inlet channel. Using a finer mesh in the y direction led to the particle spout being reproduced.

In the void fraction distribution of Figure 7.14, the shape of the bubble at the base is similar between the three methods. The differences exist towards the top of the bubble. The PCM results in more air pockets in the upper packing represented by the whitish blue and light red colors on top of the bubble. This explains the difference in bed height between the methods even though the bubble size is similar. The QCM gives a good representation for the top of the bubble while for the SPM and the PCM, we notice a kink at the top of the bubble.

We demonstrated that the QCM is cheaper than the SPM when simulating a large number of particles but still more expensive than the PCM. However, the void fraction is calculated only once per CFD time step, therefore, the cost is relatively modest. Also, the continuity in space and time of the QCM manifested itself in the convergence of the VANS equations where the number of Newton iterations was 6 ± 1 for the QCM, 8 ± 1 for the PCM, and 7 ± 1 for the SPM resulting in 25 % and 14.5 % reduction per CFD time step compared to PCM and SPM respectively. Overall, the total simulation time was 7700 s for PCM, 7400 for SPM, and 6640 s for QCM reducing the simulation time by 16 % compared to PCM and 11.5 % compared to SPM. This is in principle due to the enhancement of the condition number of the linear systems solved.

Moreover, we study the mass conservation properties of the three methods. We monitor the global continuity error (mass conservation error) that is the solution of the continuity equation as well as the maximum local continuity error in an element. The continuity error is defined as the continuity equation of the VANS equations:

$$E = \int_{\Omega} \rho_f \frac{\partial (\varepsilon_f)}{\partial t} + \rho_f \nabla \cdot (\varepsilon_f \mathbf{u}_f) d\Omega \quad (7.17)$$

where Ω is the simulation domain over which the error is being calculated.

Figure 7.15 shows the continuity error fluctuations with time normalized by the spout inlet velocity of 20 m/s. The QCM results in more homogeneous mass source term compared to the PCM and SPM. Among the compared methods, it is the most mass conservative.

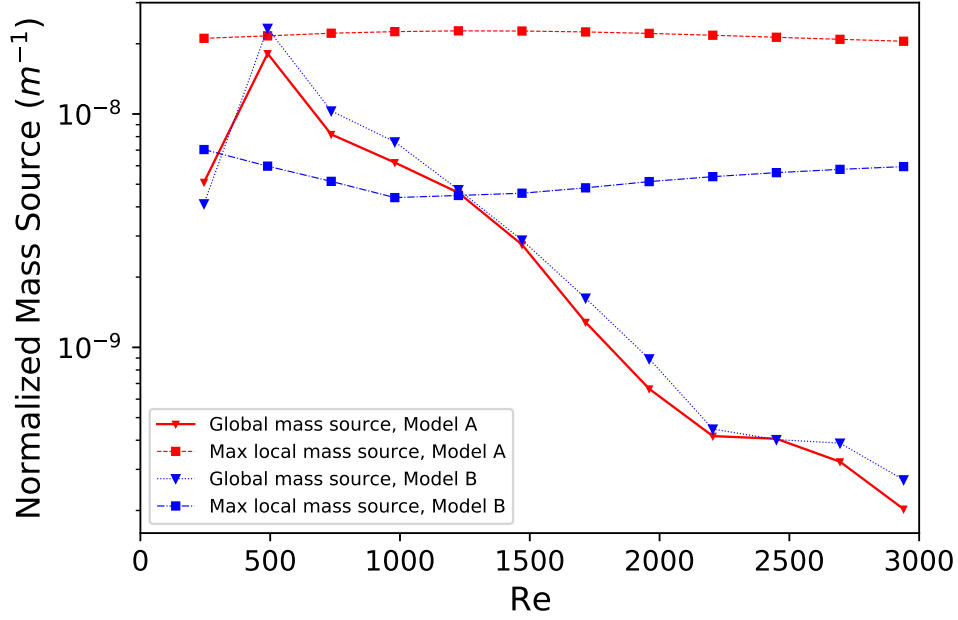


Figure 7.15 Global and maximum local continuity error for: (a) PCM; (b) SPM; and (c) QCM. The y-axes are scaled to the order of magnitude of the mass conservation error. The QCM results in a significantly lower mass conservation error in comparison to the PCM and SPM.

The order of magnitude of the normalized global mass source term is lowest for the QCM at 10^{-10} followed by the PCM and SPM at 10^{-7} and 10^{-5} respectively. The normalized maximum local mass conservation error order of magnitude for all methods is around 10^{-6} . In general, the QCM leads to the least fluctuations in the mass source term and the SPM leads to the most fluctuations specifically at certain CFD time steps when the mass source jumps four orders of magnitude and then drops instantly.

7.6 Conclusion

In this paper, we develop a new scheme to calculate the void fraction of solid-fluid systems in CFD-DEM simulations. It is mass conservative, stable and space and time continuous. Since no intersection between the particles and the cells are calculated, this method is valid on both structured and unstructured meshes. We demonstrate that the method is well-posed in the limit of $\Delta t \rightarrow 0$ and the element size when the radius of the virtual sphere is fixed. This leads to a very stable and robust void fraction scheme.

Additionally, a comparison of the results obtained by the different methods for the flat bub-

bling spouted bed demonstrate the significant error obtained from using the PCM where the bed height was higher than the experimental observation and the void fraction distribution was uneven. In comparison, the QCM correctly predicted the bed height and resulted in a compact distribution of the void fraction. Moreover, the improved accuracy and continuity in the calculation of the void fraction reduced the overall simulation time by 11-16 % by enhancing the condition number of the linear systems solved and reducing the number of non-linear iterations.

The implementation of the QCM void fraction scheme is advantageous in the simulation of applications with large void fraction fluctuations in time such as bubbling fluidized beds, high void fraction gradients such as packed beds, and dense solid-liquid systems. This method alleviates the need to artificially smooth the void fraction scheme when solving the $\mathcal{L}^2$ projection system as it is by nature continuous in both time and space, thus resulting in better representation of the void fraction field. Furthermore, the QCM scheme greatly reduces the limitations on unresolved CFD-DEM concerning the size of mesh elements and the CFD time step, thus ensuring better spatial and temporal accuracy. Finally, the continuity of QCM and its enhancement of the condition number of the linear systems solved allows it to be readily coupled with lesser robust high order velocity and pressure schemes without aggravating the stiffness of the linear system, thus additionally improving accuracy of results. Although we developed the QCM in the context of the Finite Element Method (FEM), it could readily be extended to the Finite Volume Method (FVM) by calculating the intersection between the particles and the volume averaging sphere at the centroid of the cells to obtain the void fraction within the cells.

7.7 Acknowledgements

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CHAPTER 8 ARTICLE 4 : SOLID-LIQUID ROTARY KILNS: AN EXPERIMENTAL AND CFD-DEM STUDY

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Declaration: The author of this thesis has contributed to the literature review, experimental studies, simulation and modelling, analysis of the results and the writing of the article.

Abstract: Experiments for the validation of unresolved CFD-DEM software for solid-liquid flows are often expensive, time consuming and generally provide little insight into the local particles dynamics. Additionally, several DEM parameters such as the particle surface properties are often obtained from experiments in air and used for all CFD-DEM simulations even when the fluid is a liquid. We design and perform a simple and time efficient gas-solid and liquid-solid rotary kiln benchmark for the purpose of creating a validation case for unresolved CFD-DEM software which we use to validate the unresolved CFD-DEM model of the open-source software Lethe. This case, which contains dense solid-solid contacts and strong solid-fluid forces gives insight on the importance of proper calibration of DEM surface properties in solid-liquid flows as well as on the importance of the lift force. Furthermore, it is highly sensitive to the accuracy of the CFD discretization.

8.1 Introduction

The popularity of computational fluid dynamics coupled with the discrete element method (CFD-DEM) has been increasing over the last few decades due to its accuracy in modelling multiphase solid-fluid flows [43,105,162]. Nevertheless, the user defined parameters that need to be inputted before a simulation can be run are numerous and an appropriate choice of these parameters is vital to obtain accurate and physically-realistic results.

Among these parameters, the choice of particle-fluid interactions plays a important role in the correct prediction of solid-fluid flows. Traditionally, CFD-DEM simulations focus mainly on the following forces: gravity and buoyancy, drag force, pressure gradient force, and shear force. The lift force is sometimes applied and sometimes neglected depending on the application being simulated. In general, in modelling solid-gas flows such as gas fluidized and spouted beds, the lift force is entirely neglected as it is considered to be of negligible magnitude compared to the dominant drag force. This is not true in solid-liquid flows. This has been demonstrated by Ferreira et al. [163] where enabling the Saffman lift force allowed

for better prediction of liquid fluidized beds since the pluming effect of the particles at the top of the bed significantly diminished as a result of reduced channelling due to Saffman lift. As such, it is important to correctly choose particle-fluid interactions.

On the other hand, the DEM parameters, specifically those related to the solid particles are among the most important parameters that should be chosen carefully. In general, they include material properties and surface properties. Material properties are those related directly to the material from which is made the particles and walls such as the density, Young's modulus, and Poisson's ratio. Surface properties include the rolling and sliding friction coefficients as well as the coefficient of restitution. The latter are usually calibrated based on the surface of dry particles. In other words, experiments are performed in air and the parameters are deduced. These dry parameters are then used for solid-liquid CFD-DEM simulations. This is the case for most modelling work done and, often, no specifications about the source of these parameters is given. Blais and Bertrand [164] found that DEM surface parameters such as the sliding and rolling friction coefficients and the coefficient of restitution play a role in the dynamics of solid-liquid flows. However, a thorough clarification about this topic and the true effect of the choice of such parameters has not been fully addressed in the literature.

It is unrealistic and unreliable to work solely with the parameters obtained from dry experiments as these particle properties tend to change when the state of the fluid changes. For example, a particle, upon hitting the ground, will usually bounce more in air than it would in water. Therefore, the coefficient of restitution of the particle is larger in dry settings than it would be in wet settings. This has been demonstrated by Joseph et al [165] where a bouncing particle experiment showed that the particle coefficient of restitution decreases with an increase in the viscosity of the fluid in which it is bouncing due to lubrication forces. The decrease becomes sharp for higher viscosities.

In the literature, the calibration of DEM properties has been mainly performed for dry materials such as the calibration of DEM parameters of cohesive bulk material using an angle of repose test [166] and the calibration of DEM properties of sticky adhesive powders for the simulation of segregation [167]. The influence and effects of the microscopic DEM parameters is discussed by Groger and Katterfeld [168] where they explain the need for the development of new calibration methods. Other researchers developed bench-scale experiments to calibrate and investigate DEM parameters such as the sliding and rolling friction coefficients, the coefficient of restitution, and the inter-particle cohesion forces from the presence of liquid bridges [169]. To the knowledge of the authors, the calibration of DEM properties for solely solid-liquid simulations has not been addressed in the literature.

There exist several experiments that allow the deduction of such parameters. Among them, we mention rotary kiln experiments where a lab-scale cylindrical bed is filled with particles, or a combination of particles and a fluid and are allowed to rotate. Depending on the velocity of the rotation, the flow regime inside the rotary kiln changes. This change is often determined by the rotational Froude number [170]. This dimensionless number is defined as the ratio of centrifugal forces to gravity and is given by the following [170]:

$$Fr = \frac{\omega^2 R}{g} \quad (8.1)$$

where ω is the kiln rotational velocity in rad s^{-1} , R is the kiln radius in m, and g is the gravity in m s^{-2} . For a specific range of Froude numbers, the particles exhibit a certain regime inside the rotary kiln. Figure 8.1 demonstrates the different regimes that can be observed in a rotary kiln as a function of the Froude number.

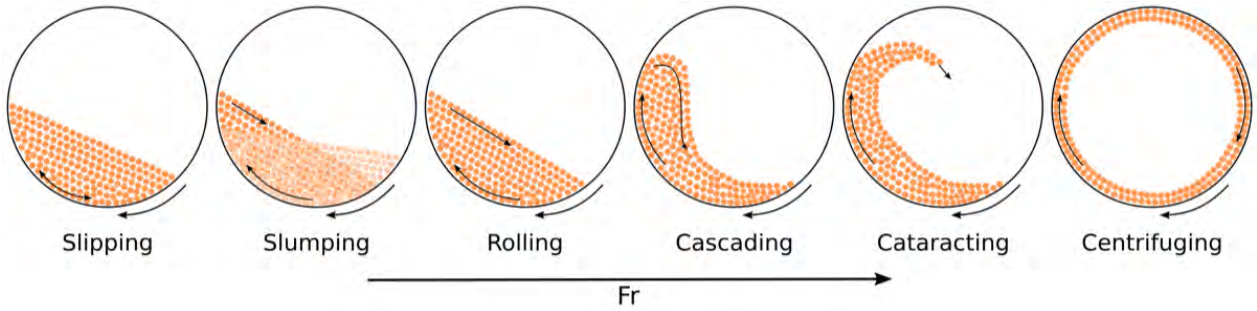


Figure 8.1 Particles flow regimes in rotary kilns as a function of Froude number. Reproduced from [171].

Increasing the Froude number allows the flow to transition from one regime to another. It is not necessary that all flow regimes are exhibited for every experiment. Sometimes, the flow transitions from one regime to another while skipping a certain regime. This is because the velocity range for the skipped regime is so small that it is not captured during the experiment. The regime at the lowest rotational speed is the slipping regime where particles slip along the wall of the bed and they can be seen to barely move. The slumping regime comes next where the particle bed behaves like a see-saw with the bed moving in an up and down motion. At higher rotational speeds is the rolling regime where particles start moving along the wall and then roll downwards after reaching the top of the packing. The cascading regime occurs when the surface layer arches resulting in a crescent shape. The cataracting regime results when particles start to be thrown away into free space, falling into the bed of particles and

then reattaching towards the base in a cascading motion. The centrifuging regime occurs when the $Fr > 1$, meaning that the centrifugal forces outweigh the gravitational forces. The particles adhere to the wall of the kiln and perform full rotations.

It is important to note that the Froude number is not always very reliable in determining the regime change intervals because even for a constant Froude number, the behavior of the drum can be affected by the volumetric fill level of the kiln and the friction coefficients between the kiln wall and the particles [171]. For example, filling the kiln to lower levels or increasing the sliding friction coefficient can lead to more cataracting or centrifuging motion. Additionally, the Froude number is determined based on the particles motion in air. There is no mentioning of the effect of different fluids on the Froude interval for the regime change of the flow. This is because the gravity in the fluid is countered by the buoyancy force and as such it is expected that a new weaker gravitational acceleration should be considered in Eq. 8.1 when the fluid inside the kiln is a liquid. Furthermore, the Froude number does not take into account the fluid viscosity and therefore, on its own, it can not be used as a measure for regime change with fluids of high viscosities.

In general, not many studies of solid-liquid rotary kilns have been performed in the literature. Many researchers experimentally studied the mixing of solid materials in air inside a rotary kiln and investigated the effects of particle types and densities, kiln loading, rotational speed and wall friction on the mixing rates in the bed [172,173]. Parsons et al. [174] experimentally studied the solid-liquid mass transfer in slurries agitated inside a rotary kiln. Tang et al. [175] modelled a three-phase gas-solid-liquid flow using CFD-DEM coupled with volume of fluid (VOF) to study gas-solid-liquid flows and mixing behaviors in rotary kilns taking into account inter-particle collisions, inter-phase interactions, and interface morphology. Additionally, mills such as semi autogenous grinding (SAG) mills, which have many similarities to solid-liquid rotary kilns in the cataracting regime if breakage is ignored, are studied using either DEM [176] where rock breakage mechanisms and the life cycle of rocks in mills are explored or CFD-DEM [177] where a method for calculating the efficiency of the SAG process based on the numerical results is proposed.

The aim of this work is to develop a simple and easily reproducible experimental and computational procedure that allows the calibration of the DEM surface properties and the validation of any unresolved CFD-DEM code for solid-liquid flows. For this, a lab-scale rotary kiln experiment is performed where different types of particles and fluids are used to calibrate the particle and wall properties and to determine the effect of the choice of fluid on the DEM surface properties. This experiment is chosen specifically because of its simplicity and due to the complicated regimes exhibited by the particles in the rotary kiln at the various

rotational velocities it is subjected to.

8.2 CFD-DEM Model

In this section, the governing equations, particle-fluid interactions and DEM parameters are described briefly. No matter the type of CFD-DEM simulations, the governing equations are mainly separated into those related to the fluid phase and they are the volume-averaged Navier-Stokes (VANS) equations and those related to the solid phase and they are Newton's equation of motion and Euler's equation of angular momentum.

8.2.1 Fluid Phase Modelling

The VANS equations are divided mainly into two models: A and B. As we will only use model A in this work, we introduce it in this section. For further description of the two models and for a detailed discussion about their differences and similarities, we refer the reader to the article by El Geitani et al. [160]. The VANS equations are made up of the continuity equation and the momentum equation. The continuity equation is given by:

$$\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}) = 0 \quad (8.2)$$

where $\mathbf{u}$ is the fluid velocity, and ε_f is the void fraction calculated using one of many available particle projection schemes. The momentum equation is given by:

$$\rho_f \left[\frac{\partial \varepsilon_f \mathbf{u}}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u} \otimes \mathbf{u}) \right] = -\varepsilon_f \nabla p + \varepsilon_f \nabla \cdot \boldsymbol{\tau} - \mathbf{F}_{pf} \quad (8.3)$$

where p is the pressure, and $\boldsymbol{\tau}$ is the shear stress tensor and is given by:

$$\boldsymbol{\tau} = \mu_f \left[(\nabla \cdot \mathbf{u}) + (\nabla \cdot \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u} \mathbf{I}) \right] \quad (8.4)$$

μ_f is the dynamic viscosity, $\mathbf{I}$ is the identity matrix and $\mathbf{F}_{pf}$ in equation (8.3) is the fluid-particle interactions vector and is given by:

$$\mathbf{F}_{pf} = \frac{1}{\Delta V_\Omega} \sum_i^{N_p} (\mathbf{f}_{pf,i} - \mathbf{f}_{\nabla p} - \mathbf{f}_{\nabla \cdot \boldsymbol{\tau}} - \mathbf{f}_b) \quad (8.5)$$

where $\mathbf{f}_{pf,i}$ is the sum of particle-fluid interaction forces such as drag ($\mathbf{f}_d$), Saffman lift ($\mathbf{f}_{\text{Saff}}$), Magnus lift ($\mathbf{f}_{\text{Mag}}$), virtual mass ($\mathbf{f}_{\text{vm}}$), and Basset force ($\mathbf{f}_B$). $\mathbf{f}_{\nabla p}$ is the pressure gradient force, $\mathbf{f}_{\nabla \cdot \boldsymbol{\tau}}$ is the shear stress force, and $\mathbf{f}_b$ is the buoyancy force. In this work, only Saffman lift ($\mathbf{f}_{\text{Saff}}$), Magnus lift ($\mathbf{f}_{\text{Mag}}$) and drag ($\mathbf{f}_d$) are considered for the particle-fluid interaction forces since the remaining forces are of negligible magnitude. This is because the fluid to solid density ratio is relatively small allowing to neglect the virtual mass force. Additionally, there exist no expression for these forces in the case of a swarm of particles as they were derived for individual particles. This gives for a particle i , the particle-fluid force as:

$$\mathbf{f}_{pf,i} = \mathbf{f}_{d,i} + \mathbf{f}_{\text{Saff},i} + \mathbf{f}_{\text{Mag},i} + \mathbf{f}_{\nabla p} + \mathbf{f}_{\nabla \cdot \boldsymbol{\tau}} + \mathbf{f}_b \quad (8.6)$$

The particle-fluid interactions implemented in this work are summarized in Table 8.1 where d_p represents the particle diameter, V_p the particle volume, and $\mathbf{v}_p$ the particle velocity.

Table 8.1 Implemented Particle Fluid Interactions.

Forces and Parameters	Equations
Pressure Force	$\mathbf{f}_{\nabla p} = V_p \nabla p$
Shear Force	$\mathbf{f}_{\nabla \cdot \boldsymbol{\tau}} = V_p \nabla \cdot \boldsymbol{\tau}$
Buoyancy Force	$\mathbf{f}_b = V_p \rho_f \mathbf{g}$
Drag Force	$\mathbf{f}_d = \frac{1}{2} \rho_f C_D \frac{\pi d_p^2}{4} \mathbf{u} - \mathbf{v}_p (\mathbf{u} - \mathbf{v}_p)$
Particle Reynolds Number	$Re_p = \rho_f \epsilon_f \mathbf{u} - \mathbf{v}_{p,i} d_p / \mu_f$
Drag Coefficient [98]	$C_D = \left(0.63 + \frac{4.8}{\sqrt{Re_p}} \right)^2 \mathbf{u} - \mathbf{v}_p \epsilon_f^\eta$
Saffman Lift Force [178–180]	$\mathbf{f}_{\text{Saff}} = 1.161 C_S d_p^2 (\mu_f \rho_f)^{1/2} \boldsymbol{\omega}_c ^{-1/2} [(\mathbf{u} - \mathbf{v}_p) \times \boldsymbol{\omega}_c]$
Vorticity	$\boldsymbol{\omega}_c = \nabla \times \mathbf{u}$
Saffman Lift Coefficient	$C_S = \begin{cases} (1 - \beta) e^{(-Re_p/10)} + \beta, & \text{for } Re_p \leq 40 \\ 0.0524 (\alpha Re_p)^{1/2}, & \text{for } Re_p > 40 \end{cases}$
Magnus Lift Force [52]	$\mathbf{f}_{\text{Mag}} = \frac{1}{2} \rho_f A_p C_{LR} \mathbf{v}_p - \mathbf{u} (\mathbf{v}_p - \mathbf{u})$
Magnus Lift Coefficient [53]	$C_{LR} = \frac{d_p \omega_p}{ \mathbf{u} - \mathbf{v}_p }$
Vortical Torque [181]	$\mathbf{M}_{vor} = \pi d_p^3 \mu_f (0.5 \omega_{c,i})$
Rotational Dissipation Torque [181]	$\mathbf{M}_{rot} = -\pi d_p^3 \mu_f (\omega_{p,i})$
η	$2 - \left[3.7 - 0.65 e^{-(1.5 - \log_{10}(Re_p))^2 / 2} \right]$
α	$\alpha = [d_p / (2 \mathbf{u} - \mathbf{v}_p)] \boldsymbol{\omega}_c $
β	$\beta = 0.3314 \alpha^{1/2}$

There exist several models for the calculation of the drag force. The drag model used in this

work is the DiFelice drag model [98] as it is shown to give good results and is often used in the literature. Other drag models, such as the Rong drag model [100], were tested within the present work and led to similar results as the DiFelice model. Both the Saffman and Magnus lift forces are applied in this work. Considering the large shear rate that occurs in the vicinity of the wall and the large particle angular velocity observed experimentally (discussed in a later section), these forces are no longer negligible in liquids and they might have an effect on the simulation results. When the Magnus lift force is applied, a rotational dissipation torque as given in Table 8.1 should be applied to the particles. This will allow the dissipation of the particles rotational velocities and prevent them from spinning uncontrollably which can result in nonphysical values of the Magnus lift as it is proportionally dependent on the particles rotational velocities.

8.2.2 Solid Phase Modelling

The solid particles are individually tracked by integrating Newton's equation of motion and Euler's angular momentum equation. Newton's equation is:

$$m_i \frac{\partial \mathbf{v}_{p,i}}{\partial t} = \sum_{j \in C_i} \mathbf{f}_{ij} + \sum_w \mathbf{f}_{w,i} + m_i \mathbf{g} + \mathbf{f}_{fp,i} \quad (8.7)$$

where m_i is the mass of particle i , $\mathbf{v}_{p,i}$ is the particle i velocity, $\mathbf{f}_{ij}$ are the contact forces between particle i and particle j , C_i includes all particles in the contact list of particle i , $\mathbf{f}_{w,i}$ are the interactions between particle i and the walls where w loops over all walls in contact with particle i , $\mathbf{g}$ is the gravitational acceleration and $\mathbf{f}_{fp,i} = -\mathbf{f}_{pf,i}$ are the interactions between the fluid and particle i which represent the coupling forces between the two phases.

The particle rotational movement is described by:

$$I_i \frac{\partial \boldsymbol{\omega}_{p,i}}{\partial t} = \sum_{j \in C_i} \left(\mathbf{M}_{ij}^t + \mathbf{M}_{ij}^r \right) + \mathbf{M}_i^{ext} \quad (8.8)$$

where I_i is the moment of inertia of particle i , $\boldsymbol{\omega}_{p,i}$ is the angular velocity of particle i , $\mathbf{M}_{ij}^t$ and $\mathbf{M}_{ij}^r$ are respectively the tangential and rolling friction torques due to the contact between particles i and j , and $\mathbf{M}_i^{ext}$ denotes all other external torques. In this work, an external torque known as viscous torque is applied as described by Derksen [181] that takes into account the fluid vorticity at the particle position (vortical torque $\mathbf{M}_{vor}$) and the particle angular velocity (rotational dissipation torque $\mathbf{M}_{rot}$). DEM is described briefly in this section.

For more detailed information about DEM, we refer the reader to the paper by Golshan et al. [105].

Since we are dealing with dense solid-fluid systems, the soft-sphere DEM model is used where artificial overlaps and a set of imaginary springs and dash-pots are used for the modelling of contact forces and torques resulting from particle collisions. This allows for multiple collisions that last several time steps and allows for overlap between the particles during collision. The particle contact force can be calculated using several contact models such as the linear visco-elastic model, non-linear visco-elastic model, and the elastic perfectly plastic models. In this work, we use a non-linear visco-elastic model. The particle contact force ($\mathbf{f}_{ij}$) can be decomposed into its normal and tangential components as [3]:

$$\mathbf{f}_{ij} = \mathbf{f}_{n,ij} + \mathbf{f}_{t,ij} = -k_{n,ij}\delta_{n,ij} - \gamma_{n,ij}\dot{\delta}_{n,ij} - k_{t,ij}\delta_{t,ij} - \gamma_{t,ij}\dot{\delta}_{t,ij} \quad (8.9)$$

where k and γ are the spring stiffness and damping coefficients and are a function of the Young's modulus (Y), the coefficient of restitution (e_r), and the Poisson ratio (ν). δ is the overlap, and $\dot{\delta}$ is the time derivative of the overlap which represents the velocity. The tangential overlap $\delta_{t,ij}$ is limited by Coulomb's criterion [3]:

$$\delta_{t,ij} \leq -\mu_{d,ij} |\mathbf{f}_{n,ij}| \frac{\delta_{n,ij}}{|\delta_{n,ij}|} \quad (8.10)$$

where μ_d is the coefficient of dynamic friction [3]. The tangential, rolling, and viscous torques are obtained as:

$$\mathbf{M}_{t,ij} = \mathbf{r}_i \times (\mathbf{f}_{ct,ij}) \quad (8.11)$$

$$\mathbf{M}_{r,ij} = -\mu_{r,ij} |\mathbf{f}_{ct,ij}| \frac{\boldsymbol{\omega}_{p,ij}}{|\boldsymbol{\omega}_{p,ij}|} R_{e,ij} \quad (8.12)$$

$$\mathbf{M}_{viscous,i} = \pi d_p^3 \mu_f \left(\underbrace{0.5\omega_{c,i}}_{\mathbf{M}_{vor}} - \underbrace{\omega_{p,i}}_{\mathbf{M}_{rot}} \right) \quad (8.13)$$

where $\mu_{r,ij}$ is the coefficient of rolling friction, $R_{e,ij}$ is the effective radius, $\mathbf{r}_i$ is the distance between particle i and the contact point, and $\boldsymbol{\omega}_{p,ij}$ is the relative angular velocity of particle i with respect to particle j . In this work, only the rotational dissipation torque portion of

the viscous torque is enabled to allow for the dissipation of the particle angular velocity and prevent unrealistic values of the Magnus lift force. The vortical torque is not applied as the fluid vorticity is deemed to be not sufficiently resolved to obtain realistic and stable results.

The necessary DEM parameters and their respective equations are given in Table 8.2.

Table 8.2 Normal and tangential spring and damping constants for the visco-elastic model.

Parameters	Equations
Normal spring constant	$k_n = \frac{4}{3}Y_e\sqrt{R_e\delta_n}$
Normal damping coefficient	$\gamma_n = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_n m_e}$
Tangential spring constant	$k_t = 8G_e\sqrt{R_e\delta_n}$
Tangential damping coefficient	$\gamma_t = -2\sqrt{\frac{5}{6}}\beta\sqrt{S_t m_e}$
Effective mass	$\frac{1}{m_e} = \frac{1}{m_i} + \frac{1}{m_j}$
Effective radius	$\frac{1}{R_e} = \frac{1}{R_i} + \frac{1}{R_j}$
Effective shear modulus	$\frac{1}{G_e} = \frac{2(2-\nu_i)(1+\nu_i)}{Y_i} + \frac{2(2-\nu_j)(1+\nu_j)}{Y_j}$
Effective Young's modulus	$\frac{1}{Y_e} = \frac{(1-\nu_i^2)}{Y_i} + \frac{(1-\nu_j^2)}{Y_j}$
β	$\beta = \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}}$
S_n	$S_n = 2Y_e\sqrt{R_e\delta_n}$
S_t	$S_t = 8G_e\sqrt{R_e\delta_n}$

The DEM time step is commonly chosen to be between 10 % and 20 % of the critical time step (Δt_{crit}) required for stability of the DEM simulation. To calculate the critical time step, the Rayleigh characteristic time is used where the smallest Rayleigh time step among all particles is taken to be the critical time step. It is determined as [3, 132]:

$$\Delta t_{crit} = \min_{i \in N_p} \left(\frac{\pi r_i}{0.1631\nu_i + 0.8766} \sqrt{\frac{\rho_i}{G_i}} \right) \quad (8.14)$$

where N_p is the total number of particles, ρ_i is the particle density, G_i is the particle shear modulus, ν_i is the particle Poisson's ratio, and r_i is the particle radius.

8.3 Experimental and Simulation Setup

In the present section, the materials and experimental setup as well as the simulation parameters and setup are introduced.

8.3.1 Rotary Kiln Experiment

Several types of particles are mixed with various fluids having different densities and viscosities and made to rotate in a lab-scale rotary kiln using a rotating ball mill in an attempt to create a simple validation test case with complex fluidization regimes for CFD-DEM simulations.

Ball Mill Setup

The lab-scale rotary kiln is made from acrylic and has a removable lid on its top wall which allows its filling and emptying. The lid is fixed onto the kiln using 15 screws. Below the lid exists a water tight gasket that prevents any leakage. The rotary kiln is of cylindrical shape with a length of 0.185 m and a radius of 0.069 m . The experimental setup is shown in Figure 8.2.

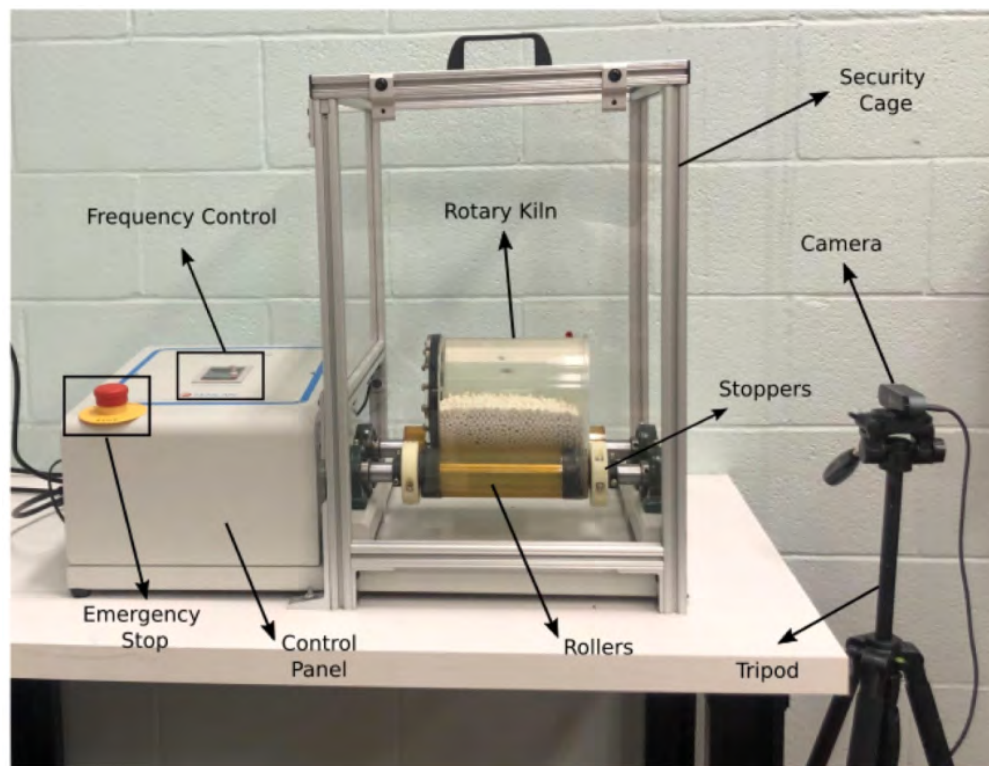


Figure 8.2 The experimental setup showing the rotary kiln and the rotating ball mill.

The water-tight rotary kiln is constructed in-house in the lab of Polytechnique Montreal. It is placed on an off-the-shelf lab roll ball mill with the following specifications: manufacturer Changsha Tianchuang Powder Technology Co., LTD, model QM-5, dimensions 70x415x260 mm, net weight 32 kg and motor operating frequency range of 0 Hz-600 Hz. The setup is

easily reproducible at a modest cost. The front roller is connected to the motor shaft located inside the control panel and is the one that rotates. The back roller is a passive roller which is entrained by the motion of the front roller and its position can be changed depending on the size of the rotary kiln. The camera used is a Logitech Brio camera with an operating range of 30-60 frames per second.

Characteristics of the Particles

We used three types of particles to carry out the experiments: acrylonitrile butadiene styrene (ABS) and two sizes of glass beads which are relatively cheap to buy. All particles are considered to be completely spherical with a sphericity of 1 and a uniform particle size distribution. The diameter of the ABS particles is 5.95 mm and their density is 1813 kg m^{-3} . The glass beads used were of diameters 3 mm and 5 mm and a density of 2500 kg m^{-3} . The different particles are represented in Figure 8.3.

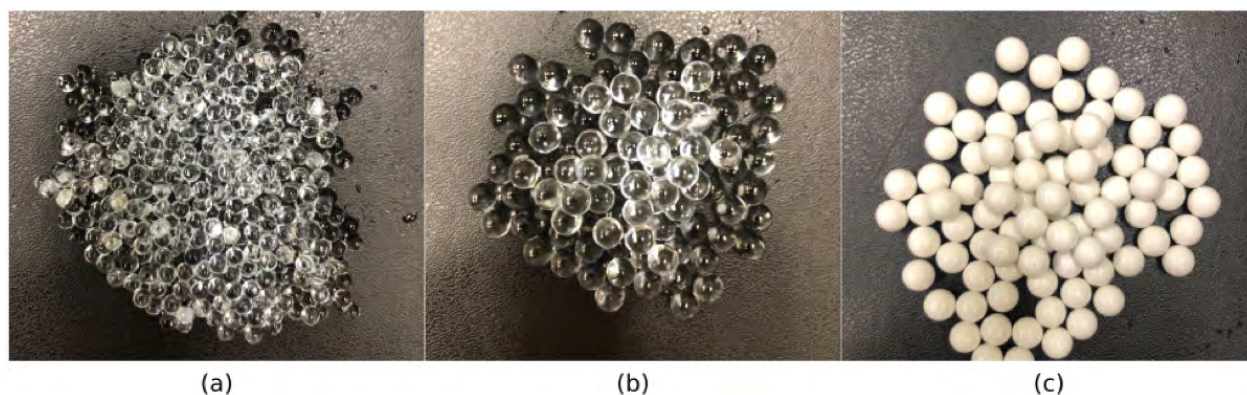


Figure 8.3 The different particles used in the experiment: (a) 3 mm glass beads, (b) 5 mm glass beads, and (c) 5.95 mm ABS particles.

Synthesis of the Fluid

Since the goal is to create a simple validation experiment with no complex equipment, the fluids with varying viscosities used were air, water, and sucrose aqueous solutions with 50 %, 66.66 %, and 100 % w_s/w_w sucrose to water weight fractions. The sucrose solutions are prepared by mixing 3 L of water corresponding to 2.991 kg with the equivalent mass of table sugar which is the main cost related to the synthesis of the viscous solutions. The properties of each fluid are shown in Table 8.3. The densities of the sucrose solution are interpolated from the data tables by Cerdeirina et al. [182] while the viscosities are interpolated from the data tables by Telis et al. [183] for a temperature of 25°C .

	Air	Water	Sucrose Solution		
Sucrose Fraction (w_s/w_w)	0 %	0 %	50 %	66.66 %	100 %
Sugar Mass (kg)	0	0	1495.5	1993.8	2991
Fluid Mass (kg)	0	0	2991	2991	2991
Density (kg m^{-3})	1.225	997	1138.5	1175.62	1229.25
Viscosity ($\text{mPa} \cdot \text{s}$)	0.016	1	3.49	5.17	11.5

Table 8.3 Fluids used in the experiment and their composition.

2 L of hot water are mixed with the table sugar and stirred continuously until most of the sugar is dissolved. Then, 1 L of room temperature water is added to the mixture and stirred manually to homogenize the temperature of the mixture and ensure all table sugar is dissolved. The mixture is left several hours until it cools down to room temperature and the mixture color turns clear.

Experimental Procedure

Particles are emptied inside the rotary kiln until a height of packing of 6.7 cm is reached and the fluid of choice is poured over the particles until they become fully submerged. They are left to soak for several hours while shaking the kiln several times during the soaking period in order to remove as many air bubbles as possible from the particle packing. Later, the kiln is completely filled with the fluid of choice. Finally, the lid of the kiln is screwed in place and the kiln is checked for any potential leakages before being placed on the rotating ball mill. The rotating mill is started and the velocity of rotation is controlled by manipulating the frequency of the motor.

Frequency (Hz)	20	60	140	200	300	400	500
Velocity (rps)	0.13	0.35	0.8	1.13	1.6	2.2	2.8
Velocity ω (rad s^{-1})	0.8164	2.198	5.024	7.0964	10.048	13.816	17.584

Table 8.4 Kiln rotational velocities as a function of motor frequencies.

The studied velocities in this experiment for all particle and fluid types are given in Table 8.4. For each frequency, the behavior of the rotating kiln is captured using the camera where a video is recorded and snapshots of the video are analyzed comparing them to those of the simulations.

8.3.2 Rotary Kiln Simulation

The simulations are carried out in Lethe [89, 105, 130, 160], an open source CFD, DEM, and CFD-DEM software based on the finite element method. The detailed parameters for the simulation setup is given in Table 8.5. The number of particles is calculated based on the experimental packing height of 6.7 cm and an average packing solid fraction of $\varepsilon_s = 1 - \varepsilon_f = 0.62$. The simulations are run for different finite element orders (Q1-Q1, Q2-Q1, Q3-Q2, and Q4-Q3) for both velocity and pressure to determine the effect of the finite element order on the simulation results. We recall that element order p leads to $p + 1$ order of accuracy.

Table 8.5 Simulation parameters.

Parameter	ABS	Glass	Glass
Simulation time (s)	5	5	5
Time integration method	BDF1	BDF1	BDF1
CFD time-step (Δt_{CFD})(s)	0.01	0.005	0.01
Coupling Frequency (f)	200	100	200
Radius of the kiln (R)(m)	0.069	0.069	0.069
Length of the kiln (H_b)(m)	0.185	0.185	0.185
Mesh ($\Delta_r \times \Delta_z$)	8×10	16×20	8×10
Number of particles (N_p)	6000	45362	9490
Diameter of the particles (d_p)(mm)	5.95	3	5
Density of the particles (ρ_p)(kg m ⁻³)	1813	2500	2500
Young's modulus (Y)(MPa)	2.4	3	3
Poisson ratio (ν)	0.37	0.25	0.25
VANS model type	A	A	A
Void fraction calculation scheme	QCM	QCM	QCM
Void fraction smoothing length	$2d_p$	$2d_p$	$2d_p$
Boundary conditions at the walls	Dirichlet	Dirichlet	Dirichlet
Drag model	DiFelice [98]	DiFelice [98]	DiFelice [98]
Gravity (g)(m s ⁻²)	9.81	9.81	9.81

The DEM time step is determined by dividing the CFD time step by the coupling frequency f . The coupling is performed at each CFD time step. The first order backward difference (BDF1) scheme is used for time-stepping. Lethe models turbulence using implicit Large Eddy Simulations (ILES) through the finite element stabilized formulation of the volume-averaged Navier-Stokes equations [130].

As the 3 mm particles are smaller than the other particles, the mesh used for the simulation of these particles is finer than that used for the larger particles. Figure 8.4 shows the difference in the mesh for the smaller and larger particle types.

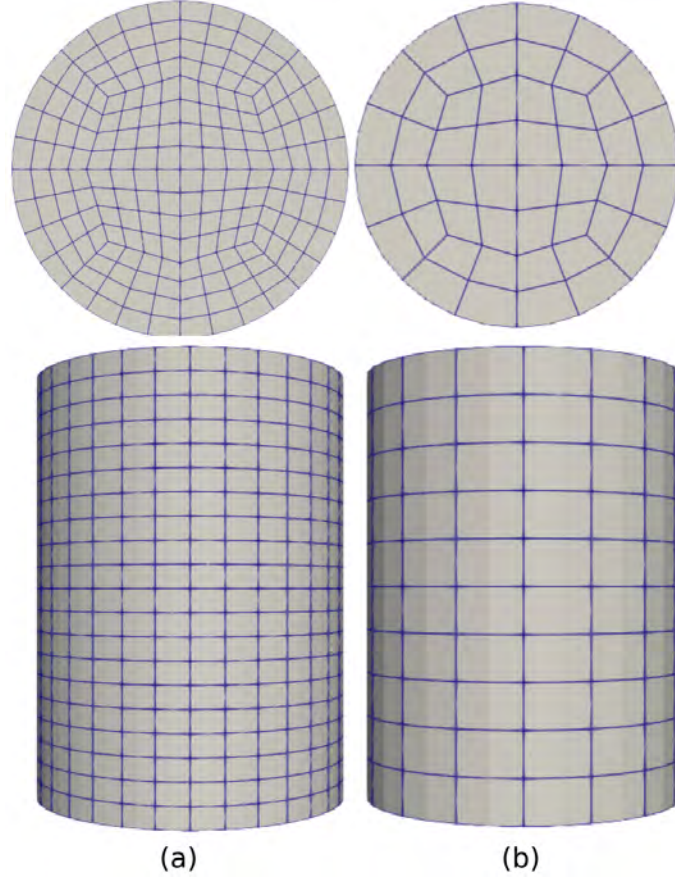


Figure 8.4 Top and side views of the two meshes used in the simulation for: (a) 3 mm glass beads, (b) 5 mm glass beads, and 5.95 mm ABS particles.

The mesh is chosen to better resolve the fluid closer to the particle scale; therefore, the smaller the particles, the finer the mesh should be. However, unresolved CFD-DEM limits the size of mesh elements to around $3 d_p$. Therefore, going below this limit is not feasible as the volume averaging assumptions that govern the VANS equations will no longer be valid leading to inaccurate calculation of the void fraction and affecting the stability of the solver. This is why the boundary layer cannot be resolved better than it already is. One solution would be to use a finer mesh at the boundary but this is unfeasible in unresolved CFD-DEM because if a particle goes towards the boundary, the void fraction becomes incorrect for the finer mesh portion. Another solution to improve the resolution of the fluid near the walls would be to use wall functions, however we are not aware of wall-function formulations which are adequate for the low Reynolds number considered in this work and which take into account the effect of particles. Thus, they cannot be used in unresolved CFD-DEM. This is one of the reasons we propose the use of high order elements for unresolved CFD-DEM where the boundary is better resolved without having to refine the mesh since the higher order polynomials allow for a steeper velocity gradient in the vicinity of the walls. The CFD time step chosen for the

simulations depends on the Courant-Friedrichs-Lewy (CFL) condition number for which a $\text{CFL} \lesssim 1$ is aimed for. As the mesh for the 3 mm glass beads is refined once, that is the mesh elements are divided once in each direction, then the CFD time step is also halved once to obtain stable simulations at higher velocities. Isoparametric elements are used in cells close to the rotating wall to ensure consistency of the high-order finite element method.

The void fraction is calculated using the quadrature centered method (QCM) [184] as it is an analytical method that results in a void fraction profile that is continuous in time and space. To enhance numerical stability of the VANS solver, the void fraction is smoothed using a smoothing length $L = 2d_p$ which is added to the $\mathcal{L}^2$ projection equation of the void fraction resulting in the following:

$$\int_{\Omega} \varphi_i \varepsilon_{f,j} \varphi_j d\Omega + \int_{\Omega} L^2 \nabla \varphi_i \nabla \varphi_j \varepsilon_{f,j} d\Omega = \int_{\Omega} \varepsilon_{f,i} \varphi_i d\Omega \quad (8.15)$$

where $\varepsilon_{f,i}$ and $\varepsilon_{f,j}$ are respectively the cell value and the projected nodal value of the void fraction, and φ is the finite element basis function. We refer the reader to the article by El Geitani et al. [130] for details about the smoothing strategy.

The simulation time was chosen to be 5 s to ensure that steady state has been reached inside the kiln. Multiple snapshots of the results are taken and compared to the experimental results. For the various velocities, fluids, and particle types, the sliding and rolling friction coefficients as well as the coefficient of restitution are calibrated. This is done by examining the angle of inclination of particles in the kiln for the rolling flow regime and comparing the results between experiments and simulations. Moreover, the effect of these parameters on the transitioning between regimes is determined.

8.4 Results and Discussion

In this section, the experimental results are extracted and analyzed, followed by a detailed comparison between experimental and simulation results in an attempt to better understand the effect of surface parameters, particle-fluid interactions, and the order of the numerical scheme on the accuracy of predictions of CFD-DEM simulations of rotary kilns.

8.4.1 Dimensional Analysis of the System

The system is non-dimensionalized to remove all physical dimensions, resulting in a simplified and parameterized description. This clarifies the relative size and importance of the different terms and makes solving the system at different limits straightforward. The following

variables are considered in the dimensional analysis of this problem: the radius of the rotary kiln (R), the diameter (d_p) and density (ρ_p) of the particles, the rotational velocity (ω) of the kiln, the density (ρ_f) and viscosity (μ_f) of the fluids, and the gravitational acceleration (g). These quantities as well as the dimensionless numbers characterizing the problem are summarized in Table 8.6.

Table 8.6 Dimensions and dimensionless numbers associated with the physical quantities for the rotary kiln.

Physical Quantities	SI Units	MLT System
R	m	L
d_p	m	L
ω	s^{-1}	T^{-1}
μ_f	$kg\ m^{-1}\ s^{-1}$	$ML^{-1}T^{-1}$
ρ_p	$kg\ m^{-3}$	ML^{-3}
ρ_f	$kg\ m^{-3}$	ML^{-3}
g	$m\ s^{-2}$	LT^{-2}
Dimensionless Numbers	Expression	
Π_1	$\frac{R}{d_p}$	-
Π_2	$\frac{\mu_f}{\rho_f d_p^2 \omega}$	-
Π_3	$\frac{\rho_p}{\rho_f}$	-
Π_4	$\frac{g}{d_p \omega^2}$	-

The basis of length (L), time (T), and mass (M) are taken to be d_p , ω^{-1} , and $\rho_f d_p^3$ respectively. From the dimensional analysis performed, four dimensionless numbers are obtained. Π_1 represents the size ratio between the rotary kiln and the particles. Π_2 represents $1/Re_\omega$ where Re_ω is the particle rotational Reynolds number where a new definition of velocity ωd_p is obtained. Π_3 represents the density ratio between the fluids and the particles. Π_4 represents $1/Fr_p$ where the length used in Fr_p is the diameter of the particle instead of the radius of the kiln. As such, in order to determine the regime change in the rotary kiln, the dimensionless numbers considered are those that take into account the rotational velocity of the kiln upon which the the flow regime is highly dependent.

8.4.2 Regime Change in Rotary Kiln

For varying values of Π_2 and Π_4 , the regime type has been plotted to create a map of regimes as shown in Figure 8.5. For the same particle type, the regime change is dependent on both Π_2 and Π_4 where it is seen that for a given particle diameter, the relation between both dimensionless numbers and the regime change is always linear. As both Π_2 and Π_4 decrease,

meaning Fr_p and Re_ω increase, the regime changes mostly from rolling to cascading. Some cases exhibit cataracting regime while others exhibit centrifuging regime as their end regimes.

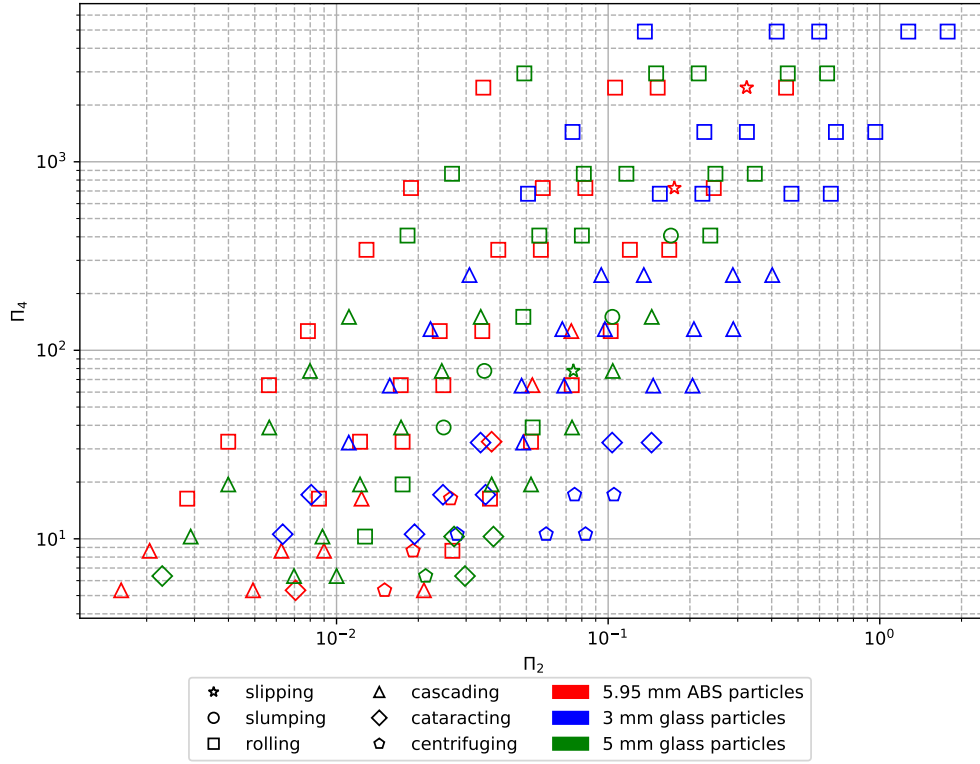


Figure 8.5 Rotary kiln regime map as a function of Π_2 and Π_4 .

For each particle type, the largest value of Π_2 represents the experiment with air where the value of Π_3 is the smallest and the smallest value of Π_2 represent the experiment with water. The 3 mm glass particles are the only particles that exhibit centrifuging regime in air.

Additionally, for the region with a low Fr_p ($\Pi_4 > 3 \times 10^2$), the dominant regime is the rolling regime for all particle types and fluids except for the 5.95 mm ABS particles at 100 % sucrose solution where a sliding regime is observed for the smallest rotational velocities. For $\Pi_4 < 3 \times 10^2$, the regime changes and evolves as a function of increasing Fr_p . The centrifuging regime is dominant at small Π_4 numbers and large Π_2 numbers which signifies that the fluid viscosity plays an important role in accelerating the regime transition. Only 5 mm glass beads produce the slumping regime for 66.66 % and 100 % sucrose solutions. It is important to note that despite all efforts taken in ensuring that the rotary kiln does not slip over the rollers of the rotating ball mill, the heavier the contents of the rotary kiln are and the larger the rotational velocity is, the less certain we are that the experiments are slip free. Therefore, it might be that some regimes that should have manifested in the experiment did not as an effect of the slight slip.

For most of the cases and particle-fluid combinations, the trend of the regime change is straightforward where in general the regimes follow what is shown in Figure 8.1. The choice of the fluid as a liquid with varying viscosities plays a role in accelerating the appearance of the regimes, that is making the same regime appear at lower rotational velocities, and in making visible some regimes that would otherwise not appear in air, specifically the sliding and slumping regimes.

8.4.3 Rotation of Particles in Kiln

The application of the Magnus lift force and the rotational dissipation torque is valid if the particles are spinning inside the rotary kiln. To determine whether or not the particles are rotating, we mark 10 ABS particles with a black marker on one side and a red marker on the other and place them inside the rotary kiln along with the remainder of the particles. The kiln is rotated at various rotational velocities and the results are captured using the Logitech camera. Figure 8.6 demonstrate that the particles rotate significantly in both gas and liquids. As such, the application of the Magnus lift force as well as the rotational dissipation torque is justified.

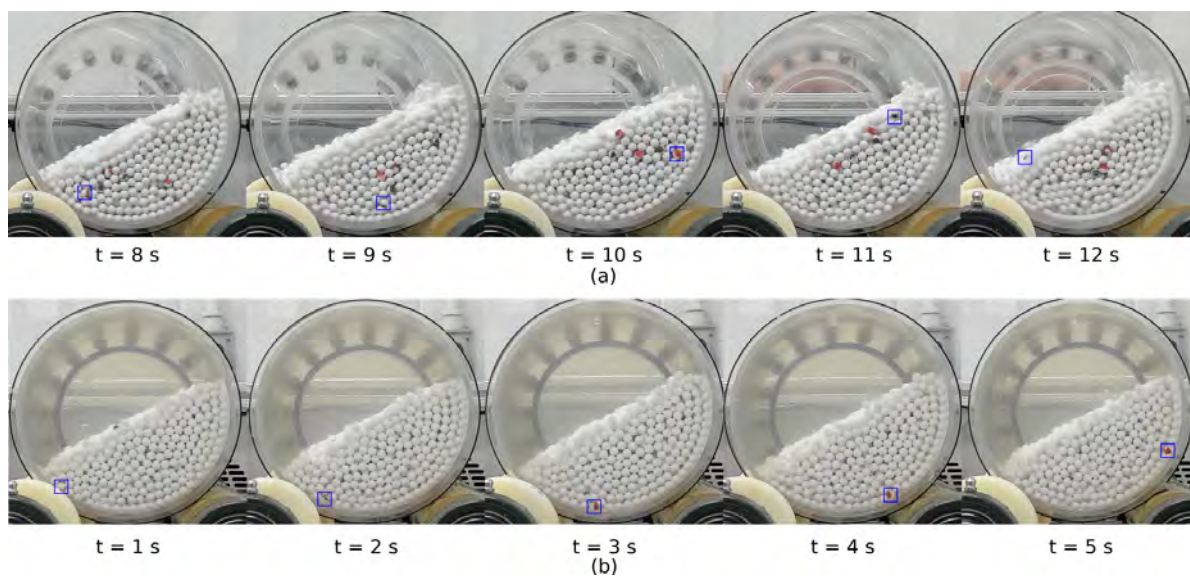


Figure 8.6 Snapshots of ABS particles in rotary kiln with (a) air and (b) 50 % sucrose solution where marked particles rotate considerably in a short time interval.

8.4.4 Effect of the Finite Element Order on Regime Change

Different finite element orders are used in the simulation to determine the effect of accurately resolving the fluid on the regime change in the rotary kiln. For this, simulations of ABS

particles and 100 % sucrose solution using Q1-Q1, Q2-Q1, Q3-Q2, and Q4-Q3 elements are run and results are compared. Figure 8.7 demonstrates the regime obtained as well as the fluid boundary layer for a motor frequency of 140 Hz using the four finite element orders.

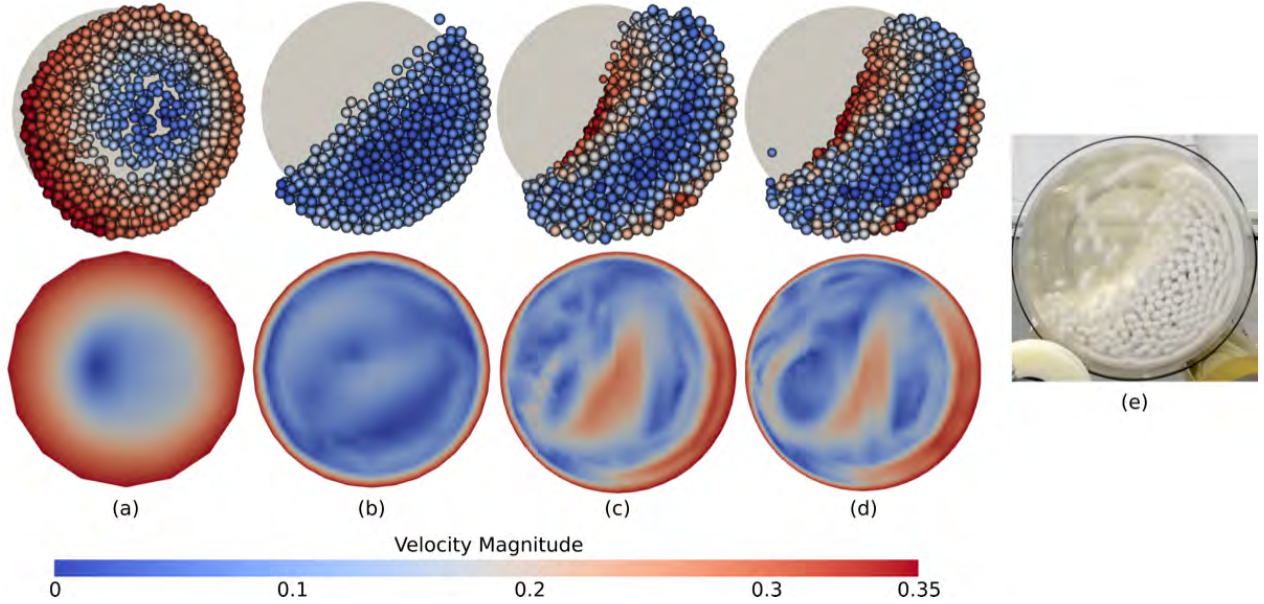


Figure 8.7 The regime of particle motion and the time-averaged steady-state velocity magnitude of particles and fluid as a function of finite element orders and the sliding friction coefficient for (a) Q1-Q1 and $\mu_s = 0$, (b) Q2-Q1 and $\mu_s = 0.24$, (c) Q3-Q2 and $\mu_s = 0.8$, (d) Q4-Q3 and $\mu_s = 0.8$, and the comparison with (e) experimental result.

At low rotational velocities, Q1-Q1 simulations lead to angles of inclination larger than those obtained in the experiments. Additionally, for higher velocities, it can be seen that Q1-Q1 simulations result in the wrong regime compared to the experimental result as shown in Figure 8.7. This is explained by the presence of a large boundary layer equivalent to two particle diameter due to the diffusion of the fluid velocity within a cell when using Q1-Q1 elements as shown in Figure 8.7 (a). This large boundary layer traps the particles at and near the wall and translates them with the same velocity as the fluid. This results in a fake centrifuging regime caused by the diffused boundary layer even for a sliding friction coefficient of 0. This is also visible looking at the fluid where a minimal velocity is observed in the center of the kiln and a maximum velocity at the boundary.

On the other hand, the low rotational velocity simulations show good agreement in the angle of inclination of the particles in the kiln between the simulation and the experimental results for Q2-Q1, Q3-Q2, and Q4-Q3 elements. However, only Q3-Q2 and Q4-Q3 simulations correctly capture and reproduce the inflection point in the middle of the inclined plane.

Additionally, for higher velocities, the higher order elements lead to similar results and allow the correct regime to be obtained. This is because the boundary layer for these higher order elements is smaller than a single particle diameter as it is not as diffused as for the case of Q1-Q1 elements. As such, it is considered to move the particles correctly with a lesser effect of numerical dissipation. Nonetheless, the accuracy in resolving the fluid changes considerably between Q2-Q1, Q3-Q2, and Q4-Q3 simulations. Q3-Q2 and Q4-Q3 elements result in the most accurate predictions as shown in Figure 8.7 where the fluid velocity profile is similar, contrary to Q2-Q1 simulations where the fluid velocity profile differs considerably. This translates into accurate regime prediction for the two highest orders studied.

As the element order increases and the boundary layer becomes smaller, the sliding friction coefficient in the simulations need to be increased in order to obtain correct flow regimes until it converges to a certain value and becomes independent of the order. This can be concluded from Figure 8.7 where using $\mu_s = 0.24$ gives correct results for Q2-Q1 and using $\mu_s = 0.8$ gives correct results for Q3-Q2 and Q4-Q3 simulations. For Q1-Q1 simulations, no matter the value of μ_s , a complete regime change is observed where the boundary layer is large and even smaller sliding friction coefficients lead to the centrifuging regime at intermediate velocities. This means that μ_s changes between element orders as it takes into account mesh inadequacies and aims at compensating for them. Therefore, Q2-Q1 elements where μ_s is still mesh dependent, and Q3-Q2 elements where μ_s becomes mesh independent are chosen for all the simulations, because using Q4-Q3 elements has an increased computational cost with similar accuracy in the prediction of regimes, requires increased computational resources and results in large simulation times compared to using Q3-Q2 elements. It is important to mention that the calibrated data using Q2-Q1 are only valid for Q2-Q1 and Q2-Q2 simulations but those calibrated for Q3-Q2 are valid for Q3-Q2 and all higher order elements as these properties become order independent.

8.4.5 Calibration of Surface Properties and their Effect on Regime Change

Three main particle surface properties should be calibrated for each particle type. These are the sliding friction coefficient (μ_s), the rolling friction coefficient (μ_r) and the coefficient of restitution (e_r). These parameters are calibrated by simulating the rotary kiln for each particle and fluid type at low velocities in the rolling regime and measuring the angle of inclination comparing it to the angle obtained experimentally. To determine the effect of μ_r , several simulations have been launched for the same fluid and particle types while varying only μ_r . It was found that a choice of μ_r in the range of 0.2-0.3 works well for all simulations and any change in the value within the given range has a negligible effect on the angle of

inclination and at higher velocities did not play a role in the regime change. For the higher kiln rotational velocities, the choice of $\mu_r < 0.2$ affected the rotational velocity of the particles where using a $\mu_r = 0$ led to much higher rotational velocities of the particles. Therefore, since the start, we set $\mu_r = 0.2$ for all simulations of the ABS particles and $\mu_r = 0.3$ for the 3 mm and 5 mm glass beads considered in this work.

The remaining parameters requiring calibration are μ_s and e_r . μ_s was calibrated based on the angle of inclination in the rolling regime while e_r was determined as the value that allows for the centrifuging regime where possible. The calibrated values are given in Table 8.7 for Q2-Q1 simulations and in Table 8.8 for Q3-Q2 simulations.

Particle Type	Surface Property	Fluid Type				
		Air	Water	50 % Sucrose	66.66 % Sucrose	100 % Sucrose
ABS ($d_p = 5.95$ mm)	μ_s	0.3	0.24	0.24	0.24	0.24
	e_r	0.9	0.2	0.2	0.2	0.2
Glass ($d_p = 3$ mm)	μ_s	0.4	0.3	0.3	0.3	0.3
	e_r	0.97	0.2	0.2	0.2	0.2
Glass ($d_p = 5$ mm)	μ_s	0.45	0.35	0.35	0.35	0.35
	e_r	0.97	0.2	0.2	0.2	0.2

Table 8.7 Calibrated surface properties μ_s and e_r for Q2-Q1 simulations.

Particle Type	Surface Property	Fluid Type				
		Air	Water	50 % Sucrose	66.66 % Sucrose	100 % Sucrose
ABS ($d_p = 5.95$ mm)	μ_s	0.3	0.33	0.37	0.39	0.8
	e_r	0.9	0.2	0.2	0.2	0.1
Glass ($d_p = 3$ mm)	μ_s	0.4	0.42	0.5	0.55	0.6
	e_r	0.97	0.2	0.2	0.2	0.1
Glass ($d_p = 5$ mm)	μ_s	0.45	0.5	0.52	0.55	0.7
	e_r	0.97	0.2	0.2	0.2	0.1

Table 8.8 Calibrated surface properties μ_s and e_r for Q3-Q2 simulations.

Both parameters are affected by the particle and fluid types. They change drastically when moving from air to liquid. Even though Joseph et al. [165] show that the particle coefficient of restitution decreases with an increase in the viscosity of the fluid, we find that in Q2-Q1 simulations, it decreases significantly between air and water and that for the sucrose solution with increasing viscosities, using the same e_r and μ_s as water works well. This means that

in Q2-Q1 simulations, the angle of inclination as well as the regime observed are still mesh dependent. The same trend is observed for the coefficient of restitution in Q2-Q1 and Q3-Q2 simulations meaning that as long as the coefficient of restitution is small in liquids, the correct regime is obtained.

However, for the sliding friction coefficient (μ_s) calibrated using Q3-Q2 simulations, the value increases with an increase in the viscosity of the fluid. This allows us to deduce that the regime change and the angle of inclination are no longer mesh dependent. The increase in the sliding friction coefficient observed is explained by the lubrication force that is not explicitly applied in the unresolved CFD-DEM solver but that is compensated for by the sliding friction coefficient. The values of μ_s and e_r shown in Tables 8.7 and 8.8 above allow for a good agreement between experimental and simulation results for all motor frequencies as shown in Figure 8.8 for Q2-Q1 simulations and in Figure 8.9 for Q3-Q2 simulations.

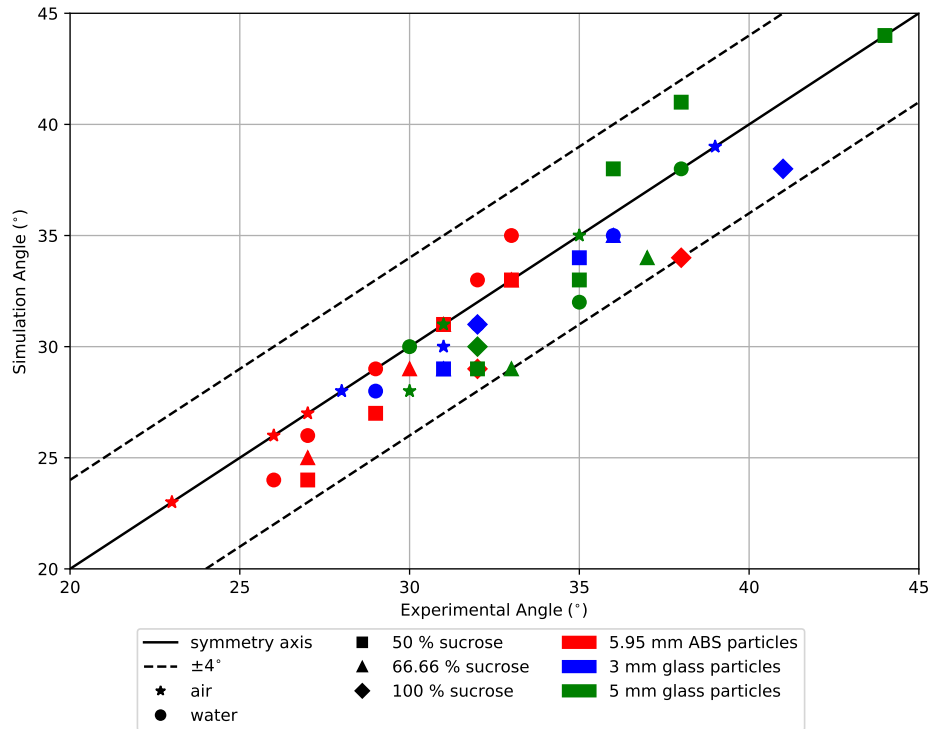


Figure 8.8 Comparison between the angle of inclination obtained from both experiments and Q2-Q1 simulations for all particle types.

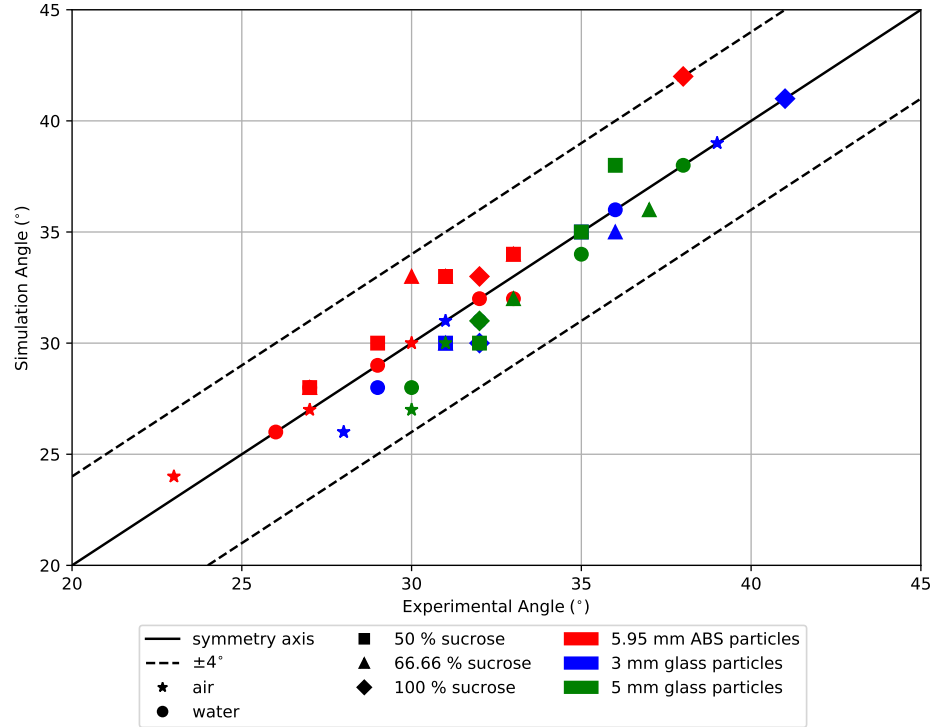


Figure 8.9 Comparison between the angle of inclination obtained from both experiments and Q3-Q2 simulations for all particle types.

Table B.1 and Table B.2 show the angle of inclination obtained through the experiments and the corresponding simulations. All dashes in the tables represent a change from the rolling regime where an angle of inclination can no longer be measured. Parity plots showing the variation of the angle of inclination between the simulations and the experiments are shown in Figure 8.8 for Q2-Q1 simulations and Figure 8.9 for Q3-Q2 simulations.

The maximum angle difference between the simulations and experiments is of 4° while the minimum is 0° where the experiment and simulation agree 100 %. The choice of both μ_s and e_r affects the regime change in the rotary kiln. For example, in the sucrose solution where experimentally we observe the centrifuging regime, if an $e_r > 0.2$ is chosen, the particles will not centrifuge at the correct kiln velocity and will remain in the cascading or cataracting regime. Similarly, the choice of μ_s is important. If the chosen μ_s is smaller than the calibrated value, the angle of inclination would be much smaller than the experimental value and the regime change would be delayed, meaning a much higher kiln rotational velocity is required to move from one regime to the other compared to the experiment. If the chosen μ_s is greater than the calibrated value, then regimes might change much more quickly than they should and at lower kiln rotational velocities than observed experimentally. This can lead, for the

same rotational velocity, to a completely different regime than the one manifested in the experiments.

Additionally, Q3-Q2 simulations show better agreement with the experimental angles of inclination compared to Q2-Q1 simulations. This is demonstrated by Figure 8.9 where the points are closer to the centerline compared to those in Figure 8.8. As such, Q3-Q2 simulations lead to better predictions of the angle of inclination.

Figures 8.10 and 8.11 show the regime change of the particles flow inside the kiln for the different kiln velocities of both experiments and simulations. For most of the simulations, predictions agree well with what is obtained experimentally. In some simulations, the regime change is faster than that of the experiments. This can be attributed to the slipping of the kiln on the rotating ball mill, since even slight slipping can reduce the kiln velocity and prevent the correct regime from manifesting itself. The slipping and slumping regimes observed experimentally for the 5 mm glass particles are not reproduced computationally. These regimes might have appeared experimentally due to certain particle or kiln properties that are not taken into account in the simulations. Nonetheless, the overall regime transition follows well what is observed experimentally.

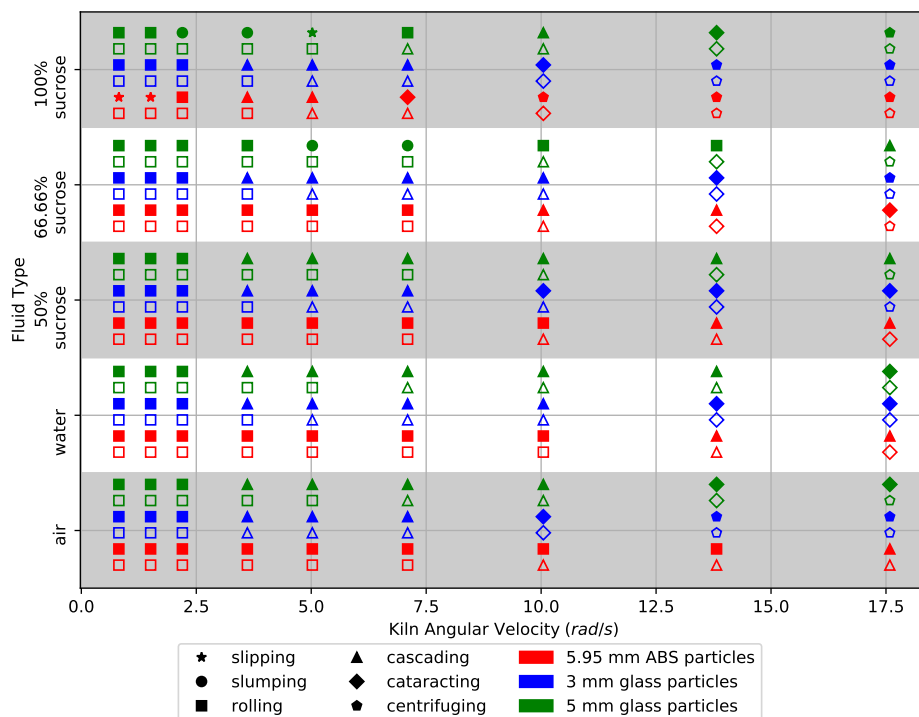


Figure 8.10 Comparison between the regime for experiments (filled) and Q2-Q1 simulations (hollow) at several kiln rotational speeds and for all particle types.

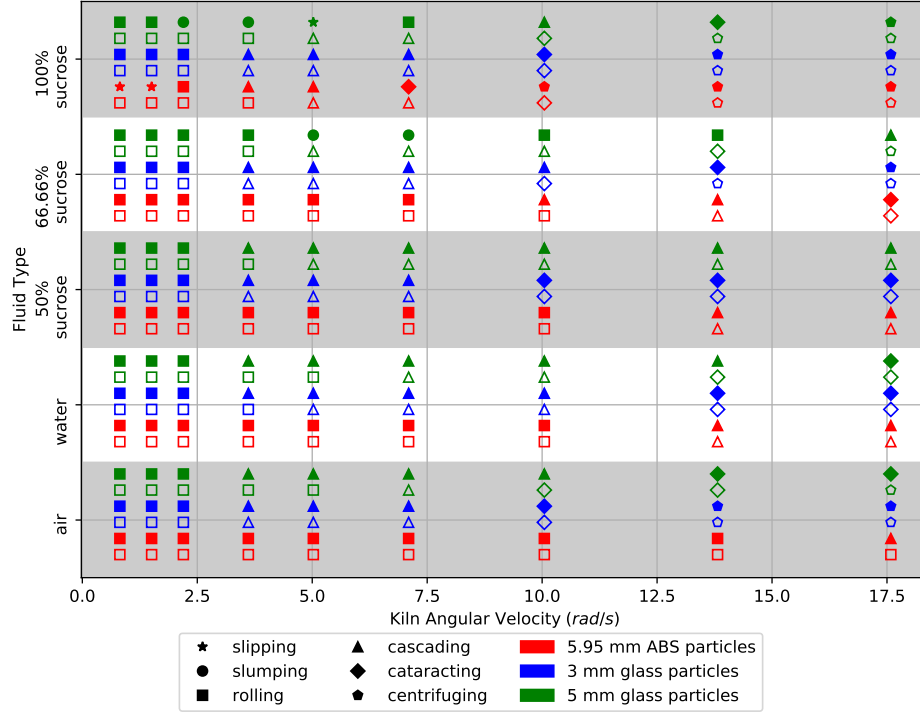


Figure 8.11 Comparison between the regime for experiments (filled) and Q3-Q2 simulations (hollow) at several kiln rotational speeds and for all particle types.

We calculate the percentage accuracy of the prediction as the fraction of velocities for which the regimes agree to the total number of velocities studied for all fluid types. For Q2-Q1 simulations, the percentage accuracy of regime prediction is roughly 87 % for 3 mm glass particles, 58 % for 5 mm glass particles, and 73 % for 5.95 mm ABS particles while for Q3-Q2 simulations, the percentage accuracy of regime prediction is 96% for 3 mm glass particles, 58 % for 5 mm glass particles, and 84 % for 5.95 mm ABS particles. In general, the accuracy of regime prediction improves considerably from Q2-Q1 to Q3-Q2 simulations; however, simulations of 5 mm glass particles suffer for both orders. These particles possess the highest particle Reynolds number (Re_p) which might explain why their results are not as accurate. As such, the weak accuracy of the 5 mm glass beads for both orders means that the problem is not related to the fluid flow but can be an issue with the experimental setup or with the particles properties themselves.

8.4.6 Effect of Lift Force on Regime Change

Usually, unresolved CFD-DEM simulations account for the following forces between the solid and fluid phases: gravity including buoyancy, drag force, pressure gradient force, and shear

stress force. Lift force is sometimes implemented depending on the application as demonstrated by Ferreira et al. [163]. The lift force being discussed is the combination of both Saffman lift force and Magnus lift force which has a contribution to the particles translational momentum. The Saffman lift force appears when the pressure on the two sides of the particle is different due to a velocity gradient in the fluid above and below the particle and thus it is termed continuous-phase vorticity-induced lift. The Saffman lift force acts in the direction from the lower relative velocity to the higher relative velocity between the particle and the fluid. The Magnus lift on the other hand is generated due to the rotation of particle and is perpendicular to the direction of particle motion and fluid flow. In gaseous fluids, the lift force is usually negligible compared to the drag force. However, in liquids, lift can play an important role. Consequently, we studied the influence of the lift force on the regime transition and manifestation as a function of the kiln rotational velocity. We simulated ABS particles at a frequency of 400 Hz for a 100 % sucrose solution with a combination of lift forces and with no lift force. The simulation results as well as the experimental results are shown in Figure 8.12

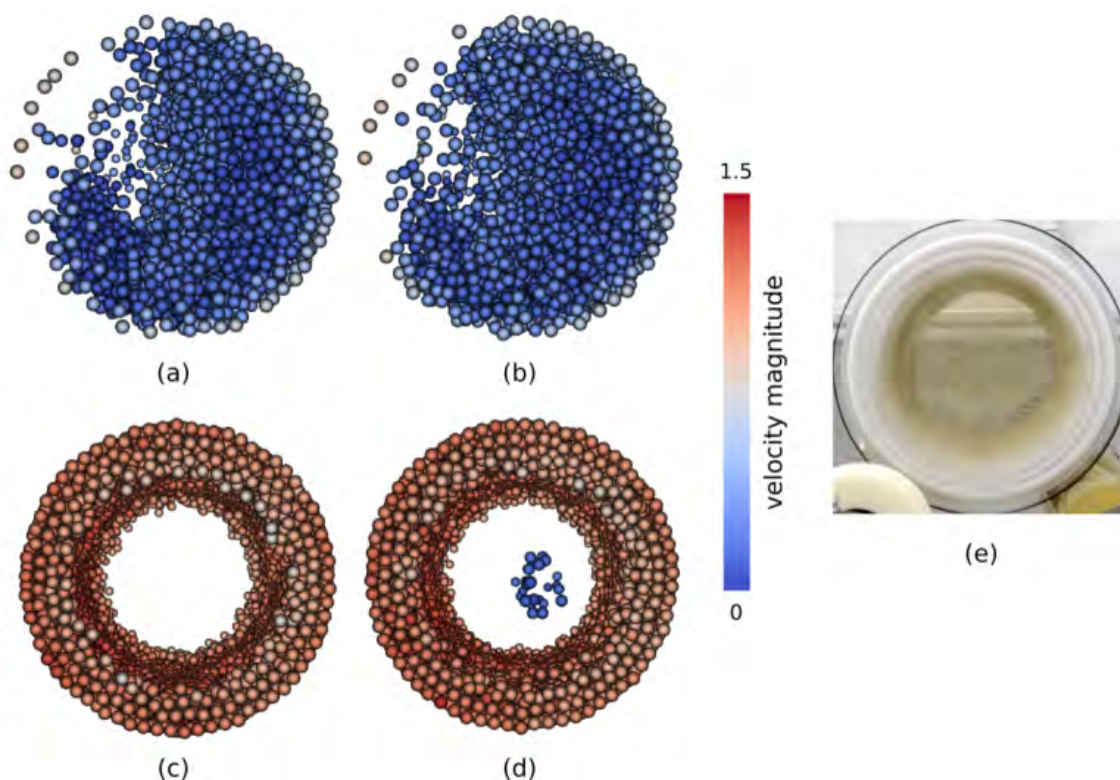


Figure 8.12 ABS particles flow regimes in 100 % sucrose solution at 400 Hz for Q2-Q1 simulations with: (a) no lift force, (b) Saffman lift force only, (c) Saffman and Magnus lift force and (d) Magnus lift force only, and its comparison with (e) experimental result.

In the complete absence of the lift force and in the presence of only the Saffman lift force, the particles do not centrifuge at the high velocities, which contradicts the experimental result. The simulation gives the correct regime when both the Saffman and Magnus lift forces are enabled and when only the Magnus lift force is enabled. This shows that the Magnus force is the dominant component of the overall lift force at high kiln rotational velocities. According to the conclusions drawn by Loth [185], for particles with low particle Reynolds number (Re_p), the Saffman lift force dominates, while for higher Re_p , the Magnus lift becomes substantial and might dominate the overall lift force. As such, for the rotary kiln simulation, Re_p is around 140 and thus, the Magnus lift plays an important role in the characterization of the flow regime inside the rotary kiln. This is amplified by the rotational nature of the confined flow in the kiln. Figure 8.13 demonstrate the main force balance acting on a single particle in the rotary kiln.

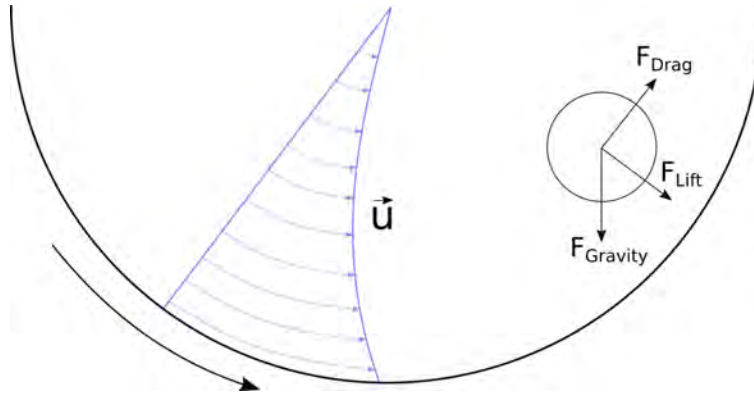


Figure 8.13 Forces acting on a single particle in a rotary kiln under the effect of a shear velocity flow $\vec{u}$.

Since the fluid velocity is maximum at the wall of the rotary kiln and lower towards the center of the kiln, the lift force is expected to act perpendicular to the rotary kiln wall and outwards toward the wall. Therefore, at high velocities, the lift force pushes the particles towards the wall and when it is large enough overcomes drag and gravity and prevents them from falling into the middle of the kiln, thus creating what is known as the centrifuging regime.

8.5 Conclusions

This work presents a simple and effective experimental validation benchmark for unresolved CFD-DEM using a liquid-filled rotary kiln. It is a strong validation experiment since it exhibits many regime transitions which can be used to validate the unresolved CFD-DEM model. Another advantage of this experimental procedure is its simplicity, time efficiency

and construction costs compared to other experiments used for CFD-DEM validation such as fluidized and spouted beds. Additionally, the different parameters and interactions that have a major effect on the results were analyzed and discussed. We found that the choice of particle surface properties such as the sliding friction coefficient and the coefficient of restitution and the order of the finite elements as well as accounting for the different components of the lift force play an important role in determining the simulation fidelity. We proved that the particles spin around themselves inside the kiln and thus explained the importance of applying the Magnus lift in order to obtain the centrifuging regime where applicable. Finally, the rigorous validation and parameter calibration applied in this work can be used in any unresolved CFD-DEM software as it is readily reproducible. The rolling ball mill can be purchased from the manufacturer, while the cylinder can be cheaply manufactured using acrylic. The particles are commercially available, while the sucrose solution only requires table sugar for its preparation.

8.6 Acknowledgements

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CHAPTER 9 GENERAL DISCUSSION

The main objective of this thesis can be reformulated as follows:

Development of a robust unresolved CFD-DEM numerical model for the accurate prediction of multiphase flows and their behavior in industrial scale fluidized and spouted beds.

This objective is complicated to achieve straight away. Therefore, it was divided into several sub-objectives, each helped in realizing the overall objective of this thesis. As solid-gas flows are the flows of interest in this work, it is important to be able to model each phase separately before the coupling can be confidently achieved.

In Chapter 5 (Article 1), the fluid phase, more specifically the gaseous phase, is modelled through the development of a high-order parallelized VANS solver. Both models A and B of the VANS equations are discretized using the finite element method and stabilized using SUPG, PSPG, and grad-div stabilization techniques. This allows the implicit modelling of turbulence using ILES and results in a VANS scheme with shock capturing capabilities as it is demonstrated in Appendix A. The scales that are dissipated using ILES are controlled by the truncation error and the residual of the VANS equations and as such, more scales are resolved the finer the mesh is. However, the presence of particles can act as a source term within the cells at the same scale and hence adverse effects can result from the two contributions.

The finite element weak form differs between both models especially for the shear stress and pressure terms of the momentum equation. The use of the method of manufactured solutions allows the verification of the solver and its high order capabilities in both time and space through convergence analysis studies. The drag force exerted by the solid particles on the fluid is implemented and this is validated using a packed bed test by measuring the pressure drop observed in the bed. Nevertheless, the pressure is an integral value, so it can hide many inaccuracies. It would have been more extensive to consider a canonical case to validate that the choice of stabilization can yield the expected results in modelling turbulence instead of directly moving from the method of manufactured solutions to the packed bed test case. Such case can involve the creation of a source term that imitates the motion of a particle. Thus, the artificial viscosity introduced by ILES could be compared to the Smagorinsky eddy viscosity..

Since the shear force and the pressure gradient force differ between the two models, and to

keep the models mathematically equivalent, the drag force is also implemented differently between the models. So far, the solver does not allow the motion of particles, where it can only treat the solid phase as fixed objects around which the fluid can flow. The fluid is aware of the particles due to the void fraction projection schemes implemented at that stage which are the PCM and SPM schemes.

To extend the VANS solver to an unresolved CFD-DEM solver capable of modelling the motion of both the solid and fluid phases, a coupling strategy is adopted in Chapter 6 (Article 2). This necessitates the identification of important particle-fluid interactions that cannot be neglected. To this effect, the following forces are identified: drag force, buoyancy force, shear force, and pressure force. These forces are calculated for both the fluid and the solid phases to respect Newton's third law of action and reaction. The forces exerted by the fluid on the particles allow the latter to fluidize once the fluid velocity is greater than a certain velocity known as the minimum fluidization velocity. The implementation of the particle-fluid interactions specifically the drag and lift forces are limited in their accuracy as they represent empirical correlations. As such, there is a chance that the higher-order solutions obtained are controlled by the correlations errors which will render the high-order capabilities of the solver ineffective. This has not been investigated within the context of this work, and thus it is open to debate and further works should be done to determine the limitations of the high-order scheme in this regard.

The majority of unresolved CFD-DEM solvers uses a coupling solver to couple between independent CFD and DEM solvers. This limits the possible computational speed that can be obtained from them. This is why we adopted a unified architecture for the unresolved CFD-DEM solver in Lethe. This architecture allowed for improved speeds and performance as the communication of information between the phases was on the spot and did not require the transfer of information between solvers. Additionally, in an attempt to reduce the overall computational cost and take full advantage of the parallelization of both the VANS and the DEM solvers, load balancing is added to the unresolved solver. The model was verified and validated using several test cases.

So far, the developed unresolved CFD-DEM model works well; however, it suffers from certain limitations mainly related to the particle projection scheme. There exists several particle projection schemes in the literature ranging between analytical schemes and approximate schemes. Since analytical schemes are expensive to implement and greatly reduce the speed of the solver, approximate schemes such as PCM and SPM are often used. The PCM and SPM are simple to implement but they suffer from discontinuity in time and space. This can lead to instabilities in the simulation especially at lower time steps. Additionally, they limit

the minimum size of the mesh elements that can be used which prevents more accuracy in solving the fluid when it is needed. Therefore, the analytical QCM scheme is proposed in Chapter 7 (Article 3) and aims at decoupling the averaging volume of the VANS equations from the mesh elements. This scheme is continuous in both time and space, thus allowing for smaller time steps and finer meshes using relatively inexpensive calculations. Mesh elements smaller than the particle size can be used which is only possible with few other projection schemes. Several schemes have been developed in the literature to couple CFD and DEM when the particle size is larger than the mesh elements. For example, Zhang et al. [186] developed in the context of unresolved CFD-DEM a novel coupling method that is designed for simulations with large-sized particles and a sub-particle scale mesh. The coupling includes both smoothing the particle point data and filtering the gas field data. Their method is also efficient in parallel computing. This allows better resolution of the fluid at the particle scale. Moreover, it is computationally efficient when compared to other analytical schemes and allows for improved convergence of the CFD solver. This results in enhanced performance of the simulation and considerably reduces the computational time required.

Our solver is not limited by the CFL number as it is fully implicit. Several test cases included a CFL number greater than 1 and resulted in physical simulations. Nonetheless, such simulations required a larger number of non-linear iterations for the solver to converge. Moreover, for certain cases, having a CFL number larger than 1 led to unrealistic DEM results, where the relative particle to fluid velocity required for the calculation of particle-fluid interactions was large which resulted in very large values of these forces and led the particles to move much faster than they should. Particles were crossing boundaries unrealistically as the contact detection step in DEM could not locate them. On the other hand, a trade-off is expected between the h-refinement of the mesh and the use of high-order schemes. However, since we use unresolved CFD-DEM, we are limited by the element size which is dependent on the particle size, h-refinement is not always possible, and the use of high-order schemes offers a solution.

In an attempt to further validate the unresolved CFD-DEM solver and to study the effect of the choice of DEM surface properties on the overall fidelity of the CFD-DEM simulations, a solid-gas and solid-liquid rotary kiln benchmark is developed and the particles motion inside the kiln is studied both experimentally and numerically in Chapter 8 (Article 4). The particles inside the rotary kiln exhibit different behaviors and regimes as a function of the kiln's rotational velocity. This is the main variable affecting the regime change; however, it is not the only one. In addition to the kiln's rotational velocity, the roughness of the particles and kiln wall and the fill level of the kiln play a role in defining the regime observed. Numerically, the regime manifested is sensitive to several parameters within the unresolved

CFD-DEM simulation. It is shown that the choice of the order of the CFD discretization, the choice of the solid-fluid interactions to be implemented, the type of fluid used as well as the choice of the correctly calibrated DEM surface properties influence the results of the simulations considerably and can affect the regimes observed. Therefore, these variables should be considered and surface parameters should be accurately calibrated before correctly modelling any solid-fluid system. Beside the new calibration benchmark, this experimental procedure is advantageous and can help validate other unresolved CFD-DEM solvers. This is because our benchmark possesses a relatively small number of particles for unresolved CFD-DEM simulations and thus can adequately validate solvers without requiring heavy and time consuming simulations unlike the majority of experimental validation cases.

Appendix C extends the solver to liquids by implementing additional forces in the balance of particle-fluid interactions. The study is performed using solid-liquid fluidized beds where an experimental benchmark is developed to validate and further study the unresolved CFD-DEM simulation results. Notably, the Saffman lift force is no longer negligible and needs to be added as it plays an important role in producing physically sound simulations. In the absence of Saffman lift, particles were pluming unrealistically at the top of the bed due to the presence of preferential paths within the fluidized bed. In the presence of the lift force, these plumes disappeared rendering the results more physical and in accordance with what was observed experimentally. The validation of the extension to liquids is carried out through the pilot-scale cylindrical fluidized bed where simulations precisely reproduced the overall mass balance in the system. The effect of several simulation variables such as the drag model used and the mesh topology is addressed as well in this article.

The chronological implementation of these sub-objectives to systematically develop a robust unresolved CFD-DEM solver with high-order capabilities and a continuous void fraction projection scheme allowed to achieve the main objective of this thesis.

CHAPTER 10 CONCLUSION

In conclusion, a concise summary of the works accomplished as part of this thesis is done to demonstrate the contributions to the literature. Additionally, the limitations of the proposed and developed model are introduced as well as possible extensions and future works.

10.1 Summary of Works

In this thesis, an unresolved CFD-DEM model is developed. It is capable of modelling both solid-liquid and solid-gas flows although the focus of this thesis is on solid-gas flows. Through the Eulerian-Lagrangian approach, it is capable of modelling solid phases through the tracking of individual particles and fluid phases through resolving the VANS equations. In DEM, the velocity and position of particles are determined by solving Newton's equation of motion and Euler's equation of angular momentum. The DEM integration scheme used throughout the thesis is the Velocity Verlet scheme as it is second order accurate. In CFD, the stabilized finite element method is implemented to solve the VANS equations. The SUPG/PSPG stabilization technique used in this thesis allows to implicitly model turbulence through Implicit Large Eddy Simulations (ILES) which captures turbulent structures. The high-order capabilities of the solver result in improved accuracy in modelling the fluid phase without the need for finer meshes. This is achieved through higher order interpolation functions within each element. This is advantageous especially in regions of the domain with high velocity gradients such as the fluid inlet of spouted beds.

The developed model is fully parallelized and supports dynamic load balancing in a unified architecture which makes it, to the knowledge of the author, the first CFD-DEM model implementing such architecture and supporting load balancing at the coupling stage. This developed architecture allows for better simulation speeds where the communication of information between the CFD and the DEM solvers is fast and occurs only once at each CFD iteration. As such, the bottleneck which exists in the coupling of most parallelized CFD-DEM solvers concerning the transfer of information between processors is eliminated in the given architecture. Promising results are demonstrated when strong scaling studies are performed where the use of up to 64 processors led to impressive speedups of the solver. All of this is possible thanks to the deal.II [78] library.

The stage by stage verification and validation of the solver as it is developed allowed for a robust model. Chronologically, the VANS solver is written, verified using the method

of manufactured solutions and then validated using a packed bed case where the packing of particles is fixed. This is followed by the coupled solver which was also verified using a particle sedimentation case and validated using several cases such as the Rayleigh-Taylor instability, a fluidized bed and a spouted bed. The improvement of the model is established with a new void fraction scheme and its behavior is compared to other available schemes where the newly developed analytical scheme is continuous in both time and space and allowed for better convergence of the non-linear solver.

An experimental benchmark for the validation of unresolved CFD-DEM solvers is developed. A solid-fluid lab-scale rotary kiln is set up and the regime change of the particles inside the kiln is studied. This benchmark is simulated as well using Lethe, and good agreement between both experimental and numerical results is found. It is found that the regime change of particles inside the kiln is dependent on the order of CFD discretization, the choice of particle-fluid interactions implemented, and the DEM surface properties used. The developed benchmark can be used to validate any unresolved CFD-DEM solver.

The main contribution of this work is the unresolved CFD-DEM model and its novel components that allowed not only to better understand the underlying phenomena of solid-fluid flows but also to accurately predict and quantify important variables such as velocity, pressure, and void fraction. It is important to note that this model is a suitable tool for the design, optimization and scale-up of applications involving solid-liquid or solid-gas flows.

10.2 Limitations

Even though the unresolved CFD-DEM model developed in this work has numerous advantages, and even if several of the limitations of unresolved CFD-DEM in the literature discussed in section 2.5.2 were addressed in this thesis, the developed model has some weaknesses and limitations.

One of the major limitations is the computational time required for the simulations. Even though large simulations with number of particles of the order of 10^6 have been achieved in this work using high performance computing, the computational time is still considered big for simulations with a larger numbers of particles ($> 10^7$). This is because the speedup achieved with the CFD-DEM solver was optimal up to 64 processors. This poses a limit on the size of the domains that can be simulated efficiently. Recent improvements to the DEM data structures diminish this issue, but computational cost remains a problem.

Another limitation that is inherent to unresolved CFD-DEM is that the accuracy of the model depends on the accuracy of solid-fluid interactions' correlations. As discussed in this thesis,

there exist several correlations for the drag force, each resulting in different values for the drag force. This is obvious especially in Appendix C where some drag models resulted in realistic representations of the liquid fluidized bed while others did not. Similarly, this applies to the other interaction forces that are important when the fluid is a liquid such as Saffman and Magnus lift forces and the virtual mass force. Moreover, such models were developed based on the undisturbed fluid flow velocity which is not the case in fluidized and spouted beds where transient structures and eddies result in a disturbed flow. As such, using the disturbed fluid flow velocity to determine these forces is a source of error in the underlying assumptions of the used force correlations. Furthermore, SUPG based stabilization techniques inherently introduce dissipation to ensure that the scheme remains stable, which additionally affects the accuracy of the particle-fluid interaction models.

The current solver is limited to fully spherical particles. In this sense, it can not be used in its current state to model more complex shapes of particles. This limitation arises due to the collision models being used which are based on spherical geometries as well as the Quadrature Centered Method (QCM) which was developed in this thesis and which only calculates the void fraction for spherical particles.

10.3 Future Research

In order to solve the aforementioned limitations, or to improve the developed model, several extensions are possible:

- The addition of coarse graining (CG) capabilities to the unresolved CFD-DEM model would allow the modelling of much larger systems where applications with a number of particles in the order of 10^7 would be feasible. Coarse graining works by agglomerating particles into parcels, thus decreasing the number of overall particles to be simulated. Additionally, improving the data structures of our solver would help in speeding up simulations.
- The use of machine learning or artificial neural networks coupled with resolved CFD-DEM could allow the development of better and more accurate correlations for the particle fluid interactions that take into account the position of each particle and its surroundings. This can be done through data collection from experiments or resolved CFD-DEM simulations of a swarm of particles. These data will then be used to train the neural networks where the effects of particles would be directly incorporated into the developed correlations, resulting in correlations with improved accuracy that take into account the disturbed flow velocity.

- The model being developed primarily for the modelling of fluidized and spouted beds can be extended to model other applications such as pneumatic conveying. This is what is currently being done in our group as part of a masters project.
- The model being solely a hydrodynamic model can be extended to include a multi-physics interface which would enable the simulation of multiphase flows with mass transfer such as the dissolving of particles or chemical reactions. This will allow to model fluidized and spouted reacting beds. It can also be extended to model heat transfer between both phases as well as with the boundaries of the domain. This will allow the simulation of exothermic and endothermic reactions as well as drying processes in fluidized and spouted beds.
- The simulation of the breakage of particles which is a common phenomenon in such applications can also be done through the addition of a particle attrition-breakage model.
- An interesting idea involves the development of a solver which includes both resolved CFD-DEM in which the boundary layer around particles is resolved and unresolved CFD-DEM in which the fluid is solved in a volume averaging sense based on the application to be modelled. The transition between them will happen based on the number of particles to be modelled as well as the particle to the mesh element cell size. This transition involves semi-resolved CFD-DEM. An important and non-trivial aspect should be considered in this case, that is the parallelization of the solver where the notion of ghost particles does not exist in resolved CFD-DEM.
- Another possible work includes the comparison of certain simulations between using sub-grid scale (SGS) models and with/out filtering to verify the use of ILES is comparable, verified, and settled.
- The solver could be extended to model smaller particles in the Geldart groups C and A. This can be achieved through the incorporation of inter-particle force models such as electrostatic and van der Waals forces in the unresolved CFD-DEM solver.

10.4 Final Word

Nowadays, computational simulation and modelling, specifically CFD, has become an indispensable tool for analyzing and optimizing process intensification techniques, namely in the chemical engineering industry. This is because such tools allow engineers to gain insights

into the underlying phenomena governing complex systems in industrial applications such as flow patterns, and heat and mass transfer, leading to informed design decisions.

The future of CFD in process intensification is promising. As a result of continued advancements in computational power and sophistication in modelling strategies, simulations are becoming more accurate, faster, and capable of capturing finer details of multiphase turbulent flows. Possibly, innovation in automated design and optimization of intensified processes will become feasible due to the integration of machine learning algorithms within CFD-DEM, resulting in the acceleration of the development of sustainable industrial solutions. One possibility would be the use of machine learning to develop better particle-fluid interactions correlations especially those that are related to the history of the flow such as the Basset force since the implementation of this force is currently difficult. This will eventually lead to more accurate and robust CFD-DEM solvers.

In summary, the future of simulation in engineering fields is set to revolutionize the methods of complex systems design and optimization, giving engineers the ability to discover new uncharted territories and unlock new levels of efficiency, innovation, and sustainability.

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APPENDIX A GRAD-DIV STABILIZATION

In this appendix, we demonstrate the effect of proper grad-div stabilization on the stability of the VANS solver in the presence of a sharp void fraction gradient. A step function for the void fraction is defined as:

$$\varepsilon_f = \begin{cases} 1 & \text{if } x < -0.5 \text{ or } x > 0.5 \\ 0.5 & \text{if } -0.5 \leq x \leq 0.5 \end{cases} \quad (\text{A.1})$$

and an inlet velocity $\mathbf{u} = 1$ is defined in a square domain $[-1, 1]^2$. The simulation is performed with and without the grad-div stabilization. The results obtained are shown in Figure A.1

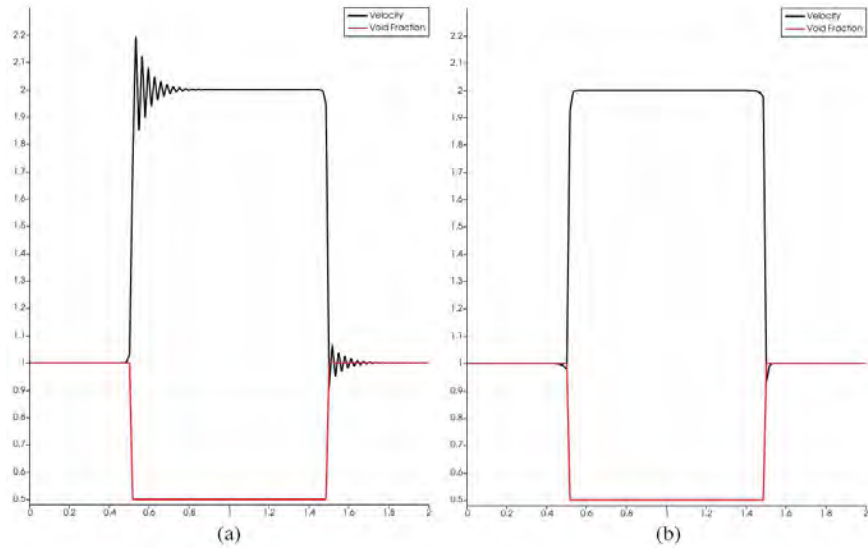


Figure A.1 Comparison of simulation results of a fluid flow through a section with a sharp void fraction gradient with SUPG stabilization only (a) and with SUPG and grad-div stabilization (b).

The simulation with only SUPG and PSPG stabilization is not enough to dampen the spurious oscillations in the velocity field arising from the sharp void fraction gradients at the location of the discontinuities. When grad-div stabilization is implemented, the oscillations disappear which makes the simulation much more stable. For our solver, using this grad-div stabilization method alleviates the need of a shock capturing scheme to diffuse the spurious oscillations.

APPENDIX B VALUES OF THE ANGLE OF INCLINATION FOR THE EXPERIMENTS AND SIMULATIONS

B.1 Values of the Angle of Inclination for the Experiments And Simulations

The tables below summarize the angle of inclination in the rolling regime for the rotary kiln cases in both experiments and simulations. The dashes in the table represent a change from the rolling regime where an angle of inclination can no longer be measured.

		Motor Frequency (Hz)									
		20		60		140		200		300	
Particle Type	Fluid Type	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.
ABS (5.95 mm)	Air	23	23	26	26	27	27	29	29	30	30
	Water	26	24	27	26	29	29	32	33	33	35
	Sucrose										
	50 %	27	24	29	27	31	31	33	33	-	-
	66.66 %	27	25	30	29	31	31	33	33	-	-
	100 %	32	28	38	34	-	-	-	-	-	-
Glass (3 mm)	Air	28	28	31	30	39	39	-	-	-	-
	Water	29	28	32	31	36	35	-	-	-	-
	Sucrose										
	50 %	31	29	35	34	44	-	-	-	-	-
	66.66 %	31	29	36	35	44	-	-	-	-	-
	100 %	32	31	41	38	-	-	-	-	-	-
Glass (5 mm)	Air	30	28	31	31	35	35	-	-	-	-
	Water	30	30	35	32	38	38	-	-	-	-
	Sucrose										
	50 %	32	29	35	33	36	38	-	-	-	-
	66.66 %	33	29	37	34	-	-	-	-	-	-
	100 %	32	30	-	-	-	-	-	-	-	-

Table B.1 Inclination angle comparison between experiments and simulations for Q2-Q1 simulations.

		Motor Frequency (Hz)									
		20		60		140		200		300	
Particle Type	Fluid Type	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.
ABS (5.95 mm)	Air	23	24	26	26	27	27	29	29	30	30
	Water	26	26	27	28	29	29	32	33	32	35
	Sucrose										
	50 %	27	28	29	30	31	33	34	33	-	-
	66.66 %	27	28	30	33	31	33	34	33	-	-
	100 %	32	33	38	42	-	-	-	-	-	-
Glass (3 mm)	Air	28	26	31	31	39	39	-	-	-	-
	Water	29	28	32	31	36	36	-	-	-	-
	Sucrose										
	50 %	31	60	35	35	44	-	-	-	-	-
	66.66 %	31	30	36	35	44	-	-	-	-	-
	100 %	32	30	41	41	-	-	-	-	-	-
Glass (5 mm)	Air	30	27	31	30	35	35	-	-	-	-
	Water	30	28	35	34	38	38	-	-	-	-
	Sucrose										
	50 %	32	30	35	35	36	38	-	-	-	-
	66.66 %	33	32	37	36	-	-	-	-	-	-
	100 %	32	31	-	-	-	-	-	-	-	-

Table B.2 Inclination angle comparison between experiments and simulations for Q3-Q2 simulations.