



Titre: Multi-Scale Modeling of Adhesion Forces in Gas-Solid Fluidized Beds
Title:

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Author:

Date: 2024

Type: Mémoire ou thèse / Dissertation or Thesis

Référence: Badran, Y. (2024). Multi-Scale Modeling of Adhesion Forces in Gas-Solid Fluidized Beds [Thèse de doctorat, Polytechnique Montréal]. PolyPublie.
Citation: <https://publications.polymtl.ca/62494/>

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URL de PolyPublie: <https://publications.polymtl.ca/62494/>
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Programme: Génie chimique
Program:

POLYTECHNIQUE MONTRÉAL

affiliée à l'Université de Montréal

Multi-scale modeling of adhesion forces in gas-solid fluidized beds

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et

Spécialité: dynamique des fluides

Institut National Polytechnique de Toulouse

Thèse en cotutelle présentée en vue de l'obtention du diplôme de *Philosophiæ Doctor*

Génie chimique

Novembre 2024

POLYTECHNIQUE MONTRÉAL

affiliée à l'Université de Montréal

Cette thèse intitulée :

Multi-scale modeling of adhesion forces in gas-solid fluidized beds

présentée par **Youssef BADRAN**

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

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DEDICATION

To God and my beloved family.

ACKNOWLEDGEMENTS

I would like to thank my research supervisors, Renaud Ansart, Jamal Chaouki, and Olivier Simonin, for their guidance, support, and encouragement. Thank you, Renaud, for your trust and for being there when I needed you. Thank you, Jamal, for your support and encouragement. Thank you, Olivier, for your assistance and expert guidance.

Thank you to my family. Your boundless love and support have been the driving force behind my successful completion of this PhD journey.

Thank you, Gerard, for welcoming me into your place. Your kindness and generosity made my stay incredibly comfortable. Thank you, Almir and Pablo, for the good times we spent together.

I would like to express my gratitude to Prof. Vincent Moureau for his assistance and guidance in the developments we made in the YALES2 code during this PhD. I would like to thank Dr. Dorian Dupuy for his contributions and collaboration on key aspects of the YALES2 code developments made during this PhD. I am sincerely grateful to Prof. Bruno Blais for sharing his expertise in CFD-DEM modeling and for the insightful discussions I had with him. I would also like to thank Dr. Ainur Nigmatova and Dr. Yann Dufresne for sharing their experiences with the YALES2 code.

Finally, thank you to the members of my thesis committee for agreeing to review my PhD thesis and for their feedback.

RÉSUMÉ

Divers secteurs industriels, principalement les processus chimiques et pétrochimiques, utilisent largement des réacteurs à lit fluidisé gaz-solide. Le développement de modèles capables de prédire les divers phénomènes de transport au sein d'un lit fluidisé gaz-solide est crucial pour sa conception, son optimisation et sa mise à l'échelle. Les forces interparticulaires affectent l'hydrodynamique du lit fluidisé et son efficacité opérationnelle. L'omission des forces interparticulaires est l'un des principaux points de désaccord entre les chercheurs dans l'analyse de l'hydrodynamique des lits fluidisés gaz-solide.

Cette recherche doctorale vise à développer une fermeture de contrainte pour un modèle macroscopique qui prend en compte l'influence des forces de Van der Waals interparticulaires afin de prédire le comportement de fluidification observé dans les expériences pratiques. Nous avons utilisé une approche de modélisation multi-échelle pour atteindre cet objectif.

Le dépassement de la chute de pression du lit à la vitesse minimale de fluidisation, qui se produit pendant la transition d'un état de lit fixe à un état de lit fluidisé, est un phénomène courant pour les particules fines classées dans le groupe A selon la classification de Geldart. Ces particules présentent une hystérésis entre les courbes de chute de pression pour les trajectoires de vitesse de gaz décroissante et croissante. Cette étude utilise deux modèles de pression de particules adhésives dans des simulations de modèles à deux fluides pour incorporer l'influence de la force de Van der Waals interparticulaire, dans le but de prédire le dépassement de la pression. Le premier modèle de pression adhésive, développé dans le cadre de la théorie cinétique des écoulements granulaires rapides, n'a pas réussi à capturer le dépassement en raison de la prévalence de contacts multiples et prolongés dans les lits fixes. Nous avons proposé une fermeture alternative basée sur le nombre de coordination, générant une contribution adhésive significativement plus élevée que le modèle de la théorie cinétique et reproduisant avec succès le dépassement de la chute de pression.

En outre, nous avons construit une base de données numériques CFD-DEM (Computational Fluid Dynamics-Discrete Element Method) pour prédire l'hystérésis dans la chute de pression. Cette base de données peut guider la formulation d'une équation de transport eulérienne pour le nombre de coordination, permettant l'incorporation des effets de l'historique des déformations. Nous avons étudié l'impact de la force de Van der Waals et de la friction statique sur la fluidisation des solides fins à l'échelle moyenne en utilisant des simulations CFD-DEM et leur rôle dans l'apparition du phénomène de dépassement de pression. Notre analyse examine des paramètres tels que la chute de pression du gaz, le vide du lit, le nombre

de coordination, les pressions répulsives et adhésives des solides, le gradient vertical de vitesse des solides, le tenseur de tissu et la contrainte de cisaillement particule-paroi tout au long des processus de défluidisation et de fluidisation. Nous avons démontré qu’il est nécessaire de prendre en compte l’adhésion de Van der Waals pour prédire l’expansion homogène du lit sur toute la gamme des vitesses, du minimum requis pour la fluidisation au minimum pour le bullage. L’ensemble de données CFD-DEM généré peut guider le développement de fermetures de contraintes solides pour les modèles à deux fluides afin d’incorporer les effets de l’adhésion de Van der Waals et de la friction statique sur l’hydrodynamique de la fluidisation, ce qui permet de prédire l’hystérésis dans la chute de pression du lit à l’échelle macroscopique.

Dans ce travail, nous avons incorporé un modèle de frottement statique-dynamique dans le code CFD-DEM massivement parallèle YALES2 à l’aide d’un algorithme en deux étapes, afin de remédier aux lacunes du modèle de frottement dynamique de Coulomb, qui est pratique pour les écoulements granulaires rapides mais ne s’applique pas aux lits stationnaires. Nous avons validé notre mise en œuvre par une série de tests à macro- et micro-échelle. En outre, nous avons introduit dans YALES2 les forces de Van der Waals entre particules et entre particules et parois, et validé cet ajout à l’échelle microscopique. En outre, nous avons postulé une expression de relaxation pour le terme source dans l’équation de transport des nombres de coordination et déterminé le temps de relaxation des nombres de coordination à l’aide de données de simulation CFD-DEM. En outre, nous avons utilisé une technique de pénalisation pour coupler de manière semi-implicite les phases gazeuse et solide, en particulier par le traitement implicite des forces de traînée et d’Archimède. Cette approche vise à résoudre les problèmes de stabilité rencontrés lorsque le couplage interphase est explicite.

ABSTRACT

Various industrial sectors, mainly chemical and petrochemical processes, extensively employ gas-solid fluidized bed reactors. Developing models capable of predicting the diverse transport phenomena within a gas-solid fluidized bed is crucial for its design, optimization, and upscaling. Interparticle forces affect fluidized bed hydrodynamics and operational efficacy. The omission of interparticle forces is a primary point of contention among researchers in analyzing gas-solid fluidized bed hydrodynamics.

This doctoral research aims to develop a stress closure for a macroscopic model that considers the influence of interparticle Van der Waals forces to predict the fluidization behavior witnessed in practical experiments. We employed a multi-scale modeling approach to achieve this goal.

The overshoot in bed pressure drop at the minimum fluidization velocity, occurring during the transition from a fixed to a fluidized bed state, is a common phenomenon for fine particles categorized under Group A according to Geldart's classification. These particles exhibit hysteresis between the pressure drop curves for the decreasing and increasing gas velocity paths. This study employs two adhesive particle pressure models within two-fluid model simulations to incorporate the influence of interparticle Van der Waals force, aiming to predict the pressure overshoot. The first adhesive pressure model, developed within the kinetic theory of rapid granular flows framework, failed to capture the overshoot due to the prevalence of multiple and prolonged contacts in fixed beds. We proposed an alternative closure based on coordination number, generating a significantly higher adhesive contribution than the kinetic theory model and successfully reproducing the pressure drop overshoot.

In addition, we constructed a Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) numerical database to predict hysteresis in pressure drop. This database can guide the formulation of an Eulerian transport equation for the coordination number, enabling the incorporation of deformation history effects. We explored the impact of Van der Waals force and static friction on the fluidization of fine solids at the mesoscale using CFD-DEM simulations and their role in causing the pressure overshoot phenomenon. Our analysis examines parameters such as gas pressure drop, bed voidage, coordination number, repulsive and adhesive solid pressures, vertical solid velocity gradient, fabric tensor, and particle-wall shear stress throughout the defluidization and fluidization processes. We demonstrated that it is necessary to consider the Van der Waals adhesion to predict the homogeneous expansion of the bed across the range of velocities from the minimum required for fluidization to the

minimum for bubbling. The generated CFD-DEM dataset can guide the development of solid stress closures for two-fluid models to incorporate the effects of Van der Waals adhesion and static friction on fluidization hydrodynamics, allowing for the prediction of hysteresis in bed pressure drop at the macroscale.

In this work, we incorporated a static-dynamic friction model into the massively parallel CFD-DEM code YALES2 using a two-step algorithm, aiming to address the shortcomings of the Coulomb dynamic friction model, which is practical for fast granular flows but not applicable to stationary beds. We validated our implementation through a series of macro- and microscale tests. Furthermore, we introduced interparticle and particle-wall Van der Waals forces into YALES2 and validated this addition at the microscale. Additionally, we postulated a relaxation expression for the source term in the coordination number transport equation and determined the coordination number relaxation time using CFD-DEM simulation data. Moreover, we employed a penalization technique to semi-implicitly couple gas and solid phases, specifically through the implicit handling of drag and Archimedes forces. This approach aimed to resolve the stability issues encountered when the interphase coupling is explicit.

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LIST OF SYMBOLS AND ACRONYMS

IPF	Interparticle Forces
VDW	Van der Waals
LES	Large-Eddy Simulation
DEM	Discrete Element Method

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CHAPTER 1 INTRODUCTION

The primary source of debate among researchers studying bed hydrodynamics is disregarding Interparticle Forces (IPF) [13]. Traditional correlations based solely on hydrodynamics, like the Ergun [14] and Carman–Kozeny [15] equations, fail to provide reliable predictions for the minimum fluidization velocity when IPF are significant [1]. In a dry ambient setting, the primary force governing interactions among fine particles is the Van der Waals (VDW) adhesive force [16]. Despite some existing knowledge regarding how this interparticle force impacts fluidized bed dynamics, a comprehensive understanding remains elusive. Therefore, this research aims to develop a macroscopic model for the VDW force and offer a deeper understanding of its influence on fluidization dynamics. The objective is to create an adhesive solid stress model that can be integrated into the two-fluid model for accurately simulating gas-solid fluidized beds at an industrial scale.

1.1 Gas-solid fluidized beds

1.1.1 Applications

Gas-solid fluidized beds find application across various industrial processes including coal combustion, olefin polymerization, gasification, fluid catalytic cracking (FCC), and ore roasting [17]. These beds are favored for their ability to handle diverse feedstocks, promote efficient solid mixing, and exhibit advantageous mass and heat transfer properties [13, 18].

1.1.2 Flow regimes

Various flow regimes occur within a fluidized bed, based on the operational conditions. These regimes are illustrated in Figure 1.1 and can be delineated as follows:

1. **Fixed bed:** This regime is manifested when the gas forces acting on the particles are insufficient to counterbalance the particles' weight, IPF, and particle-wall friction.
2. **Homogeneous fluidization:** This regime is observable with Geldart A particles. The onset of this state is demarcated by the minimum fluidization velocity (U_{mf}). Here, the system solely comprises an emulsion phase. Notably, Geldart B particles do not exhibit this regime; instead, they promptly form bubbles once the superficial gas velocity surpasses U_{mf} .

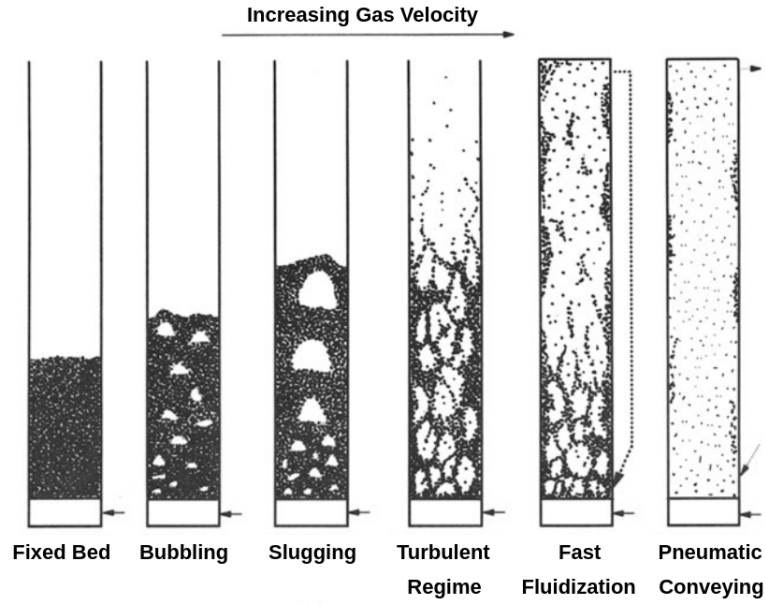


Figure 1.1 Flow regimes within a gas-solid fluidized bed. Adapted from [2].

3. **Bubbling**: Upon reaching the minimum bubbling velocity (U_{mb}), the excess gas in the emulsion phase emerges as bubbles that aid in solid mixing.
4. **Slugging**: When bubble size becomes comparable to the bed diameter, the regime is termed slugging [19].
5. **Turbulent regime**: With an increase in gas velocity, bubble coalescence and breakup intensify. This turbulent regime is characterized by vigorous solid mixing, making it advantageous for numerous industrial applications [20].
6. **Fast fluidization**: Further elevation of gas velocity results in substantial particle entrainment. In this state, the gas volume fraction notably decreases towards the column wall.
7. **Pneumatic conveying**: At extremely high gas velocities surpassing the particles' terminal velocity, all particles are transported by the gas out of the column. In this regime, solids are conveyed up the column as individual particles dispersed widely within the gas.

1.1.3 Classification of particles

According to Geldart [21], particles can be categorized into four groups based on their size and the disparity between particle and gas densities, as illustrated in Figure 1.2. These

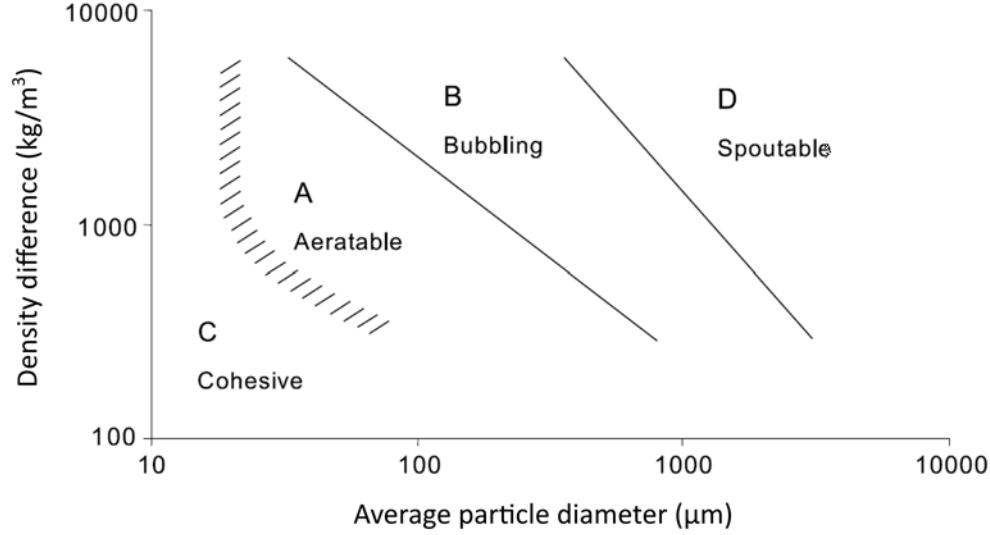


Figure 1.2 Geldart diagram for powder classification. Adapted from [3].

groups are distinguished by their fluidization characteristics:

- **Group C:** This group comprises very fine particles that exhibit adhesion and limited flowability due to significant IPF. Typically, the fluidization of such materials leads to channel formation and restricted particle mobility, necessitating supplementary methods for proper fluidization [22].
- **Group A:** This group encompasses particles with small mean diameter and/or low density (less than approximately 1400 kg/m^3), characterized as aeratable and undergoing homogeneous fluidization before bubbling. Many catalysts employed in fluidized bed reactors belong to Group A [23], with the FCC catalyst serving as a notable example.
- **Group B:** This group includes particles ranging from 40 to $500 \text{ } \mu\text{m}$ in size and between 1400 and 4000 kg/m^3 in density. Upon fluidization of these particles, bubble formation initiates once the bed attains the fluidization state ($U_{mb} = U_{mf}$). Sand is an exemplar of particles belonging to Group B.
- **Group D:** This group consists of particles that are large and/or highly dense, challenging to fluidize in deep beds and prone to channeling or spouting. Coal particles involved in gasification are categorized as D-type particles.

A summary of various fluidization regimes based on the Geldart classification is depicted in Figure 1.3. Geldart's classification pertains to fluidization under ambient conditions solely with air. It's demonstrated that the behavior of the bed can transition from one particle group

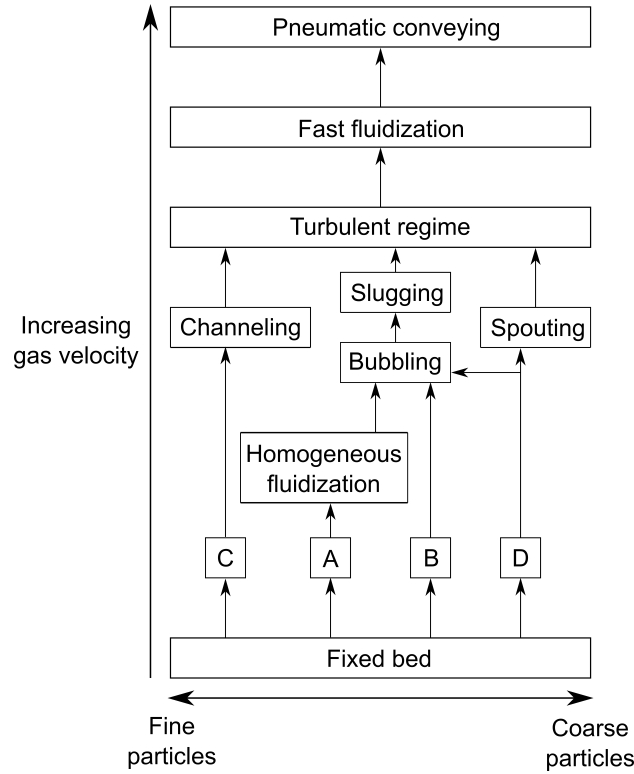


Figure 1.3 The fluidization behaviors of particles as per the Geldart classification. Adapted from [4].

to another under increased pressure and temperature [24]. For instance, in high-pressure olefin polymerization, particles classified under Geldart group B may exhibit behavior akin to Geldart group A particles [25]. Elevated temperatures can accentuate IPF' impact, causing Geldart A particles to behave similarly to Geldart C particles [26]. A modification to Geldart's classification by Yang [27] accommodated fluidization under elevated conditions with gases of varying properties.

1.2 Interparticle forces in fluidization

The primary IPF involved in fluidization comprise Van der Waals forces, material bridge forces, and electrostatic forces [22,28]. These IPF' magnitude is influenced by various factors like operational parameters and the characteristics of both the particles and the gas. A substantial presence of these forces greatly impacts the dynamics within a gas-solid fluidized bed.

1.2.1 Van der Waals forces

VDW interactions comprise dipole-dipole, instantaneous dipole-induced dipole, and dipole-induced dipole forces occurring between atoms and molecules. The instantaneous dipole-induced dipole force, also referred to as the London dispersion force, arises from the asymmetrical electron distribution around the nuclear protons within a neutral atom, leading to an instantaneous dipole moment [29]. This moment induces an electric field that leads to the polarization of neighboring neutral atoms, creating a mutual attraction between their dipoles. The VDW interaction between an instantaneous dipole and induced dipole is shown in Figure 1.4. According to London [30], the dispersion interaction potential between a pair

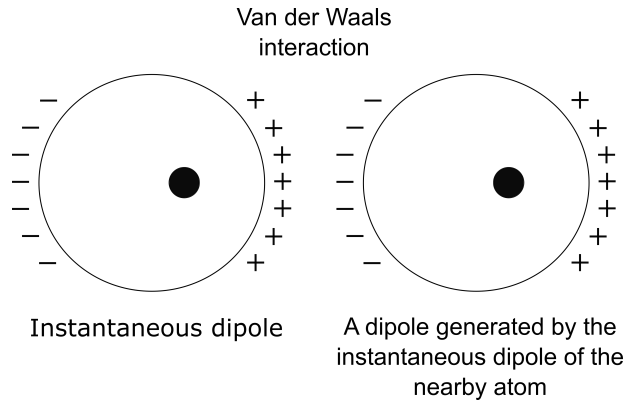


Figure 1.4 Instantaneous dipole-induced dipole Van der Waals interaction.

of atoms can be quantified by:

$$E_a = -\frac{K_{lv}}{l_a^6} \quad (1.1)$$

where K_{lv} denotes the London-Van der Waals constant and l_a is the interatomic distance. As per Hamaker [31], determining the force acting between macroscopic bodies involves combining the forces between all pairs of individual atoms. The total interaction potential between two particles is determined by integrating the interaction energy specified in Equation (1.1) over all atoms according to:

$$E_{tot} = \int_{v_1} dn_1 \int_{v_2} E_a dn_2 \quad (1.2)$$

where n_1 , n_2 , v_1 and v_2 designate atom densities and volume elements for each of the two particles. For a pair of identical spherical particles, this integration leads to:

$$E_{tot} = -\frac{AR}{12S} \quad (1.3)$$

where the symbols A , R , and S represent the Hamaker constant, the radius of the spheres, and the distance between their surfaces, respectively. The VDW force is then found by differentiation with respect to S :

$$F_{vw} = \frac{\partial E_{tot}}{\partial S} = \frac{AR}{12S^2} \quad (1.4)$$

According to Equation (1.4), the attractive force F_{vw} is inversely proportional to S^2 . It was postulated by some researchers that there exists a minimum separation distance S_0 (equals $4\text{\AA}$), where the force reaches its highest value [32].

Lennard-Jones [33] suggested extending the atom-to-atom interaction energy:

$$E_a = -\frac{K_{lv}}{l_a^6} + \frac{C}{l_a^{12}}. \quad (1.5)$$

In this equation, C is equal to $K_{lv}l_{a,c}^6/2$, where $l_{a,c}$ represents the characteristic separation distance between the atoms within the particle. The first term in Equation (1.5) represents the attraction due to the VDW force, while the second term represents the repulsion due to the overlap of atomic orbitals. The Lennard-Jones potential between two atoms is shown in Figure 1.5. Upon integrating the Lennard-Jones potential (Equation (1.5)) over all atoms within the particles as per the Hamaker expression (Equation (1.2)), the resultant interaction energy between a pair of identical spheres is determined to be [32]:

$$E_{tot} = \frac{AR}{12S} \left[-1 + \frac{1}{420} \left(\frac{l_{a,c}}{S} \right)^6 \right] \quad (1.6)$$

The net force acting between the spheres is then determined by taking the derivative with respect to S :

$$F_{net} = \frac{\partial E_{tot}}{\partial S} = \frac{AR}{12S^2} \left[1 - \frac{1}{60} \left(\frac{l_{a,c}}{S} \right)^6 \right] \quad (1.7)$$

The ratio of VDW force (which scales with R) and particle weight (which scales with R^3) is inversely proportional to R^2 . Therefore, the importance of VDW force is generally higher for smaller particles. In a dry setting, particles smaller than about $100 \mu\text{m}$ usually exhibit a greater magnitude of the VDW force compared to other IPF [22]. Multiple scholars have applied the CFD-DEM approach to forecast fluidization behaviors when Van der Waals forces are present [34–37]. Conversely, there is a scarcity of literature concerning two-fluid models that incorporate Van der Waals forces [38, 39].

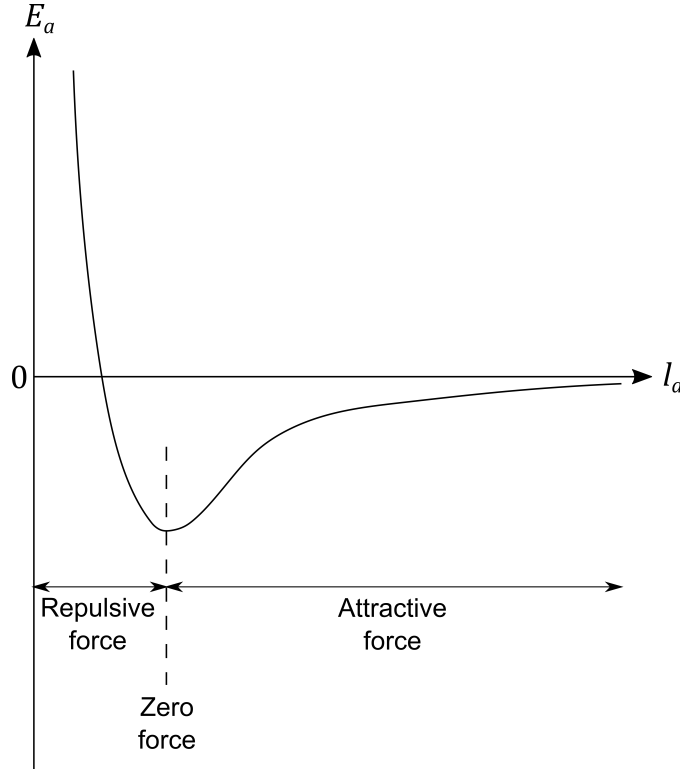


Figure 1.5 Lennard-Jones potential: interaction energy vs. interatomic distance.

1.2.2 Electrostatic force

During fluidization, particles touch different surfaces and get charged through a process called tribo-electrification [40]. The presence of electric charges in motion leads to the creation of an electromagnetic field. An interaction through the Lorentz force can occur between the electrically charged particles. The Lorentz force, caused by electromagnetic fields, acts on a point charge [41]. It is given by:

$$F_L = qE_f + q(V_q \times M_f) \quad (1.8)$$

where qE_f is the force experienced by a particle of charge q in an electric field E_f created by the existence of another charged particles, and $q(V_q \times M_f)$ is the force arising from the magnetic field M_f . Here, V_q represents the velocity vector of the particle with charge q . Given that the velocity of the particle is significantly smaller than the speed of light, the magnetic force can be disregarded. In this context, the Lorentz force simplifies to the electrostatic Coulomb force:

$$F_e = qE_f \quad (1.9)$$

Generally, the electrostatic force is minor next to the VDW force. In a moist environment, this kind of force becomes weaker and loses its relative importance as the system undergoes discharge [22]. The long-range electrostatic force can cause problems such as agglomeration of particles, for example in gas phase polymerization [42]. The impact of electrostatic forces on fluidization dynamics has been explored by various researchers through CFD-DEM [43] and a two-fluid approach [41, 44, 45].

1.2.3 Material bridge forces

Material bridge forces can be categorized into two major types: liquid bridge force and sintering force. The magnitudes of these forces significantly exceed those of VDW and electrostatic forces [46].

Liquid bridge force

A liquid bridge force, resulting from a liquid meniscus formed between two particles, manifests as an attractive force. Figure 1.6 depicts a liquid bridge connecting a spherical particle to another identical one. The formation of the meniscus can occur through capillary condensation

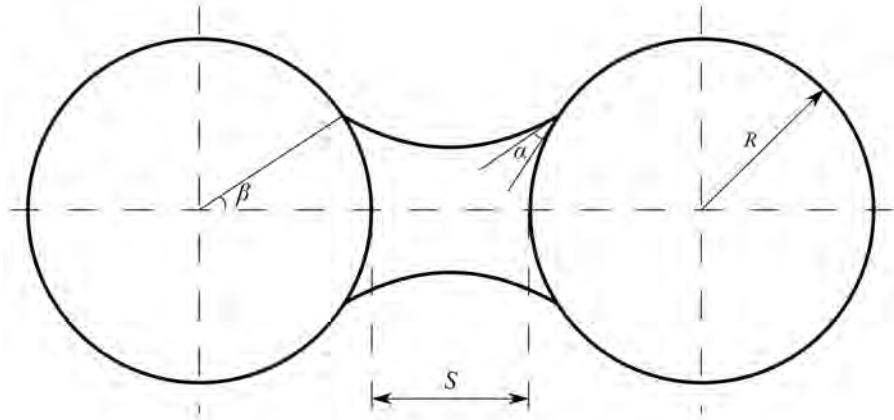


Figure 1.6 Liquid bridging two spherical particles.

or by introducing liquid into the system. When two solid surfaces exhibit lyophilic properties towards the surrounding vapor and the gap between them is adequately narrow, the vapor undergoes condensation into a liquid through capillary condensation phenomenon [47]. Upon addition of a liquid to the system, as in wet granulation [48], the liquid deposits on the solid surfaces. Subsequently, when these surfaces come into contact, a liquid bridge forms.

The force originating from the liquid bridge comprises capillary and viscous components.

The capillary force is given by [49]:

$$F_{cap} = 2\pi\gamma R \sin \beta \sin(\beta + \alpha) + \pi R^2 \Delta p \sin^2 \beta. \quad (1.10)$$

Here, γ represents the surface tension of the liquid, R denotes the sphere radius, α symbolizes the contact angle, β signifies the half-filling angle, and Δp stands for the pressure differential across the interface between the gas and the liquid, which is determined by the Laplace-Young expression [50]:

$$\Delta p = \left(\frac{1}{R_{c1}} - \frac{1}{R_{c2}} \right) \gamma \quad (1.11)$$

where R_{c1} and R_{c2} represent the principal radii of the liquid bridge curvature. The viscous force is expressed as [51]:

$$F_{vis} = \frac{3}{2} \mu_l \frac{u_r \pi R^2}{S} \xi^2 \quad (1.12)$$

where μ_l is the liquid dynamic viscosity, u_r is the velocity difference between the two spheres, S is the surface separation distance, and ξ is determined by:

$$\xi = 1 - \left(\frac{2V_l}{R\pi S^2} + 1 \right)^{-0.5} \quad (1.13)$$

where V_l is the volume of the liquid bridge. Liquid bridge force plays a crucial role in several processes such as drying and agglomeration [22]. The fluidization of powders in the presence of liquid bridge forces has been investigated by numerous researchers employing the CFD-DEM model [52, 53] and a two-fluid model [54–56].

Sintering force

At a specific temperature threshold known as the minimum sintering temperature (T_s), the particle surface undergoes thermal softening, initiating a process of sintering. This phenomenon is observable in fluidized beds operating at temperatures equal to or greater than T_s , where particle-to-particle contact results in material migration towards the contact zone, forming a neck between the particles. The material migration is mainly due to diffusion and/or viscous flow [57]. Higher temperatures correlate with an accelerated sintering rate. The growth of the neck region between two particles over time is described by an analytical equation in the form of [58]:

$$\left(\frac{r_n}{R} \right)^a = \frac{C}{R^b} t_c \quad (1.14)$$

where r_n represents the neck radius, R indicates the particle radius, and t_c denotes the contact time. a , b , and C are constants that are characteristic of the specific transport mechanism

involved, such as surface diffusion, volume diffusion, viscous flow, etc. The sintering force is written as [59]:

$$F_s = \pi r_n^2 \sigma_{tn} \quad (1.15)$$

where σ_{tn} represents the tensile strength of the neck. Sintering can pose significant challenges in fluidized beds operating at high temperatures, for example, those used in gasification and combustion [28, 60]. It can result in the formation of large agglomerates within the bed, potentially leading to defluidization issues. Some studies have focused on simulating gas-solid fluidized beds with consideration of sintering forces using the CFD-DEM approach [61, 62].

1.3 Effect of interparticle forces on bed hydrodynamics

An elevation in the intensity of IPF due to the rise in temperature leads to increased voidages in the static and minimum fluidization states for particles of B and A types [63, 64]. Raising the magnitude of IPF leads to higher minimum fluidization velocity [65]. Elevating IPF' levels may lead to the emergence of a particulate fluidization state in beds of B-type particles, shifting the behavior towards type A or even type C behavior [66, 67]. Augmenting IPF' levels intensifies the emulsion phase's resistance to modifications in its structure and diminishes solids mixing quality [13]. In beds with large IPF' magnitudes, reduced bubble activity occurs because bubbles traverse a strengthened emulsion phase, raising the velocity of the transition from bubbling to a turbulent state. IPF' levels increase when operating conditions are elevated, leading to particle agglomeration and potential defluidization [57, 68].

1.3.1 Pressure-drop overshoot

The presence of IPF plays a role in the overshoot in the gas pressure drop across the bed witnessed in experiments involving fine particles. Typical variations in bed pressure drop as superficial gas velocity increases and decreases are displayed in Figure 1.7. Below the critical gas velocity U_{mf} , particles remain in a static state. The pressure drop in this state can be approximated using the Ergun [14] correlation:

$$\frac{\Delta P_g}{H_b} = 1.75 \rho_g \frac{\alpha_p U_g^2}{\alpha_g^3 \varepsilon_p d_p} + 150 \mu_g \frac{\alpha_p^2 U_g}{\alpha_g^3 (\varepsilon_p d_p)^2} \quad (1.16)$$

where H_b is the bed height, α_g is the voidage of the bed, α_p is the volume fraction of the solid particles, μ_g is the gas dynamic viscosity, U_g is the superficial gas velocity, ε_p is the particle sphericity, d_p is the mean diameter of the particles, and ρ_g is the density of the gas phase. Upon exceeding U_{mf} , the bed fluidizes, and the pressure drop stabilizes at a value

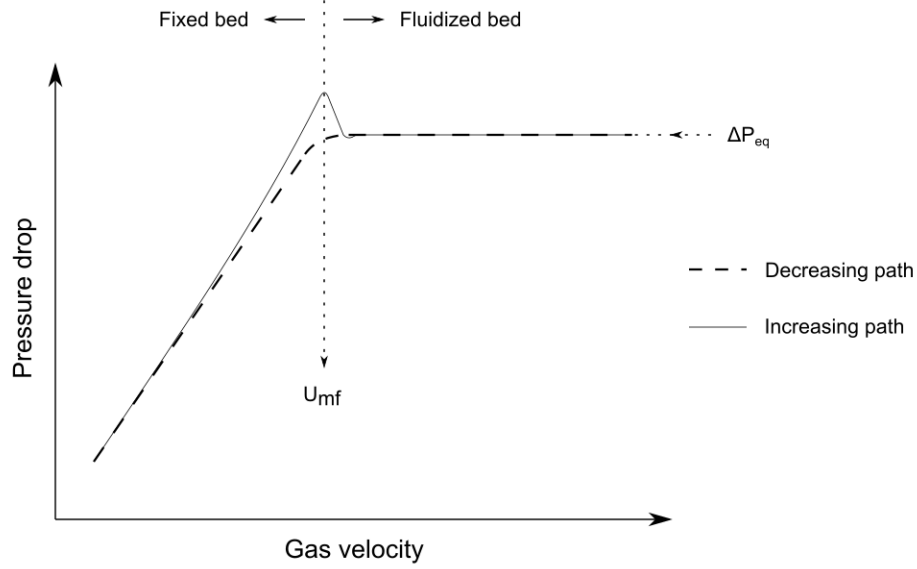


Figure 1.7 Variation of total bed pressure drop with superficial gas velocity throughout fluidization and defluidization cycles.

equivalent to the particles' weight ($\Delta P_{eq} = W_p/A_b$, where W_p is the particles' weight and A_b is the cross-sectional area of the particle bed). The minimum fluidization velocity (U_{mf}) is crucial in fluidized bed operation and design and can be obtained experimentally from the bed pressure drop plotted against gas velocity or calculated using a correlation like the one introduced by Wen and Yu [69]:

$$\text{Re}_{s,mf} = -33.7 + \sqrt{0.0408\text{Am} + 33.7^2} \quad (1.17)$$

where the particle Reynolds number at the minimum of fluidization, $\text{Re}_{s,mf}$, and the Archimedes number, Am , are defined as:

$$\text{Re}_{s,mf} = \frac{d_p \rho_g}{\mu_g} U_{mf} \quad (1.18)$$

$$\text{Am} = \frac{g d_p^3}{\mu_g^2} \rho_g \rho_{pg} \quad (1.19)$$

where ρ_p represents the density of particles, g stands for the gravitational acceleration, and ρ_{pg} refers to the disparity between particle and gas densities ($\rho_{pg} = \rho_p - \rho_g$). The Wen-Yu correlation is applicable under ambient conditions. However, Elahipanah [70] noted experimentally that this correlation loses validity at elevated temperatures for A-type particles due to the increased magnitude of IPF. The magnitude of the pressure drop overshoot at U_{mf} signifies the intensity of IPF. Elahipanah [70] observed a more significant overshoot at more

elevated temperatures for A-type particles, which indicates higher IPF' levels. Besides the role of IPF in pressure-drop hysteresis, wall friction also contributes to this phenomenon. However, Vanni et al. [71] observed in experiments under ambient conditions that this wall influence is only significant in beds with small diameters, specifically those less than or equal to 2 cm.

1.4 Multi-scale modeling approach

The development of robust models for gas-solid fluidized beds on an industrial scale faces significant challenges due to a limited comprehension of the underlying principles governing gas-solid flows in dense regimes. This limited knowledge encompasses critical aspects such as the interactions among particles and between particles and surfaces, as well as the interactions between gas and particles.

A key challenge lies in the substantial difference in scales involved: while the biggest structures within the flow may span meters, their behavior is linked to minute details of gas-particle and interparticle interactions occurring at the millimeter or micrometer level [72]. These interactions are captured effectively by detailed models on a small scale, which are utilized by the multi-scale modeling approach to formulate closure laws capable of representing the interactions at a macroscopic level within models suitable for large-scale simulations.

1.4.1 Meso-scale modeling

The meso-scale modeling approach, known as the CFD-DEM approach, involves characterizing the gas phase within an Eulerian context and tracking particles in a Lagrangian manner. This method describes the gas flow at a level ten times greater than the size of the particles [72]. The gas flow behavior is determined by solving the Navier-Stokes equations. Every single particle is tracked in both space and time through the application of the second law of motion posited by Newton. Contact interactions between particles and between particles and walls can be simulated via either a soft-sphere [73] or hard-sphere [74] modeling approach. Hard-sphere models assume instantaneous and binary contacts. In contrast, in the soft-sphere models, several contacts between a single particle and other particles, as well as small overlaps among particles, are taken into account.

The CFD-DEM approach enables the validation and adjustment of the kinetic-theory pressure and viscosity closure models employed in the macro-scale approach [72]. The meso-scale modeling approach allows the study of system sizes comprising typically about 10^5 particles, which is equivalent to systems of lab scale [72].

1.4.2 Macro-scale modeling

The macro-scale modeling approach, known as the two-fluid approach, is applicable for analyzing gas-particle flows within fluidized beds at both pilot and industrial levels. This method considers the gas and solid phases as interacting continuum media. By employing separate balance equations for each phase, interconnected via terms that account for the transfers between the phases, encompassing momentum, mass, and enthalpy, this model effectively captures the dynamics of the system. The solid phase is described through a kinetic equation for the probability density function and closures permitting the consideration of contact and turbulent interactions [75]. The two-fluid model has the capacity to simulate systems containing a huge number of particles. For instance, Neau et al. [6] carried out two-fluid simulations of a polymerization fluidized bed reactor at the industrial level, incorporating over 40 billion particles and using a computational grid comprising more than one billion cells.

1.4.3 Coupling of mesoscopic and macroscopic scales

Meso-scale information extracted from CFD-DEM simulations can be used for calculating macroscopic parameters and serves as a foundation for creating and verifying macro-scale closures for the two-fluid model. An illustrative example of this process is the work by Dupuy et al. [76], who developed a continuum model for the particle-wall contact shear stress through analysis of CFD-DEM simulations. Figure 1.8 presents a laboratory-scale simulation employing CFD-DEM [5], alongside an industrial-scale simulation using the two-fluid model [6]. The former can serve as a basis for developing closure models for the latter, enabling accurate macro-scale predictions.

1.5 Research hypothesis and main objective

The presence of interparticle adhesion forces significantly influences the hydrodynamics of gas-solid fluidized beds, potentially posing risks for industrial applications. The reasons for certain observed phenomena in fluidized beds operating at ambient conditions are not clearly and adequately identified, such as the overshoot in the bed pressure drop when reaching the minimum fluidization velocity while increasing the inlet gas velocity. In dry ambient settings, the prevailing interparticle force is the Van der Waals adhesion force, which obstructs the mobility of fine particles. Therefore, it is reasonable to think that **the Van der Waals force contributes to the pressure-drop overshoot, although this has never been demonstrated through macroscopic modeling**. This is our research hypothesis.

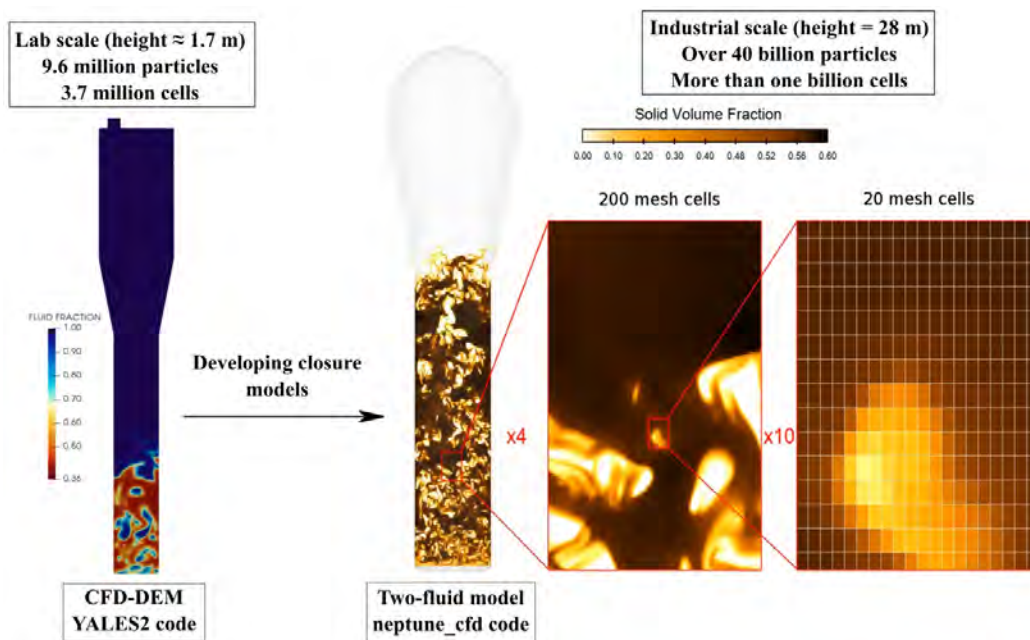


Figure 1.8 Coupling mesoscopic and macroscopic scales: from lab to industrial fluidized bed simulations [5, 6].

Taking the impact of interparticle VDW forces into account can help forecast experimental fluidization behavior. Additionally, accounting for these forces can aid in designing more suitable equipment, determining optimal operating conditions, and scaling up fluidized bed reactors. However, literature on macro-scale models that consider VDW adhesion forces is scarce, and there is a lack of suitable adhesive solid stress closures, resulting in a limited comprehension of the dynamics within the bed. Developing continuum closure models to account for the influence of VDW adhesion requires numerical data from meso-scale simulations that capture the interactions between individual particles.

Therefore, **the main objective of this thesis is to quantify the macroscopic impact of the Van der Waals adhesion force on gas-solid fluidized bed hydrodynamics using a multi-scale modeling approach.** This objective necessitates a deep understanding of bed hydrodynamics, especially during the transitions between static and fluidized states. In the next chapter, a comprehensive literature review will be presented to identify key research gaps and potential contributions to the field.

CHAPTER 2 LITERATURE REVIEW

2.1 Modeling of gas-solid flows

Various approaches are utilized for modeling gas-solid flows, such as the Eulerian-Lagrangian and Eulerian-Eulerian approaches. The former operates at the meso-scale level, whereas the latter operates at the macro-scale level.

2.1.1 Eulerian-Lagrangian approach

A computational framework has been developed by integrating the Discrete Element Method (DEM) for particle phase representation and the Large-Eddy Simulation (LES) method for gas phase representation within the YALES2 code [5]. This computational tool uses the finite volume method and is designed to solve the filtered Navier-Stokes equations at small Mach numbers for flows with turbulence and chemical reactions. Below, we provide a brief description of the Eulerian-Lagrangian modeling approach employed in YALES2.

Modeling of gas phase

The LES equations for the gas phase are derived by filtering the Navier-Stokes equations, accounting for the local volume fraction of the gas [77]:

$$\partial_t (\tilde{\rho}_g \alpha_g) + \nabla \cdot (\tilde{\rho}_g \alpha_g \hat{\mathbf{u}}_g) = 0, \quad (2.1)$$

$$\partial_t (\tilde{\rho}_g \alpha_g \hat{\mathbf{u}}_g) + \nabla \cdot (\tilde{\rho}_g \alpha_g \hat{\mathbf{u}}_g \otimes \hat{\mathbf{u}}_g) = \nabla \cdot (\alpha_g \tilde{\boldsymbol{\varepsilon}}_g) - \nabla \tilde{P}_g + \tilde{\mathbf{I}}_{p \rightarrow g} + \tilde{\rho}_g \alpha_g \mathbf{g}. \quad (2.2)$$

Equation (2.1) is the mass conservation equation, and Equation (2.2) is the momentum transport equation. YALES2 also has the capability to solve conservation equations for energy and chemical species [78], but we have chosen not to include them in this thesis as they fall outside the scope of our study. In Equation (2.1), $\tilde{\rho}_g$ is the volume-filtered gas density, α_g is the gas volume fraction, and $\hat{\mathbf{u}}_g$ is the Favre-averaged gas velocity. In Equation (2.2), $\tilde{P}_g$ represents the pressure of the gas, $\tilde{\mathbf{I}}_{p \rightarrow g}$ denotes the momentum source term associated with gas-solid coupling, $\mathbf{g}$ signifies the acceleration due to gravity, and $\tilde{\boldsymbol{\varepsilon}}_g$ refers to the viscous strain tensor, which is calculated as follows:

$$\tilde{\boldsymbol{\varepsilon}}_g = \left(\nabla \hat{\mathbf{u}}_g + \nabla \hat{\mathbf{u}}_g^T - \frac{2}{3} (\nabla \cdot \hat{\mathbf{u}}_g) \mathbb{I} \right) [\mu_g + \mu_t], \quad (2.3)$$

where μ_g signifies the dynamic viscosity of the gas, μ_t stands for the turbulent viscosity, and $\mathbb{I}$ denotes the unit tensor.

Modeling of solid phase

The motion of a spherical particle p , encompassing both translational and rotational aspects, can be determined through the application of Newton's second law [5]:

$$\mathrm{d}_t(\mathbf{x}_p) = \mathbf{u}_p, \quad (2.4)$$

$$m_p \mathrm{d}_t(\mathbf{u}_p) = \mathbf{F}_p^e + \mathbf{F}_p^c, \quad (2.5)$$

$$I_p \mathrm{d}_t(\boldsymbol{\omega}_p) = \mathbf{M}_p^d + \mathbf{M}_p^c + \mathbf{M}_p^r. \quad (2.6)$$

The variables I_p , m_p , $\mathbf{x}_p$, $\boldsymbol{\omega}_p$, and $\mathbf{u}_p$ denote respectively the moment of inertia ($I_p = m_p d_p^2/10$), mass, position, angular velocity, and translational velocity of particle p . $\mathbf{F}_p^e$, $\mathbf{F}_p^c$, $\mathbf{M}_p^d$, $\mathbf{M}_p^c$, and $\mathbf{M}_p^r$ are respectively the overall external force acting upon particle p , the total contact force (interparticle and particle-wall contacts), the torque of gas drag force, the torque of $\mathbf{F}_p^c$, and the torque due to rolling friction. The overall external force $\mathbf{F}_p^e$ encompasses the force of gravity $\mathbf{F}_p^g$ and the forces acting upon the solid by the gas, specifically the buoyant force $\mathbf{F}_p^b$ and the drag force $\mathbf{F}_p^d$.

$$\mathbf{F}_p^e = \mathbf{F}_p^d + \mathbf{F}_p^b + \mathbf{F}_p^g. \quad (2.7)$$

The gravitational force $\mathbf{F}_p^g$ is equal to $m_p \mathbf{g}$, and the Archimedes force $\mathbf{F}_p^b$ is equal to $-V_p \nabla P_{g@p}$, where V_p denotes the volume of the particle and $\nabla P_{g@p}$ represents the gradient of gas pressure interpolated at the particle's position. The drag force $\mathbf{F}_p^d$ is computed through a method incorporating both the Wen and Yu [69] and Ergun [14] correlations (see paragraph 2.1.1). The drag torque $\mathbf{M}_p^d$ is computed using a model from the research of Dennis et al. [79].

Modeling of collisions The overall contact force $\mathbf{F}_p^c$ exerted on a particle p is calculated by summing the forces $\mathbf{f}_{q \rightarrow p}^c$ applied by all the walls and particles that are in contact with it:

$$\mathbf{F}_p^c = \sum_{q=1}^{n_s+n_w} \mathbf{f}_{q \rightarrow p}^c, \quad (2.8)$$

where n_s and n_w denote the number of particles and walls in contact with p , respectively. The collision forces $\mathbf{f}_{q \rightarrow p}^c$ are separated into components along the normal ($\mathbf{f}_{q \rightarrow p,n}^c$) and tangential

$(\mathbf{f}_{q \rightarrow p, t}^c)$ directions:

$$\mathbf{f}_{q \rightarrow p}^c = \mathbf{f}_{q \rightarrow p, n}^c + \mathbf{f}_{q \rightarrow p, t}^c. \quad (2.9)$$

The soft-sphere model, as described in reference [73], is utilized in our research to address contact interactions between particles as well as between particles and walls. This model, unlike the hard-sphere model, allows for slight overlapping between particles and enables multiple contacts and prolonged contact durations, which is a key factor in its selection for our investigation. The soft-sphere model characterizes particles in contact as a system comprising dashpot, spring, and mass elements, as depicted in Figure 2.1. In this depiction,

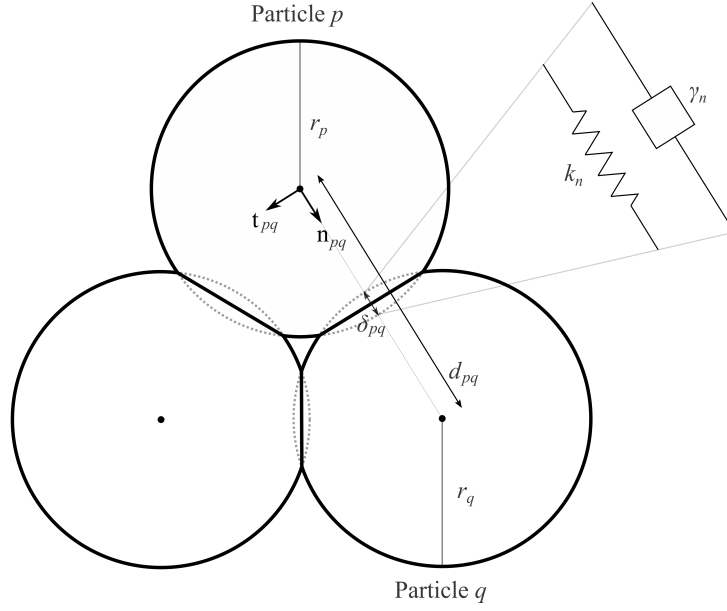


Figure 2.1 Representation of interparticle contacts using the soft-sphere model.

the distance of overlap between a pair of particles with radii r_q and r_p is denoted as δ_{pq} . The vectors $\mathbf{n}_{pq}$ and $\mathbf{t}_{pq}$ represent the unit normal and tangential vectors, respectively. The parameter d_{pq} , which is equal to $\|\mathbf{x}_p - \mathbf{x}_q\|$, denotes the separation between the centers of particles q and p . Additionally, γ_n represents the normal damping parameter, and k_n denotes the normal spring stiffness.

When two particles p and q make contact ($\delta_{pq} = r_p + r_q - \|\mathbf{x}_q - \mathbf{x}_p\| > 0$), and the condition $d_{pq} < r_p + r_q$ is satisfied, a repulsive force $\mathbf{f}_{q \rightarrow p, n}^c$ arises in the normal direction:

$$\mathbf{f}_{q \rightarrow p, n}^c = -k_n \delta_{pq} \mathbf{n}_{pq} - \gamma_n \mathbf{u}_{pq, n}. \quad (2.10)$$

The spring (k_n) serves as an energy reservoir that can potentially be discharged at a subse-

quent phase of the collision process. The normal unit vector $\mathbf{n}_{pq}$ can be written as:

$$\mathbf{n}_{pq} = \frac{\mathbf{x}_q - \mathbf{x}_p}{\|\mathbf{x}_q - \mathbf{x}_p\|}. \quad (2.11)$$

The normal damping parameter γ_n can be expressed as follows:

$$\gamma_n = \frac{-2 \ln e_n}{\sqrt{\pi^2 + \ln^2 e_n}} \sqrt{k_n m_{pq}}, \quad (2.12)$$

where e_n denotes the normal restitution coefficient, and m_{pq} stands for the effective mass given by:

$$m_{pq} = \left(\frac{1}{m_q} + \frac{1}{m_p} \right)^{-1}. \quad (2.13)$$

The relative velocity is defined as:

$$\mathbf{u}_{pq} = \mathbf{u}_p - \mathbf{u}_q + (r_p \boldsymbol{\omega}_p + r_q \boldsymbol{\omega}_q) \times \mathbf{n}_{pq}. \quad (2.14)$$

Then, the normal component of the relative velocity is determined by:

$$\mathbf{u}_{pq,n} = (\mathbf{u}_{pq} \cdot \mathbf{n}_{pq}) \mathbf{n}_{pq}. \quad (2.15)$$

The distance of overlap, denoted as $\delta_{pq}(t)$, is influenced by parameters specified by the user, like k_n and e_n , as well as the properties of the particles involved. The contact duration t_c is utilized in determining the particle time step. It is defined as:

$$t_c = \pi \left(\sqrt{\frac{k_n}{m_{pq}}} - \gamma_n^2 \right)^{-1}. \quad (2.16)$$

When k_n increases, the contact duration and particle time step decrease, which increases the computational cost. For a contact between a particle and a wall, the wall is treated akin to a particle but with zero radius and velocity, and infinite moment of inertia and mass.

For a description of modeling the tangential component of the contact force, $\mathbf{f}_{q \rightarrow p, t}^c$, please refer to Chapter 5. The overall torque, denoted as $\mathbf{M}_p^c$ in Equation (2.6), exerted by all objects q colliding with a given particle p can be computed as [5]:

$$\mathbf{M}_p^c = r_p \sum_{q=1}^{n_s+n_w} \mathbf{n}_{pq} \times \mathbf{f}_{q \rightarrow p, t}^c. \quad (2.17)$$

Gas-solid coupling

Gas-to-particle interpolation Gas-phase parameters must be interpolated from the grid nodes to the location of a given particle in order to solve its motion equations. This interpolation is illustrated through the example provided below for the velocity of the gas, $\mathbf{u}_g$, interpolated at the position of the particle, $\mathbf{x}_p$:

$$\mathbf{u}_{g@p}(t) = \sum_{k=1}^{n_k} \omega_k^p \mathbf{u}_g(\mathbf{x}_k, t), \quad (2.18)$$

where the sum is taken over all grid nodes k of the cell that contains particle p , and the interpolation weight ω_k^p is determined via trilinear interpolation [10].

Particle-to-gas projection The projection of data from the particle position onto the grid is demonstrated via the following example for the momentum transfer term:

$$\mathbf{I}_{p \rightarrow g}(\mathbf{x}_k, t) = -\frac{1}{V_k} \sum_{p \in C_k} \omega_k^p [\mathbf{F}_p^d(t) + \mathbf{F}_p^b(t)], \quad (2.19)$$

where V_k represents the control volume corresponding to node k , and $p \in C_k$ signifies that the center of particle p is positioned within one of the adjacent cells of node k . The projection weights used are the same as the interpolation weights. The instantaneous volume fraction of the gas at a given node k is determined as follows:

$$\alpha_g(\mathbf{x}_k) = 1 - \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p V_p, \quad (2.20)$$

where V_p represents the volume of the particle. The chosen projection approach utilizes the particle centroid method, which categorizes particles as belonging to a given cell if their centers are situated inside it. This method has been noted to introduce considerable discontinuities and possible instabilities when the cell size is less than $3d_p$ [80].

Gas-solid interactions The force of interaction between the gas and the particles can be expressed as the sum of drag and buoyant forces:

$$\mathbf{F}_{g \rightarrow p} = \mathbf{F}_p^d + \mathbf{F}_p^b. \quad (2.21)$$

The buoyancy contribution can be expressed in the following manner:

$$\mathbf{F}_p^b = -V_p \nabla P_{g@p}, \quad (2.22)$$

and the drag contribution can be written as follows:

$$\mathbf{F}_p^d = \frac{1}{\tau_r^d} [\mathbf{u}_{g@p} - \mathbf{u}_p] m_p, \quad (2.23)$$

where τ_r^d represents the drag relaxation time, given as:

$$\tau_r^d = \frac{4}{3} \left(\frac{\rho_p d_p^2}{\mu_{g@p} Re_p C_d} \right). \quad (2.24)$$

Here, C_d stands for the drag coefficient, and Re_p represents the particle Reynolds number, which is written as:

$$Re_p = \frac{d_p \|\mathbf{u}_{g@p} - \mathbf{u}_p\| \rho_{g@p}}{\mu_{g@p}} \alpha_{g@p}. \quad (2.25)$$

The closure model employed for C_d in our numerical simulations is the one suggested by Gobin et al. [81]:

$$C_d = \begin{cases} C_d^{W\&Y}, & \text{if } \alpha_p \leq 0.3, \\ \min(C_d^E, C_d^{W\&Y}), & \text{else.} \end{cases} \quad (2.26)$$

Here, C_d^E represents the drag coefficient according to Ergun [14]:

$$C_d^E = \frac{1}{\alpha_{g@p}} \left[\frac{7}{3} + \frac{200}{Re_p} (1 - \alpha_{g@p}) \right], \quad (2.27)$$

and $C_d^{W\&Y}$ is the Wen and Yu drag coefficient [69] defined as:

$$C_d^{W\&Y} = \begin{cases} 0.44 \alpha_{g@p}^{-2.7}, & \text{if } Re_p \geq 1000, \\ \frac{24}{Re_p} \alpha_{g@p}^{-2.7} \left(1 + 0.15 Re_p^{0.687} \right), & \text{else.} \end{cases} \quad (2.28)$$

Time advancement of gas and solids

Advancement of particles The Groot-Warren scheme [82] is employed in our simulations to solve the particle equation of motion (2.5). The particle position is advanced in the following way:

$$\mathbf{x}_p^{j+1} = \mathbf{x}_p^j + \Delta t_p \mathbf{u}_p^j + \frac{1}{2} (\Delta t_p)^2 \mathbf{a}_p^j. \quad (2.29)$$

Here, $\mathbf{x}_p^{j+1}$ denotes the particle position at time $t + \Delta t_p$, and $\mathbf{a}_p^j = \mathbf{F}_{p,tot}^j / m_p$ represents the particle acceleration at time t , where $\mathbf{F}_{p,tot}$ indicates the total force applied on particle p and Δt_p denotes the particle time step. The particle velocity is advanced using a prediction-

correction mechanism as follows:

$$\begin{aligned}
&\text{Prediction step } \left\{ \mathbf{u}_p^{*j+1} = \mathbf{u}_p^j + \xi \Delta t_p \mathbf{a}_p^j, \right. \\
&\text{Correction step } \left\{ \begin{aligned} \mathbf{a}_p^{j+1} &= \mathbf{a}_p(\mathbf{x}_p^{j+1}, \mathbf{u}_p^{*j+1}), \\ \mathbf{u}_p^{j+1} &= \mathbf{u}_p^j + \frac{1}{2} \Delta t_p (\mathbf{a}_p^j + \mathbf{a}_p^{j+1}), \end{aligned} \right.
\end{aligned} \tag{2.30}$$

where $\mathbf{u}_p^{*j+1}$ is the predicted particle velocity and ξ is a numerical parameter between 0 and 1. For $\xi = 1/2$, the equivalent of the velocity-Verlet scheme is obtained if the force were not influenced by velocity. In our tests, $\xi = 1/2$ is used. The Groot-Warren scheme is also employed to advance the angular particle velocity.

The time step for particles (Δt_p) must satisfy various conditions to guarantee accurate treatment of collisions and stability [83]. The first condition is:

$$\Delta t_p \leq \Delta t_g, \tag{2.31}$$

where Δt_g is the gas time step. This condition means that particles can advance over multiple particle time steps (sub-steps) within one gas time step. To prevent a particle from traversing multiple cells within a particle time step Δt_p , another criterion is imposed:

$$\Delta t_p \leq CFL_s \frac{\Delta h}{\|\mathbf{u}_p\|}. \tag{2.32}$$

Here, CFL_s denotes the particle CFL number, and Δh stands for the cell size. Additionally, to regulate and restrict the distance of overlap at the start of the collision, the condition below is employed:

$$\Delta t_p \leq CFL_s^c \frac{d_p}{\|\mathbf{u}_{pq,n}^i\|}, \tag{2.33}$$

where CFL_s^c denotes a coefficient that constrains the distance particles p and q can move within a single sub-step Δt_p , and $\mathbf{u}_{pq,n}^i$ represents the normal relative velocity between particles p and q at the start of the collision. The time step for particles ought to be sufficiently less than the collision time (t_c) to ensure resolving the collision accurately:

$$\Delta t_p < \frac{t_c}{n_c}, \tag{2.34}$$

where n_c represents the number of sub-steps within t_c . It is advised to choose n_c between 15

and 50 [84]. Regarding the drag, the condition of stability is expressed as:

$$\Delta t_p < \tau_r^d, \quad (2.35)$$

where τ_r^d stands for the drag relaxation time given by Equation (2.24). Concerning gravity, the stability criterion is stated as:

$$\Delta t_p < Gr \sqrt{\frac{\Delta h}{\|\mathbf{g}\|}}, \quad (2.36)$$

where Gr denotes the gravity number. Finally, the definitive sub-step is determined as the minimum value from all the aforementioned conditions:

$$\Delta t_p = \min \left(CFL_s \frac{\Delta h}{\|\mathbf{u}_p\|}, CFL_s \frac{d_p}{\|\mathbf{u}_{pq,n}^i\|}, \frac{t_c}{n_c}, \tau_r^d, Gr \sqrt{\frac{\Delta h}{|g|}} \right). \quad (2.37)$$

The same time step (Δt_p) is used for all the particles.

Advancement of gas The Navier-Stokes equations (2.1) and (2.2) are solved in time using an explicit approach. Discretization in space employs a 4th-order centered scheme, and advancement in time utilizes the 4th-order TFV4A scheme incorporating both Lax-Wendroff and Runge-Kutta approaches [85]. Gas advancement in time employs a projection technique tailored for flows with changing densities [86]. The steps used to advance the gas in time are outlined as follows [10]:

a) **Advancing the particles:** The advancement of particles is performed following the procedure outlined in paragraph 2.1.1 from time $n + 1/2$ to time $n + 3/2$, where n indicates discrete instances in time. Then, the gas volume fraction $\alpha_g^{n+3/2}$ is calculated from Equation (2.20).

b) **Prediction of density:** The predicted density $(\rho_g \alpha_g)^*$ is computed via the continuity equation (2.1) as follows:

$$(\rho_g \alpha_g)^* = (\rho_g \alpha_g)^{n+1/2} - \Delta t_g \nabla \cdot (\rho_g \alpha_g \mathbf{u}_g)^n. \quad (2.38)$$

c) **Prediction of velocity:** The predicted gas velocity is determined as:

$$(\rho_g \alpha_g \mathbf{u}_g)^* = (\rho_g \alpha_g \mathbf{u}_g)^n - \Delta t_g \left(\nabla P_g^{n-1/2} + \nabla \cdot [(\rho_g \alpha_g \mathbf{u}_g)^n \otimes \mathbf{u}_g^n] - \nabla \cdot \boldsymbol{\epsilon}_g^n \right). \quad (2.39)$$

d) **Correction of velocity:** The correction of gas velocity is carried out in the following manner:

$$(\rho_g \alpha_g \mathbf{u}_g)^{n+1} = (\rho_g \alpha_g \mathbf{u}_g)^* - \Delta t_g \nabla (\Delta P_g). \quad (2.40)$$

Here, $\Delta P_g = P_g^{n+1/2} - P_g^{n-1/2}$, where $P_g^{n+1/2}$ is determined from the Poisson equation. By applying the divergence operator to Equation (2.40) and utilizing the following continuity equation:

$$\nabla \cdot (\rho_g \alpha_g \mathbf{u}_g)^{n+1} = -\frac{1}{\Delta t_g} \left[(\rho_g \alpha_g)^{n+3/2} - (\rho_g \alpha_g)^{n+1/2} \right], \quad (2.41)$$

the Poisson equation given below can be derived:

$$\nabla \cdot \left(\nabla (\Delta P_g) \right) = \frac{1}{\Delta t_g} \nabla \cdot (\rho_g \alpha_g \mathbf{u}_g)^* + \frac{1}{\Delta t_g^2} \left[(\rho_g \alpha_g)^{n+3/2} - (\rho_g \alpha_g)^{n+1/2} \right]. \quad (2.42)$$

The linear system presented in Equation (2.42) is solved using the Deflated Preconditioned Conjugate Gradient (DPCG) method [87].

The gas time step is determined by applying the following stability conditions:

$$\Delta t_g < CFL \frac{\Delta h}{\|\mathbf{u}_g\|}, \quad (2.43)$$

$$\Delta t_g < Fo \frac{\rho_g}{\mu_g + \mu_t} \Delta h^2, \quad (2.44)$$

$$\Delta t_g < Gr \sqrt{\frac{\Delta h}{\|\mathbf{g}\|}}, \quad (2.45)$$

where CFL is the Courant-Friedrichs-Lewy number, Fo is the Fourier number, and Gr is the gravity number.

2.1.2 Eulerian-Eulerian approach

In this section, we present an overview of the multi-fluid modeling approach utilized in `neptune_cfd`.

Modeling of gas phase

Mass balance The mass balance equation for the gas can be written as [88]:

$$\frac{\partial}{\partial t} (\rho_g \alpha_g) + \frac{\partial}{\partial x_i} (\rho_g \alpha_g U_{g,i}) = 0, \quad (2.46)$$

where $U_{g,i}$ denotes the i th component of the Favre-averaged gas velocity ($\langle u_{g,i} \rangle_g$).

Momentum balance The momentum balance equation for the gas can be expressed as [88]:

$$\rho_g \alpha_g \frac{\partial U_{g,i}}{\partial t} + \rho_g \alpha_g U_{g,j} \frac{\partial U_{g,i}}{\partial x_j} = \frac{\partial \Sigma_{g,ij}}{\partial x_j} - \alpha_g \frac{\partial P_g}{\partial x_i} + I_{p \rightarrow g,i} + \rho_g \alpha_g g_i, \quad (2.47)$$

where $\Sigma_{g,ij}$ represents the gas stress tensor, and $I_{p \rightarrow g,i}$ stands for the interphase momentum transfer. The stress tensor $\Sigma_{g,ij}$ is given by the following expression:

$$\Sigma_{g,ij} = \Theta_{g,ij} - \rho_g \alpha_g R_{g,ij}, \quad (2.48)$$

where $\Theta_{g,ij}$ is the viscous stress tensor, and $R_{g,ij}$ is the Reynolds stress tensor. The Reynolds stress tensor is modeled as [81]:

$$R_{g,ij} = \langle u''_{g,i} u''_{g,j} \rangle_g = \frac{2}{3} \delta_{ij} \left(\nu_g^T \frac{\partial U_{g,l}}{\partial x_l} + k \right) - \nu_g^T \left(\frac{\partial U_{g,j}}{\partial x_i} + \frac{\partial U_{g,i}}{\partial x_j} \right), \quad (2.49)$$

where $u''_{g,i}$ is the fluctuating gas velocity, δ_{ij} is the Kronecker delta, k is the turbulent kinetic energy of the gas, and ν_g^T denotes the turbulent viscosity, expressed as:

$$\nu_g^T = \tau_g^T \left(\frac{3}{2k} + 0.51 \frac{\tau_{gp}^T}{k \tau_{gp}^E} \frac{\rho_p \alpha_p}{\rho_g \alpha_g} \left[1 - \frac{q_{gp}}{2k} \right] \right)^{-1}, \quad (2.50)$$

where $\tau_g^T = 0.135k/\varepsilon$ represents the time scale characterizing the turbulence of the gas phase, with ε indicating the rate at which turbulent kinetic energy dissipates. ρ_p and α_p are the solid density and volume fraction, respectively. τ_{gp}^T is the time of interaction between eddies and particles, τ_{gp}^E is the relaxation time of the particles, and q_{gp} is the gas-solid velocity covariance. The transport equations for k and ε can be found in Vermorel et al. [89]. The viscous stress tensor is written as [75]:

$$\Theta_{g,ij} = \mu_g \alpha_g \left(\frac{\partial U_{g,j}}{\partial x_i} + \frac{\partial U_{g,i}}{\partial x_j} - \frac{\partial U_{g,l}}{\partial x_l} \frac{2}{3} \delta_{ij} \right), \quad (2.51)$$

where μ_g stands for the dynamic viscosity of the gas. The average transfer of momentum from solid to gas is modeled under the assumption of hard-sphere particles that undergo translational motion [75, 81]:

$$I_{p \rightarrow g,i} = \frac{1}{\tau_{gp}^E} \rho_p \alpha_p U_{pg,i}^r. \quad (2.52)$$

Here, $U_{pg,i}^r$ represents the average relative velocity, which is expressed as:

$$U_{pg,i}^r = U_{p,i} - U_{g,i} - U_{gp,i}^d, \quad (2.53)$$

where $U_{gp,i}^d$ denotes the gas-solid turbulent drift velocity, the modeling of which can be found in Fotovat et al. [90]. The relaxation time of the particles, τ_{gp}^E , is written as [81]:

$$\tau_{gp}^E = \frac{4\rho_p d_p}{3\rho_g \langle \|\mathbf{u}_{pg}^r\| \rangle_p} \frac{1}{C_d(\text{Re}_p)}. \quad (2.54)$$

Here, $\mathbf{u}_{pg}^r$ denotes the relative velocity of each particle compared to the gas around it, and $C_d(\text{Re}_p)$ represents the drag coefficient. The model used for C_d is according to the work of Gobin et al. [81]. This model is the same as that used in the CFD-DEM simulations (Equation (2.26)).

Modeling of solid phase

The kinetic theory is employed to obtain balance equations for the solid [91]. A probability density function, denoted as f_p , is used to describe particle statistics. The following Boltzmann equation specifies how f_p evolves [88]:

$$\frac{\partial f_p}{\partial t} + \frac{\partial}{\partial x_j} (f_p c_{p,j}) = -\frac{\partial}{\partial c_{p,j}} \left(f_p \left\langle \frac{du_{p,j}}{dt} \middle| \mathbf{x}_p = \mathbf{x}, \mathbf{u}_p = \mathbf{c}_p \right\rangle \right) + \left(\frac{\partial f_p}{\partial t} \right)_{coll}. \quad (2.55)$$

Here, $f_p(\mathbf{x}, \mathbf{c}_p, t) \delta \mathbf{x} \delta \mathbf{c}_p$ represents the likely count of particles having a center of mass, $\mathbf{x}_p$, situated within the volume $[\mathbf{x}, \mathbf{x} + \delta \mathbf{x}]$ and possessing a velocity $\mathbf{u}_p$ between $\mathbf{c}_p$ and $\mathbf{c}_p + \delta \mathbf{c}_p$ at time t . In Equation (2.55), the last term on the right-hand side indicates the rate at which f_p varies as a result of collisions between particles. Enskog's transport equation for a given property of particles, denoted as Υ_p , can be obtained through the integration of Equation (2.55) over the entire range of particle property values:

$$\frac{\partial}{\partial t} (\langle \Upsilon_p \rangle_p \rho_p \alpha_p) + \frac{\partial}{\partial x_j} (\langle \Upsilon_p u_{p,j} \rangle_p \rho_p \alpha_p) = \rho_p \alpha_p \left\langle \frac{\partial \Upsilon_p}{\partial u_{p,j}} \frac{du_{p,j}}{dt} \right\rangle_p + \mathbf{\Gamma}(\Upsilon_p m_p), \quad (2.56)$$

where $\mathbf{\Gamma}(\Upsilon_p m_p)$ indicates the average rate of variation in the particle property resulting from collisions. Mass and momentum conservation equations for the solid are obtained, respectively, by substituting Υ_p with 1 and $u_{p,i}$ in Equation (2.56).

Mass balance The mass balance equation of the solid phase can be written as [91]:

$$\frac{\partial}{\partial t}(\rho_p \alpha_p) + \frac{\partial}{\partial x_j}(\rho_p \alpha_p U_{p,j}) = 0. \quad (2.57)$$

Momentum balance The momentum balance equation of the solid phase is expressed as [91]:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_p \alpha_p U_{p,i}) + \frac{\partial}{\partial x_j}(\rho_p \alpha_p U_{p,j} U_{p,i}) = & \rho_p \alpha_p \left\langle \frac{F_i^d}{m_p} \right\rangle_p + \rho_p \alpha_p g_i - \alpha_p \frac{\partial P_g}{\partial x_i} \\ & + \mathbf{\Gamma}(u_{p,i} m_p) - \frac{\partial}{\partial x_j} \left(\langle u_{p,j}'' u_{p,i}'' \rangle_p \rho_p \alpha_p \right), \end{aligned} \quad (2.58)$$

where $\rho_p \alpha_p \langle F_i^d / m_p \rangle_p$ represents the average transfer of momentum from the gas to the solid phase ($I_{g \rightarrow p,i}$), with F_i^d standing for the i th component of the drag force. $\langle u_{p,j}'' u_{p,i}'' \rangle_p$ denotes the kinetic particle stress tensor, and $\mathbf{\Gamma}(u_{p,i} m_p)$ takes into consideration the transfer of momentum between particles that occurs during collisions. $\mathbf{\Gamma}(u_{p,i} m_p)$ is divided into source and flux terms as follows [92]:

$$\mathbf{\Gamma}(u_{p,i} m_p) = \Psi_p(u_{p,i} m_p) - \frac{\partial}{\partial x_j} \Theta_{p,j}(u_{p,i} m_p). \quad (2.59)$$

The source term, denoted as $\Psi_p(u_{p,i} m_p)$, is negligible due to the conservation of momentum in binary collisions. The flux term, represented as $\Theta_{p,j}(u_{p,i} m_p)$, is regarded as a component of the stress tensor of the solid phase, $\Sigma_{p,ij}$. Then, the momentum balance equation of the particles can be written as:

$$\frac{\partial}{\partial t}(\rho_p \alpha_p U_{p,i}) + \frac{\partial}{\partial x_j}(\rho_p \alpha_p U_{p,j} U_{p,i}) = \rho_p \alpha_p \left\langle \frac{F_i^d}{m_p} \right\rangle_p + \rho_p \alpha_p g_i - \alpha_p \frac{\partial P_g}{\partial x_i} - \frac{\partial \Sigma_{p,ij}}{\partial x_j}, \quad (2.60)$$

with the solid stress tensor expressed as a sum of collisional and kinetic stress tensors [88]:

$$\Sigma_{p,ij} = \Sigma_{p,ij}^c + \Sigma_{p,ij}^k = \Theta_{p,ij} + R_{p,ij} \rho_p \alpha_p = \Theta_{p,ij} + \langle u_{p,j}'' u_{p,i}'' \rangle_p \rho_p \alpha_p. \quad (2.61)$$

In dilute regimes, the primary contribution to the solid stress tensor is from its kinetic component, while in dense regimes, the dominant contribution is from its collisional component. The Boussinesq approximation is employed to model the kinetic solid stress tensor [88, 93]:

$$\langle u_{p,j}'' u_{p,i}'' \rangle_p = \frac{2}{3} \left(\frac{\partial U_{p,l}}{\partial x_l} \nu_p^k + q_p^2 \right) \delta_{ij} - \left(\frac{\partial U_{p,j}}{\partial x_i} + \frac{\partial U_{p,i}}{\partial x_j} \right) \nu_p^k, \quad (2.62)$$

where ν_p^k is the kinetic viscosity of the solid phase, and q_p^2 is the fluctuant kinetic energy of the particles. The kinetic viscosity of the particulate phase is expressed as [75]:

$$\nu_p^k = \left(\frac{1}{3} q_p^2 \tau_{gp}^E [1 + \xi_c g_0 \alpha_p] + \nu_{gp}^T \right) \left(\frac{\gamma_c \tau_{gp}^E}{2 \tau_p^c} + 1 \right)^{-1}, \quad (2.63)$$

where $\nu_{gp}^T = q_{gp} \tau_{gp}^T / 3$ stands for the gas-solid turbulent viscosity, and g_0 denotes the radial distribution function. The expression for τ_p^c , which represents particle-particle collision time, can be found in Simonin et al. [94]. γ_c and ξ_c are two constants whose values are respectively $(3 - e_c)(e_c + 1)/5$ and $2(3e_c - 1)(e_c + 1)/5$, with e_c being the restitution coefficient.

The collisional component of the solid stress tensor is modeled as follows [93]:

$$\Theta_{p,ij} = - \left(\frac{\partial U_{p,j}}{\partial x_i} + \frac{\partial U_{p,i}}{\partial x_j} - \frac{\partial U_{p,l}}{\partial x_l} \frac{2}{3} \delta_{ij} \right) \nu_p^c \rho_p \alpha_p + \left(\frac{4}{3} \rho_p \alpha_p^2 g_0 q_p^2 (e_c + 1) - \Pi_p \frac{\partial U_{p,l}}{\partial x_l} \right) \delta_{ij}, \quad (2.64)$$

with $\Pi_p = \frac{4}{3} d_p \rho_p \alpha_p^2 g_0 (e_c + 1) \sqrt{\frac{2q_p^2}{3\pi}}$. ν_p^c is the collisional viscosity given by [88]:

$$\nu_p^c = \frac{4}{5} \left(d_p \sqrt{\frac{2q_p^2}{3\pi}} + \nu_p^k \right) g_0 \alpha_p (e_c + 1). \quad (2.65)$$

The radial distribution function, g_0 , is expressed as [95]:

$$g_0 = \left(1 - \frac{\alpha_p}{\alpha_{p,\max}} \right)^{-2.5\alpha_{p,\max}}, \quad (2.66)$$

with $\alpha_{p,\max} = 0.64$. The value of g_0 is 1 when the solid volume fraction is zero and increases to infinity at the close-packing volume fraction ($\alpha_{p,\max}$). Using Equations (2.62) and (2.64), the particle stress tensor can be formulated as:

$$\Sigma_{p,ij} = \Sigma_{p,ij}^c + \Sigma_{p,ij}^k = - \left[\frac{\partial U_{p,j}}{\partial x_i} + \frac{\partial U_{p,i}}{\partial x_j} - \frac{\partial U_{p,l}}{\partial x_l} \frac{2}{3} \delta_{ij} \right] (\nu_p^c + \nu_p^k) \rho_p \alpha_p + \left[P_p - \Pi_p \frac{\partial U_{p,l}}{\partial x_l} \right] \delta_{ij}, \quad (2.67)$$

where P_p is the granular pressure (solid phase pressure) expressed as a sum of collisional and kinetic pressures:

$$P_p = P_p^c + P_p^k, \quad (2.68)$$

with

$$P_p^c = \frac{4}{3} \rho_p \alpha_p^2 g_0 (e_c + 1) q_p^2, \quad (2.69)$$

$$P_p^k = \frac{2}{3} \rho_p \alpha_p q_p^2, \quad (2.70)$$

where $2q_p^2/3$ is known as the granular temperature. The transport equation for the fluctuant kinetic energy of the solid phase, $q_p^2 = \langle u_{p,i}'' u_{p,i}'' \rangle_p / 2$, can be found in the work of Simonin [91]. The governing equation for the gas-solid velocity covariance, $q_{gp} = \langle u_{g,i}'' u_{p,i}'' \rangle_p$, originally introduced by Fevrier and Simonin [96], is presented in the work of Hamidouche et al. [75].

To take into consideration the interparticle interactions via prolonged contacts when the solid volume fraction is elevated, a frictional stress tensor, denoted as $\Sigma_{p,ij}^f$, is added to the stress tensor of the solid phase. This additional stress tensor is written as [97]:

$$\Sigma_{p,ij}^f = - \left[\frac{\partial U_{p,j}}{\partial x_i} + \frac{\partial U_{p,i}}{\partial x_j} - \frac{\partial U_{p,l}}{\partial x_l} \frac{2}{3} \delta_{ij} \right] \nu_p^f \rho_p \alpha_p + P_p^f \delta_{ij}, \quad (2.71)$$

where P_p^f is the frictional pressure expressed as [98]:

$$P_p^f = Fr \frac{(\alpha_p - \alpha_{p,min})^n}{(\alpha_{p,max} - \alpha_p)^m}, \quad \text{for } \alpha_p > \alpha_{p,min}, \quad (2.72)$$

with $m = 5$, $n = 2$, and $Fr = 0.05$. $\alpha_{p,min}$ denotes the threshold particle volume fraction for friction. For detailed information about the calibration of the model presented in Equation (2.72), the reader is referred to the study of Dupuy et al. [99]. ν_p^f in Equation (2.71) is the frictional viscosity modeled as [97]:

$$\nu_p^f = \sqrt{2} \sin(\phi) \frac{P_p^f}{\rho_p \alpha_p} \left(\sqrt{\frac{8q_p^2}{3d_p^2} + D_p : D_p} \right)^{-1}, \quad (2.73)$$

where ϕ represents the angle of internal friction, and D_p denotes the strain rate tensor given by:

$$D_{p,ij} = \frac{\partial U_{p,j}}{\partial x_i} + \frac{\partial U_{p,i}}{\partial x_j} - \frac{\partial U_{p,l}}{\partial x_l} \frac{2}{3} \delta_{ij}. \quad (2.74)$$

With the addition of the frictional component, the solid stress tensor can be expressed as follows:

$$\Sigma_{p,ij} = \Sigma_{p,ij}^f + \Sigma_{p,ij}^c + \Sigma_{p,ij}^k = -D_{p,ij} \nu_p \rho_p \alpha_p + \left[P_p - \Pi_p \frac{\partial U_{p,l}}{\partial x_l} \right] \delta_{ij}, \quad (2.75)$$

where the particle viscosity and pressure are written as:

$$\nu_p = \nu_p^f + \nu_p^c + \nu_p^k, \quad P_p = P_p^f + P_p^c + P_p^k. \quad (2.76)$$

It's worth noting that `neptune_cfd` also solves equations for energy and chemical species conservation [100]. However, we have chosen not to delve into these equations because they

are beyond the scope of our work.

2.2 Modeling of Van der Waals force

The Eulerian-Lagrangian approach was employed by multiple scholars to anticipate fluidization behavior in the presence of Van der Waals force [34–37]. Conversely, studies that incorporate the Van der Waals force within the Eulerian-Eulerian approach are rare [38, 39]. A detailed review of CFD-DEM and two-fluid model investigations is presented in Section 4.1 of Chapter 4, revealing a research gap in macro-scale Van der Waals force modeling.

2.3 Measurement of Van der Waals force

Several methods have been employed to assess the extent and impact of interparticle forces, specifically the interparticle Van der Waals force, in various materials. These methods include atomic force microscopy, shearing tests, angle of repose measurement, Hausner ratio measurement, and indirect techniques for measuring IPF.

The Hausner ratio represents the ratio between the bulk density of a particle bed when it is tapped and its bulk density in a loose state. Research by Hakim et al. [101] demonstrated that nanoparticles with a Hausner ratio exceeding 1.4 exhibit behavior akin to C-type particles; those below 1.2 resemble A-type particles; and those within the 1.2 to 1.4 range may exhibit characteristics of both A-type and C-type particles. Additionally, Hakim et al. [101] categorized the flowability of nanoparticles according to their angle of repose, where higher interparticle forces lead to increased heap strength and the creation of more inclined formations, resulting in a higher angle of repose. Elahipanah [70] conducted research on the indirect measurement of interparticle forces. This method involves calculating the force required to counterbalance interparticle forces at U_{mf} as the difference between the drag force determined from experimental U_{mf} (influenced by IPF) and that determined from U_{mf} computed using a correlation that neglects the impact of IPF. In atomic force microscopy, the force between a particle fixed on an AFM tip and another particle on a glass substrate is plotted against their separation distance [102]. Shearing tests can be utilized to evaluate the friction properties and the bulk cohesion of particles [102]. Details about shear testing are included in Section 2.3.1.

2.3.1 Shear testing

In granular shear flows, the ease of particle movement is determined by the friction among particles, influenced by the Van der Waals adhesive force. Shear cells serve to assess the particles' flow characteristics by producing a yield locus that demonstrates the relationship between the normal stress exerted on a particle bed, denoted as σ , and the shear stress needed for initiating flow or failure within the particle bed, referred to as τ . The presence of interparticle adhesive forces significantly impacts the position and form of the yield locus. Adhesive particle beds exhibit a yield locus that doesn't go through the origin of the $\sigma - \tau$ plot (refer to Figure 2.2), unlike non-adhesive particle beds, where it does.

The local stress condition is visualized through Mohr circles that are tangent to the yield locus, as depicted in Figure 2.2. The tensile strength, represented as σ_t in this figure, refers

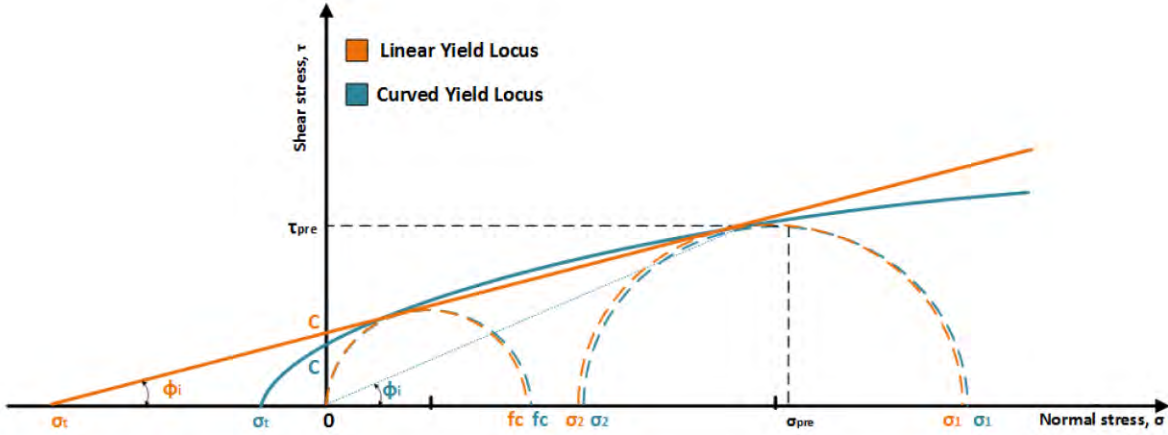


Figure 2.2 Linear and curved yield loci. σ_t : tensile strength, ϕ_i : angle of internal friction, C : cohesion, σ_1 : major principal stress, f_c : unconfined yield strength, σ_2 : minor principal stress, pre: pre-shear. Extracted from [7].

to the normal tensile stress needed to break a densely packed particle bed under no shear stresses [103]. It is located at the intersection of the yield locus with the negative region of the σ axis. The cohesion, denoted as C , refers to the shear stress required to deform a compacted particle bed when there is no normal stress present.

For many particles, the yield locus is approximately linear (see Figure 2.2), which can be represented using the Mohr-Coulomb model [104]:

$$\tau = \sigma \tan(\phi_i) + C, \quad (2.77)$$

where C is the cohesion given by the intersection between the yield locus and τ axis, and ϕ_i

is the angle of internal friction, which is the angle between the σ axis and the yield locus. There are particles that do not exhibit a linear yield locus (see Figure 2.2). Finer particles show larger yield stress and greater curvature of the yield locus due to a higher adhesion effect [103]. The Warren-Spring equation can be used to approximate the non-linear yield locus [105]:

$$\left(\frac{\tau}{C}\right)^r = 1 + \frac{\sigma}{\sigma_t}, \quad (2.78)$$

where r is the curvature index, which can be adjusted to fit experimentally measured data. García-Triñanes et al. [103] observed a high degree of agreement between the tensile strength values determined from the Warren-Spring equation and those obtained from direct experimental measurements.

To establish a connection between the macroscopic flow characteristics determined experimentally and the interparticle adhesive interactions occurring at the microscopic level, the theories of Rumpf-Molerus [106,107] and Tomas [108] can be employed. The microscopic adhesion force between particles, F_{ad} , can be calculated from the macroscopic tensile strength, σ_t , as follows [106]:

$$F_{ad} = \frac{\alpha_g}{1 - \alpha_g} d_p^2 \sigma_t, \quad (2.79)$$

where α_g is the voidage of the particle bed, and d_p is the average diameter of the particles. Tomas [109] suggested determining the properties of a granular material by employing the stationary yield locus. Mittal and Jaiswal [110] computed the average adhesion force from shear test results and found a good match with direct adhesion force measurements using atomic force microscopy.

CHAPTER 3 RESEARCH OBJECTIVES

3.1 Synthesis of the literature review

The literature review indicates that numerous studies have been carried out to examine how granular materials behave in a gas-solid fluidized bed in the presence of Van der Waals adhesion force. Various experimental and computational investigations have been conducted to study the impact of Van der Waals forces between particles. For example, these studies have demonstrated that the Van der Waals force contributes to the formation of clusters. The vast majority of computational studies that account for the Van der Waals force utilize the CFD-DEM approach. There is a scarcity of models that take into consideration the Van der Waals force at the macroscopic level. These models lack thorough testing, leading to uncertainties about their validity, primarily due to the assumptions used in their development. Moreover, there is a lack of research that can predict the pressure-drop hysteresis phenomenon using a macroscopic model, which is crucial for simulating fluidized beds on an industrial scale.

3.2 Specific objectives of the research

To achieve our previously stated main objective, which is to quantify the macroscopic impact of the Van der Waals adhesion force on gas-solid fluidized bed hydrodynamics using a multi-scale modeling approach, we define the following three specific objectives:

- Developing an Eulerian model to account for the impact of Van der Waals force in order to predict the pressure drop overshoot observed experimentally during the shift from static to fluidized bed state (Chapter 4).
- Building a CFD-DEM numerical database to guide developing the Eulerian stress closure accounting for the Van der Waals force, enabling the prediction of pressure-drop hysteresis between the fluidization and defluidization cycle curves (Chapter 5).
- Proposing a continuum transport equation for the coordination number that takes into consideration the effect of the history of deformation and predicting a hysteresis in the pressure drop via two-fluid simulations (Chapter 6).

3.3 Numerical codes

For this thesis, we have opted to use the `neptune_cfd` code for conducting two-fluid model simulations and the YALES2 code for CFD-DEM simulations.

3.3.1 The `neptune_cfd` code

`neptune_cfd` is a multiphase CFD code developed in the framework of the NEPTUNE project, financially supported by EDF, CEA (Commissariat à l'Énergie Atomique), IRSN (Institut de Radioprotection et de Sécurité Nucléaire) and Framatome. It is a proprietary code constructed based on `code_saturne`, which is open-source. `neptune_cfd` is a massively parallel C/C++ program that employs MPI for parallel computing. It is a semi-implicit solver that incorporates a second-order finite volume centered scheme for spatial discretization and a first-order implicit fractional step method for time integration [8]. `neptune_cfd` is capable of managing unstructured meshes and using cells of any type (hexahedral, tetrahedral, prismatic, etc.). This code solves transport equations for 3D multiphase flows with chemical reactions, including equations for turbulent parameters, mass fractions of chemical species, and enthalpy.

An illustration of a polydisperse fluidized bed reactor at an industrial level and high pressure, simulated using `neptune_cfd` with an 8 billion-cell mesh, is presented in Figure 3.1. Additionally, Figure 3.2 shows the speedup achieved by `neptune_cfd` on the Jean-Zay supercomputer for the same 8 billion-cell mesh. The efficiency of `neptune_cfd` for this mesh is 85% when utilizing the entire supercomputer, as depicted in Figure 3.2. Although `neptune_cfd` has been tested with larger meshes, such as 64 billion cells, challenges and limitations were encountered in these cases [8].

3.3.2 The YALES2 code

YALES2 is developed at the CORIA laboratory and maintained by researchers from CORIA and other institutions. YALES2 is capable of simulating various physical phenomena such as combustion, spray and atomization, and two-phase flows using its different solvers [111]. It utilizes a hybrid communication approach that combines MPI and OpenMP, along with domain decomposition into two levels. It is a massively parallel code that can handle unstructured meshes and features adaptive mesh refinement capabilities. YALES2 uses a projection technique to solve the Navier-Stokes equations at small Mach numbers. It employs a fourth-order centered finite volume scheme. YALES2 is written in Fortran 95.

For our tests, we used the granular flow solver in YALES2, which enables the simulation

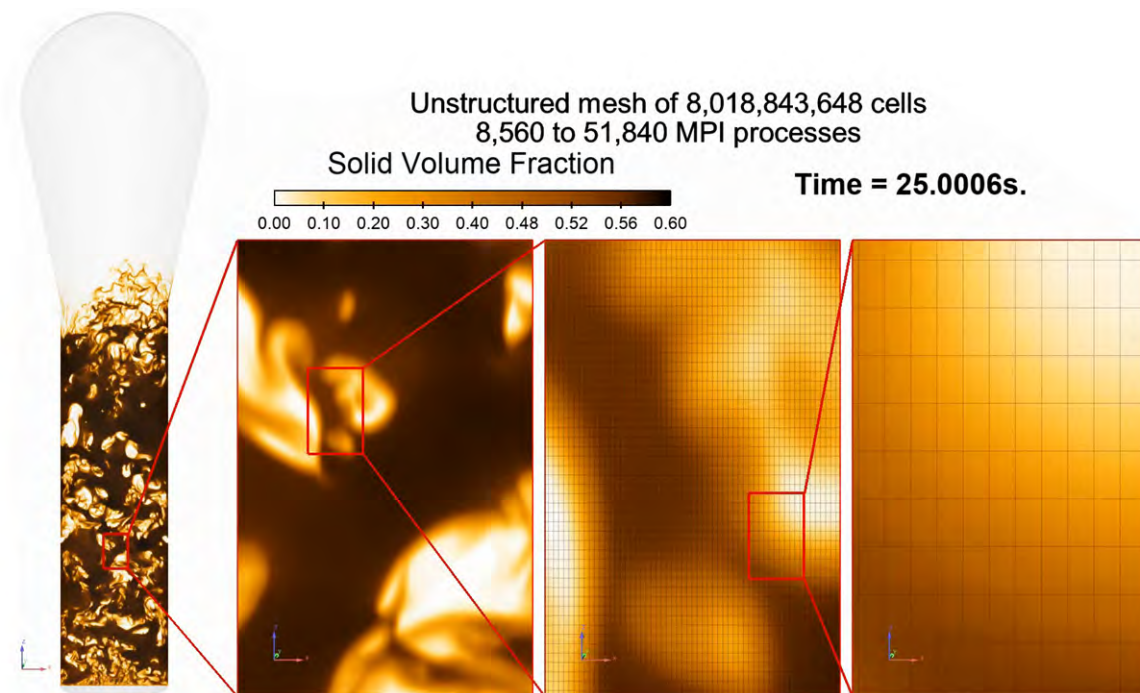


Figure 3.1 3D simulation of a polydisperse fluidized bed reactor at an industrial level and high pressure, conducted using `neptune_cfd` on the Jean-Zay (IDRIS) supercomputer. Adapted from [8].

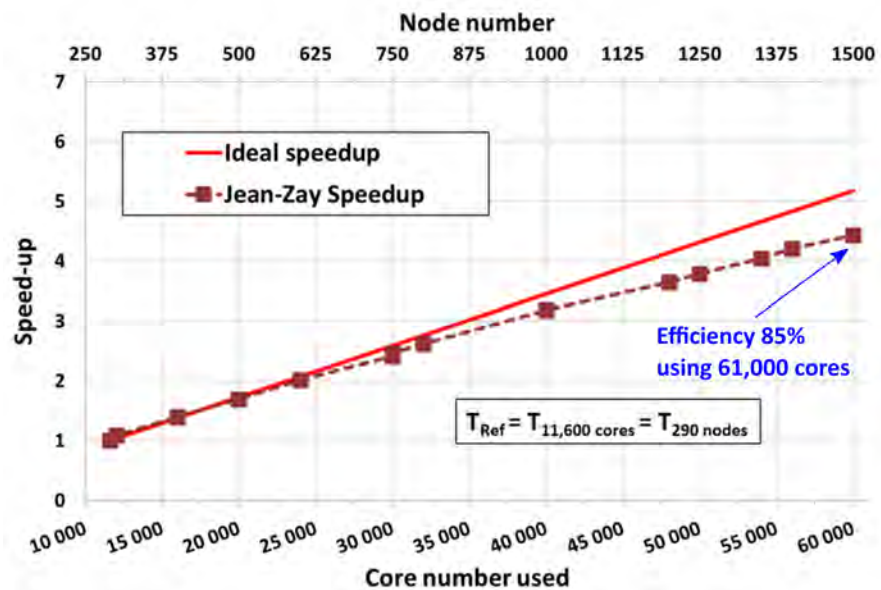
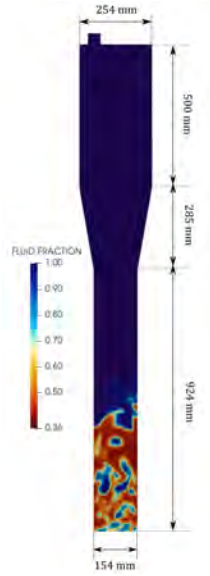
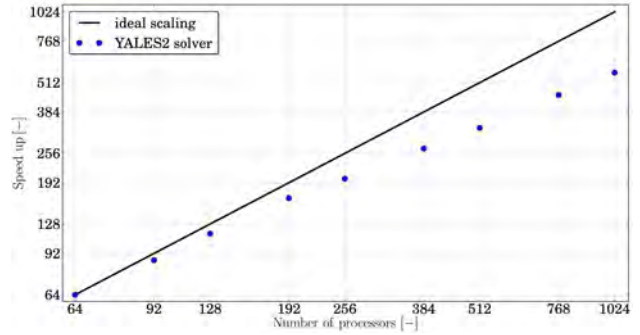


Figure 3.2 Speedup achieved by `neptune_cfd` on the Jean-Zay (IDRIS) supercomputer for a mesh with more than 8 billion cells. Adapted from [8].

of gas-solid flows with turbulence and chemical reactions using an approach that combines large-eddy simulation with the discrete element method. Figure 3.3a shows a gas volume fraction contour in a lab-scale fluidized bed containing 9.6 million particles and simulated using a mesh of 3.7 million cells. The YALES2 speedup for this simulation on the Curie (TGCC) supercomputer is illustrated in Figure 3.3b. As seen in this figure, the speedup achieved using 1024 processors is 55% of its optimal value, a reasonable outcome given the significant dispersion of particles across the processors leading to their desynchronization [5].



(a) Gas volume fraction contour.



(b) YALES2 speedup on the Curie (TGCC) supercomputer.

Figure 3.3 YALES2 simulation of a lab-scale fluidized bed containing 9.6 million particles using a mesh of 3.7 million cells. Adapted from [5].

3.4 Organization of the thesis

Each specific objective presented in the previous section represents a chapter in this thesis.

Chapter 4 delves into the macro-scale modeling of Van der Waals force, presenting two adhesive models: one based on kinetic theory and another on coordination number. These models were implemented in the `neptune_cfd` code and qualitatively validated, with the first model unable to predict a pressure overshoot due to its assumptions, while the second model successfully does so.

Chapter 5 discusses extending the coordination-number-based adhesion model to take into

account the impact of deformation history, necessitating a CFD-DEM numerical database. This chapter begins by detailing our implementation of static-dynamic friction and Van der Waals force in the massively parallel CFD-DEM code YALES2. Various data were extracted from fluidization-defluidization simulations using the CFD-DEM approach, including the bed pressure drop, bed voidage, repulsive and adhesive solid pressures, coordination number, fabric tensor, and wall shear stress.

Chapter 6 validates the static-dynamic friction and Van der Waals adhesion models through various DEM tests at micro and macro scales, including interparticle and particle-wall collision tests, as well as Janssen-effect tests. This chapter also presents a continuum transport equation for the coordination number and an assessment of its capability to predict pressure-drop hysteresis at the macroscale. A source term was computed from CFD-DEM simulations to guide the formulation of this transport equation. It is acknowledged that further refinement is needed for an accurate simulation of pressure hysteresis. Therefore, this chapter marks an initial endeavor towards predicting pressure-drop hysteresis accurately through a multi-scale approach integrating CFD-DEM and two-fluid models. Additionally, this chapter addresses a stability issue associated with gas-solid coupling and presents two potential solutions. The first solution involves adding a stability condition to restrict the time step in the case of explicit coupling, while the second achieves semi-implicit coupling through a penalization technique.

Finally, Chapter 7 provides a general discussion about the research findings, and Chapter 8 presents the conclusion drawn from this study.

CHAPTER 4 ARTICLE 1 : MACRO-SCALE NUMERICAL INVESTIGATION OF THE CONTRIBUTION OF VAN DER WAALS FORCE TO THE PRESSURE-DROP OVERSHOOT IN FINE-PARTICLE FLUIDIZED BEDS

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Published in *Powder Technology* on February 5, 2024

Abstract Interparticle Van der Waals force contributes to the overshoot in the bed pressure drop at the minimum fluidization velocity during the transition from static to fluidized bed conditions, which is a well-known phenomenon in the fluidization of fine particles. In this study, two adhesive particle pressure closures considering the effect of interparticle Van der Waals force are used in two-fluid model simulations with the intention to generate the pressure overshoot. The first adhesive pressure model developed within the context of the kinetic theory of rapid granular flows failed to produce the overshoot due to the dominance of multiple and long duration contacts in the fixed-bed flow. Another closure based on the coordination number was then proposed to represent long-lasting interparticle contacts, which gave an adhesive contribution much larger than the one of the kinetic theory model and was able to create the pressure drop overshoot.

Keywords Gas-solid fluidized beds ; Interparticle forces ; Van der Waals adhesion ; Granular media ; Two-fluid model ; Kinetic theory

4.1 Introduction

Gas-solid fluidized beds are employed in several industries, such as the polymerization of olefins, fluid catalytic cracking (FCC), coal combustion, and ore roasting [17]. Good quality solids mixing, high rates of mass and heat transfer, uniform temperature distribution, and the capability of processing a broad variety of granular materials are among the features of fluidized-bed reactors [13, 17, 18, 112, 113]. Interparticle forces, such as Van der Waals, electrostatic, liquid bridge, and solid bridge forces, may have a significant influence on fluidized bed hydrodynamics and performance [22, 42, 48, 60, 114–116].

Fine particles ranging from cohesive to aeratable are highly desirable for reactive fluidization processes due to their high surface-to-volume ratio, which results in greater reaction rates per unit volume of reactor [117]. The pressure drop overshoot at the minimum fluidization

velocity is a typically encountered phenomenon in beds of fine particles belonging to the group A of Geldart's classification [1]. A more intense overshoot and a larger hysteresis area between the fluidization and defluidization pressure-drop curves are observed upon decreasing the particle diameter towards Geldart's C group [118]. This observation is owing to the dominant role of interparticle over hydrodynamic interactions in static beds of these particles. The Van der Waals adhesive force is the dominating interaction force between fine particles in a dry ambient environment [16].

Van der Waals forces include dipole-dipole, dipole-induced dipole, and instantaneous dipole-induced dipole forces acting between atoms and molecules. The temporal average of a neutral atom's dipole moment is zero, yet at every instant there is a definite polar moment provided by the asymmetrical electron distribution around the protons that are inside the nucleus [29]. This instantaneous dipole produces an electric field, which creates a dipole moment in any adjacent neutral atom [29]. The two dipoles then interact, resulting in a force of attraction among the two atoms. The temporal average of this instantaneous dipole-induced dipole force, which is also known as the London dispersion force, is finite. Hamaker [31] obtained an expression for the Van der Waals force between macroscopic objects using the dispersion interaction potential between two atoms/molecules proposed by London [30] and an additivity hypothesis (summing up the forces over all pairs of individual atoms/molecules). The Van der Waals force between particles in contact is highly influenced by their surface roughness (i.e., asperity size) [119, 120].

Working at high temperatures and/or high pressures has an impact on the strength of Van der Waals force. The Van der Waals force increases with temperature due to greater molecular dipole pulsation and a larger particle-particle contact area induced by viscoelastic flattening [63, 120–122]. The magnitude of the Van der Waals force can rise with pressure owing to gas adsorption on the particle surfaces [13, 123, 124]. It is worth mentioning that hydrodynamic forces can increase dramatically with pressure (gas density increases with pressure), which may result in a less prominent influence of interparticle interactions on the bed hydrodynamics [13].

Stresses caused by adhesive and frictional interactions have a significant influence on the mechanical response of granular media [125]. There is, however, insufficient data on the magnitude of these stresses, which limits comprehension of the fluidization behavior reported in experimental studies. Mutsers and Rietema [126] and Tsinontides and Jackson [127] postulated that the interparticle contact adhesion and friction are responsible for the stable expansion occurring between the minimum fluidization and minimum bubbling velocities in fine-particle beds. Rietema and Piepers [128] ascribed the pressure drop overshoot at incipi-

ent fluidization to interparticle and particle-wall forces. According to these authors, the Van der Waals interaction is the source of particle-particle force. The non-sphericity can enhance the solid friction and the pressure-drop hysteresis [71, 129–131].

In the experiments carried out by Vanni et al. [71], the static wall friction effect on the pressure overshoot was only noticeable in columns with small diameters ($D = 2$ cm). The experiments of Srivastava and Sundaresan [125] also revealed a more significant overshoot in smaller columns, which they ascribed to particle-wall friction. Wang et al. [132] observed that increasing the static bed height increases the pressure overshoot intensity, which they attributed to wall friction. The effect of bed diameter and height on the significance of static wall friction (bridging) can also be seen in the vertical solid stress profiles showing the Janssen effect in silos and hoppers [133, 134].

Several researchers accounted for the Van der Waals force in the Eulerian-Lagrangian model to simulate the fluidization behavior of fine particles. Ho and Sommerfeld [34] used a criterion for agglomeration based on a critical velocity determined from an energy conservation between before and after collision that takes into account the Van der Waals force. These authors considered that when the normal relative velocity between two interacting particles is smaller than the critical velocity, agglomeration occurs. Wang et al. [35] solved a Newtonian equation of motion with a Van der Waals force term based on the Hamaker theory for each particle in a fluidized bed riser. Zhang et al. [37] investigated the cluster dynamics in circulating fluidized-bed reactors using a CFD-DEM model. Their simulations showed that when the solid volume fraction α_p is large, the Van der Waals interaction may promote the cluster formation.

On the other hand, Eulerian-Eulerian models that take into consideration the impact of interparticle Van der Waals interaction are scarce in the literature. Within the framework of the kinetic theory of granular flows, Gidaspow and Huilin [38] added a negative pressure inferred from the experimental data of radial distribution functions to the solid pressure in order to consider the effect of adhesive forces on the fluidization of FCC particles. This empirical adhesive pressure modified the kinetic theory equation of state to match the measured particle pressure. Parmentier [135] worked on incorporating the effect of Van der Waals interaction into the two-fluid model utilizing the BBGKY hierarchy. An adhesive pressure was added to the particle pressure to account for the Van der Waals attraction between particles. By comparing the magnitudes of attractive and repulsive solids pressures within a bed of Geldart A particles in the fluidized state (small attraction), Parmentier [135] concluded that the overestimation of bed expansion found in standard two-fluid model simulations is not due to neglecting the effect of the Van der Waals force. The kinetic theory based on the assumptions

of binary collision and molecular chaos may be extended from moderately dense to highly dense gas-solid flows by utilizing numerical data of discrete element simulations [136–138].

Some efforts have been made to predict the pressure-drop overshoot phenomenon observed during the fluidization of fine particles. Srivastava and Sundaresan [125] and Loezos et al. [139] utilized a one-dimensional force balance model based on Janssen’s approach in order to predict the pressure drop overshoot. This model involves determining coefficients that can combine the adhesion and friction effects together. For instance, when the particle diameter decreases, the friction coefficient of Loezos et al. [139] increases, which may be attributed to an increase in the significance of the Van der Waals adhesive interaction. Ye et al. [12] demonstrated through discrete particle simulations that the pressure overshoot is caused by particle-particle Van der Waals adhesion and particle-wall friction. Weber and Hrenya [36] conducted discrete particle simulations employing Hamaker and square-well adhesion models. Their findings reveal that the overshoot in the bed pressure drop is dominated by interparticle adhesion. The Hamaker model predicted that Van der Waals adhesive interactions with the sidewalls have a considerable impact on the pressure-drop overshoot (adhesion augments wall friction), whereas adhesive interactions with the distributor plate have minimal impact. The square-well model, on the other hand, predicted that particle-distributor plate adhesion has a considerable influence on the pressure-drop overshoot.

Interparticle adhesive forces affect both solid pressure and viscosity (normal and shear stresses) [140–142]. The influence of particle viscosity on the pressure overshoot, which is associated with a fixed arrangement of particles (zero particle velocity), is negligible. Hence, we consider only the effect of adhesion on the solid pressure. In our investigation, we take into account the short-range Van der Waals interaction between particles via an adhesive pressure gradient in the particle momentum equation within an Eulerian-Eulerian approach. We present two adhesive pressure models, one based on the kinetic theory and another based on the coordination number to represent interparticle contacts, and assess their capability of creating a pressure-drop overshoot in beds of Geldart A particles.

4.2 Prediction of overshoot in pressure drop across an aeratable-particle bed

Soleimani et al. [1] performed experimental measurements of the total bed pressure drop and bed voidage of Geldart A and Geldart B particles fluidized by air at 20 °C. The air was pre-dried by passing it through a bed of humidity adsorber. As a result, capillary forces have a negligible effect. The properties of the solids used in their study are shown in Table 4.1. The experiments were carried out in a fluidized bed of 5.25 cm in diameter and 50 cm in height. The static bed height was around 15 cm. For details about the procedure employed

to determine the experimental bed pressure drop and voidage, the reader is referred to the paper of Soleimani et al. [1].

Table 4.1 Properties of particles used in the experiments of Soleimani et al. [1].

Material	Glass beads	Glass beads
Mean particle diameter, d_p (μm)	156	67
Particle density, ρ_p (kg/m^3)	2595	2595
Sphericity	~ 1	~ 1
Geldart group	B	A
Acronym	GB-156	GB-67

The experimental bed pressure drop and voidage profiles as a function of the superficial gas velocity of the Geldart B and A glass beads determined by Soleimani et al. [1] are demonstrated in Figure 4.1. It can be seen that the increasing velocity path pressure drop curve of the Geldart B particles has no overshoot since the associated loose-fixed-bed and minimum fluidization voidages (ε_0 and ε_{mf} , respectively) are nearly equal. In contrast, a considerable pressure drop overshoot is apparent at the minimum fluidization velocity (U_{mf}) in the fluidization branch of the experiment with Geldart A particles, which is equivalent to the difference between the fixed-bed and minimum fluidization voidages.

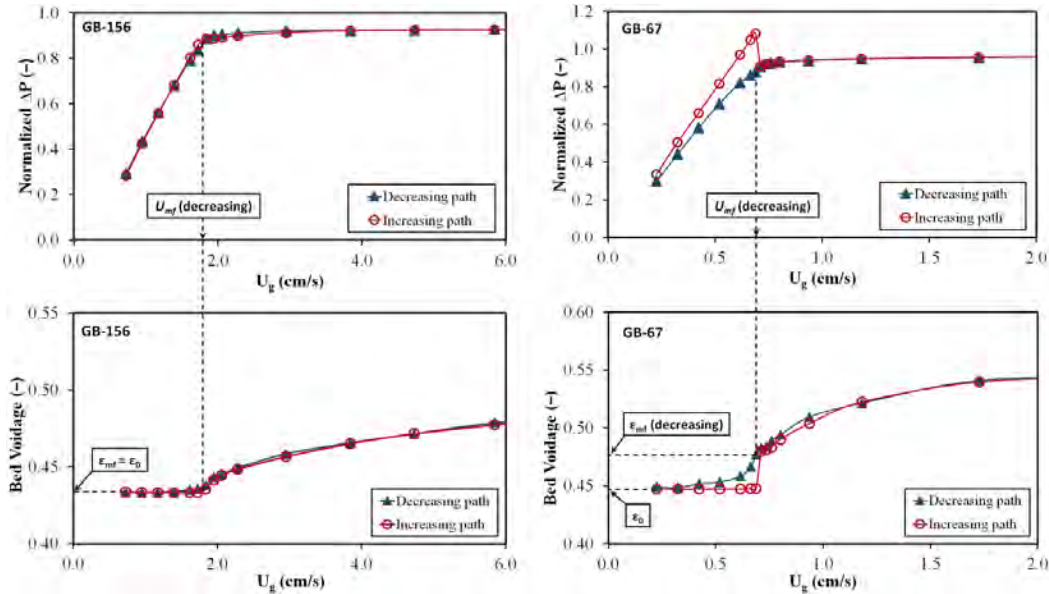


Figure 4.1 Normalized bed pressure drop and corresponding voidage profiles of Geldart B (GB-156) and A (GB-67) particles measured by Soleimani et al. [1].

In our study, we perform two-fluid simulations using the `neptune_cfd` code [6]. Transport equations and models employed in this code are reported in Ansart et al. [143]. The particle

stress in the Eulerian-Eulerian model consists of kinetic, collisional and frictional terms. The closure of the kinetic and collisional stresses is based on the kinetic theory of granular flows. In dilute flows ($\alpha_p < 1\%$), the kinetic stress is dominant, whereas in moderately dense flows ($\alpha_p > 5\%$), the collisional stress dominates. The particle friction stress is employed at high solid volume fractions to take into account the interaction of single particles with several neighbors through prolonged contact. The normal particle-particle forces are considered via the particle pressure [144]. For the particle frictional pressure, we have employed the following semi-empirical model proposed by Johnson and Jackson [97, 98]:

$$P_p^f = \begin{cases} Fr \frac{(\alpha_p - \alpha_{p,min})^n}{(\alpha_{p,max} - \alpha_p)^m} & \text{for } \alpha_p > \alpha_{p,min} \\ 0 & \text{for } \alpha_p \leq \alpha_{p,min} \end{cases} \quad (4.1)$$

where Fr , n and m are constants and $\alpha_{p,min}$ and $\alpha_{p,max}$ are respectively the threshold particle volume fraction for the activation of the frictional stress and the close-packing particle volume fraction. The values of these parameters used in our simulations are listed in Table 4.2. To account for the Van der Waals interaction among particles, a negative adhesive pressure is added to the particle pressure for all values of the particle volume fraction α_p in our work. The additional negative stress component has the effect of lowering particle repulsion. In the following sections, we propose two adhesive pressure models and investigate their ability to create a pressure drop overshoot.

4.2.1 Derivation of an adhesive pressure model based on the kinetic theory

The kinetic theory approach relies on the similarity between the random particle movement in rapid granular flow and the thermal motion of molecules in gas [91]. The adhesive pressure model derivation employing the kinetic theory of granular flows given in this subsection is based on the research of Parmentier [135]. Using the BBGKY hierarchy, the Van der Waals force can be included in the Boltzmann-Liouville equation:

$$\begin{aligned} \frac{\partial f_p}{\partial t} + \frac{\partial}{\partial x_i} (c_{p,i} f_p) + \frac{\partial}{\partial c_{p,i}} \left(\left\langle \frac{F_{p,i}}{m_p} \mid \mathbf{x}_p = \mathbf{x}, \mathbf{u}_p = \mathbf{c}_p \right\rangle f_p \right) \\ = \left(\frac{\partial f_p}{\partial t} \right)_{coll} + \left(\frac{\partial f_p}{\partial t} \right)_{ad} \end{aligned} \quad (4.2)$$

with [145]

$$\left(\frac{\partial f_p}{\partial t} \right)_{ad} = \iint \frac{\partial f_p^{(2)}}{\partial c_{p,i}} \frac{\partial}{\partial x_i} \left(\frac{V(\|\mathbf{x}^* - \mathbf{x}\|)}{m_p} \right) d\mathbf{c}_p^* d\mathbf{x}^* \quad (4.3)$$

where f_p is the one-particle probability density function defined such that $f_p(\mathbf{c}_p, \mathbf{x}, t) \delta \mathbf{c}_p \delta \mathbf{x}$ is the probable number of particles, whose center of mass, $\mathbf{x}_p$, at time t is located in the volume $[\mathbf{x}, \mathbf{x} + \delta \mathbf{x}]$ with a velocity $\mathbf{u}_p$ in $[\mathbf{c}_p, \mathbf{c}_p + \delta \mathbf{c}_p]$. $F_{p,i}$ represents the external forces acting on the particles (gravity, drag and buoyancy). $F_{p,i}/m_p = du_{p,i}/dt$ is the acceleration of a particle. $\langle F_{p,i} | \mathbf{x}_p = \mathbf{x}, \mathbf{u}_p = \mathbf{c}_p \rangle$ represents the conditional average of the external force acting on a particle at a given center position $\mathbf{x}_p = \mathbf{x}$ with the translation velocity $\mathbf{u}_p = \mathbf{c}_p$. The two terms on the right-hand side of Equation (4.2) denote the rate of change in the probability density function caused by particle-particle collision and Van der Waals adhesion, respectively. The adhesion term is given by Equation (4.3), where $f_p^{(2)}(\mathbf{c}_p, \mathbf{x}, \mathbf{c}_p^*, \mathbf{x}^*, t)$ is the two-particle probability density function and $V(\|\mathbf{x}^* - \mathbf{x}\|)$ is the interaction potential between two particles resulting in an adhesion force. According to Elimelech et al. [146], the Van der Waals interaction potential between two spheres can be expressed as follows:

$$V(\|\mathbf{x}^* - \mathbf{x}\|) = -\frac{A}{24} \left[\frac{2}{2u + u^2} + \frac{2}{(1 + u)^2} + 4 \ln \left(\frac{2u + u^2}{[1 + u]^2} \right) \right] \quad (4.4)$$

where $u = \|\mathbf{x}^* - \mathbf{x}\|/d_p - 1$ is the dimensionless distance between the two particle surfaces and A is the Hamaker constant, which relies on the composition of the particles and the interstitial fluid. The adhesive force exerted by particle p^* , with its center at $\mathbf{x}^*$, on particle p , with its center at $\mathbf{x}$, as a result of the Van der Waals potential given by Equation (4.4) can be written as:

$$\mathbf{F}_{p^* \rightarrow p}^{ad} = \frac{A}{6d_p} \frac{1}{(2u + u^2)^2} \frac{1}{(1 + u)^3} \frac{\mathbf{x}^* - \mathbf{x}}{\|\mathbf{x}^* - \mathbf{x}\|} \quad (4.5)$$

For distances between the surfaces of two particles less than a typical interatomic distance S_0 , Equations (4.4) and (4.5) are no longer applicable and the magnitude of the Van der Waals force is fixed at a maximal value in order to represent the physical particle-particle repulsion and prevent the single attraction when the surface separation distance is zero [147].

Assuming that the velocities of colliding particles are not correlated (Enskog approximation for dense flows), the two-particle probability density function is defined as follows:

$$f_p^{(2)}(\mathbf{c}_p, \mathbf{x}, \mathbf{c}_p^*, \mathbf{x}^*, t) = g(\mathbf{x}, \mathbf{x}^*) f_p(\mathbf{c}_p, \mathbf{x}, t) f_p(\mathbf{c}_p^*, \mathbf{x}^*, t) \quad (4.6)$$

with $g(\mathbf{x}, \mathbf{x}^*)$ being the two-particle radial distribution function. The adhesion term in Equation (4.3) can then be written as:

$$\left(\frac{\partial f_p}{\partial t} \right)_{ad} = -\frac{\partial}{\partial c_{p,i}} \left(\frac{F_{a,i}}{m_p} f_p \right) - \frac{\partial}{\partial c_{p,i}} \left(\frac{F_{b,i}}{m_p} f_p \right) \quad (4.7)$$

with

$$F_{a,i} = -\frac{\partial}{\partial x_i} \int n_p(\mathbf{x}^*) g(\mathbf{x}, \mathbf{x}^*) V(\|\mathbf{x}^* - \mathbf{x}\|) d\mathbf{x}^* \quad (4.8)$$

$$F_{b,i} = \int n_p(\mathbf{x}^*) \frac{\partial g(\mathbf{x}, \mathbf{x}^*)}{\partial x_i} V(\|\mathbf{x}^* - \mathbf{x}\|) d\mathbf{x}^* \quad (4.9)$$

where n_p is the particle number density. $F_{a,i}$ and $F_{b,i}$ can be approximated as follows:

$$F_{a,i} \approx -\frac{\partial}{\partial x_i} n_p(\mathbf{x}) g_0(\mathbf{x}) \int V(\|\mathbf{x}^* - \mathbf{x}\|) d\mathbf{x}^* \quad (4.10)$$

$$F_{b,i} \approx 0 \quad (4.11)$$

where g_0 is the radial distribution function at contact. A momentum balance equation for the solid phase containing a gradient of adhesive particle pressure can then be derived from the Boltzmann-Liouville equation (Equation (4.2)):

$$\begin{aligned} \alpha_p \rho_p \frac{\partial U_{p,i}}{\partial t} + \alpha_p \rho_p U_{p,j} \frac{\partial U_{p,i}}{\partial x_j} = & -\alpha_p \frac{\partial P_g}{\partial x_i} + \alpha_p \rho_p g_i + I_{g \rightarrow p,i} \\ & - \frac{\partial}{\partial x_j} (\alpha_p \rho_p R_{p,ij} + \Theta_{p,ij}) - \alpha_p \frac{\partial P_{ad}}{\partial x_i} \end{aligned} \quad (4.12)$$

where $I_{g \rightarrow p,i}$ is the mean interphase gas-to-particle momentum transfer and $R_{p,ij}$ and $\Theta_{p,ij}$ are respectively the particle kinetic and collisional stress tensors. Equation (4.12) is derived by substituting (4.7) in (4.2) and then multiplying (4.2) by $m_p \mathbf{c}_p$ and integrating over all velocities $\mathbf{c}_p$. In Equation (4.12), $-\alpha_p \partial P_{ad} / \partial x_i$ is equal to $n_p F_{a,i}$, where $F_{a,i}$ is expressed by Equation (4.10). P_{ad} represents an adhesive pressure resulting from the attraction between particles, which is given by:

$$P_{ad} \approx \frac{n_p g_0}{\pi d_p^3 / 6} \int V(\|\mathbf{x}^* - \mathbf{x}\|) d\mathbf{x}^* \quad (4.13)$$

In the case of Van der Waals interaction potential, P_{ad} may be written as:

$$P_{ad} \approx \frac{n_p g_0}{\pi d_p^3 / 6} \int_{\|\mathbf{x}^* - \mathbf{x}\| > d_p + S_0} V(\|\mathbf{x}^* - \mathbf{x}\|) d\mathbf{x}^* \quad (4.14)$$

And according to Parmentier [135]:

$$P_{ad} \approx -A n_p g_0 \ln \left(\frac{d_p}{S_0} \right) \quad (4.15)$$

The adhesion term in the momentum equation (Equation (4.12)) is written as:

$$-\alpha_p \frac{\partial P_{ad}}{\partial x_i} = -\frac{\partial P_p^a}{\partial x_i} \quad (4.16)$$

with

$$P_p^a \approx -A \frac{n_p}{\alpha_p} \ln \left(\frac{d_p}{S_0} \right) \int_0^{\alpha_p} \alpha_p \left(g_0 + \alpha_p \frac{\partial g_0}{\partial \alpha_p} \right) d\alpha_p \quad (4.17)$$

The radial distribution function, g_0 , which may be viewed as a measure for the likelihood of particle-particle collision, is given as the following expression [95]:

$$g_0 = \left(1 - \frac{\alpha_p}{\alpha_{p,max}} \right)^{-2.5\alpha_{p,max}} \quad (4.18)$$

Using Equation (4.17), the negative adhesive pressure can then be formulated as:

$$P_p^a = -\frac{B}{d_p^3} 2\alpha_{p,max}^2 \left[\frac{25}{6} + \left(-\frac{3}{2} \frac{\alpha_p^2}{\alpha_{p,max}^2} + \frac{20}{3} \frac{\alpha_p}{\alpha_{p,max}} - \frac{25}{6} \right) g_0 \right] \quad (4.19)$$

with

$$B = A \frac{3}{\pi} \ln \left(\frac{d_p}{S_0} \right) \quad (4.20)$$

where d_p is the particle diameter, α_p is the solid volume fraction, A is the Hamaker constant, and S_0 is a minimum cutoff separation distance between two particle surfaces. The adhesive pressure P_p^a given by Equation (4.19) is added to the kinetic, collisional, and frictional pressures.

4.2.2 Evaluation of the kinetic-theory-based adhesion model

The adhesive pressure model presented in Equation (4.19) is tested by adding it to the solids pressure and performing two-fluid model simulations similar to CFD-DEM simulations carried out by Hou et al. [148]. The values of the parameters used in our quasi-two-dimensional fluidized bed simulations of Geldart A particles are summarized in Table 4.2. The value of the initial solid volume fraction ($\alpha_{p,ini} = 0.6$) is chosen to be the same as that obtained from the CFD-DEM simulations of Hou et al. [148] for the fixed bed. The bottom face of the cuboid bed employed in our simulations acts as an inlet for gas and a wall with a no-slip condition for particles. The top face serves as a free outlet for both gas and solid phases with an imposed gauge pressure of zero. The left and right faces (normal to the x-axis) are walls for both phases with a no-slip condition for each phase. A symmetry boundary condition is employed for both phases at the front and back faces (normal to the y-axis).

The no-slip particle-wall boundary condition enforces zero tangential particle velocity at the wall. This boundary condition provides reliable results in the dense regime that align well with positron emission particle tracking (PEPT) data and CFD-DEM simulations [76]. Particle-wall adhesion was not considered in our two-fluid simulations. The dynamic boundary condition proposed by Dupuy et al. [76] can be extended to include particle-wall adhesion by adding the adhesion pressure to the frictional, kinetic, and collisional pressures in the Coulomb model.

Table 4.2 Simulation parameters.

Parameter	Value
Particle diameter, d_p	100 μm
Particle density, ρ_p	1440 kg/m ³
Particle-particle normal restitution coefficient, e_c	0.8
Gas density, ρ_g	1.205 kg/m ³
Gas viscosity, μ_g	1.8×10^{-5} Pa.s
Cuboid bed size, $L_x \times L_y \times L_z$	$60d_p \times 4d_p \times 200d_p$
Cell size, $\Delta x = \Delta y = \Delta z$	$2d_p$
Initial particle bed height, H_{ini}	$36d_p$
Initial particle volume fraction, $\alpha_{p,ini}$	0.6
Frictional pressure constant (Equation (4.1)), Fr	0.05 Pa
Frictional pressure constant (Equation (4.1)), n	2
Frictional pressure constant (Equation (4.1)), m	5
Threshold solid volume fraction for friction, $\alpha_{p,min}$	0.58
Close-packing solid volume fraction, $\alpha_{p,max}$	0.64
Minimum surface separation distance, S_0	1 nm
Base value of the Hamaker constant, A	2.1×10^{-21} J
Maximum Courant number, CFL_{max}	0.1

The equations for the kinetic, collisional and frictional solids stress closures employed in our simulations can be found in Ansart et al. [143]. The frictional viscosity is omitted from each simulation with adhesion (only the frictional pressure is included) since it turns negative in the region where adhesion effect is dominant over friction effect. The drag model used is that proposed by Gobin et al. [81], which is the drag correlation of Wen and Yu [149] limited by the Ergun [14] equation for dense regimes. The gas flow is assumed to be laminar (no turbulence model is used). The agitation model used for the solid phase is $q_p^2 - q_{gp}$, which includes transport equations for the particle fluctuant kinetic energy, q_p^2 , and the gas-particle velocity covariance, q_{gp} [90,91,96,150]. However, since the gas flow is assumed to be laminar, the gas fluctuating velocity $u''_{g,i}$ is zero; hence $q_{gp} = \langle u''_{g,i} u''_{p,i} \rangle_p$ equals zero.

Two sidewall pressure monitoring points at zero and $195d_p$ above the inlet were utilized to

measure the overall bed pressure drop at each superficial gas velocity in fluidization and defluidization cycles. Each superficial gas velocity was sustained for 5 s, and the pressure was averaged over the last 2 s of each of these 5 s intervals to determine the time-averaged bed pressure drop values:

$$\overline{\Delta P} = \overline{P_1} - \overline{P_2} = \frac{1}{\sum_{k=1}^{N_r} \Delta t_k} \left(\sum_{k=1}^{N_r} \Delta t_k P_{1,k} - \sum_{k=1}^{N_r} \Delta t_k P_{2,k} \right) \quad (4.21)$$

where P_1 and P_2 are the pressures at the monitoring points, Δt is the time step, and N_r is the total number of time steps in the 2 s interval. The normalized bed pressure drop is defined as the ratio of the pressure drop across the whole bed to the pressure drop equivalent to the weight of the particles, $\overline{\Delta P}/\Delta P_{eq}$. The pressure drop ΔP_{eq} can be expressed as:

$$\Delta P_{eq} = m_b g / S_b = \alpha_p \rho_p H_b g \quad (4.22)$$

where m_b is the mass of the particles bed, g is the gravitational acceleration, S_b is the cross-sectional area of the bed, and H_b is the bed height. Substituting 0.6 for α_p and $36d_p$ for H_b (see Table 4.2) in Equation (4.22) gives ΔP_{eq} equals 30.513 Pa. The spatial average of the solid volume fraction α_p is computed as follows:

$$\langle \alpha_p \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} \alpha_{p_i} \quad (4.23)$$

where N_c is the number of cells between the inlet and $34d_p$ above the inlet, which is slightly less than the bed height at the lowest superficial gas velocity. The time average of the spatially averaged α_p is determined as:

$$\overline{\langle \alpha_p \rangle} = \frac{\sum_{k=1}^{N_r} \Delta t_k \langle \alpha_p \rangle_k}{\sum_{k=1}^{N_r} \Delta t_k} \quad (4.24)$$

Then, the bed voidage is obtained as: $\overline{\langle \alpha_g \rangle} = 1 - \overline{\langle \alpha_p \rangle}$.

Bed pressure drop and voidage versus superficial gas velocity curves for fluidization and defluidization cycles with different B values (Equation (4.19)) are shown in Figure 4.2. The value of B obtained by substituting the values of A , d_p and S_0 (given in Table 4.2) in Equation (4.20) is 2.3×10^{-20} J. In addition to this value, we tested much higher B values in order to demonstrate that the adhesion provided by the kinetic theory model is several orders

of magnitude smaller than that given by the coordination number model presented later in section 4.2.3. As depicted in Figure 4.2, generating a pressure drop overshoot requires multiplying B by 10^6 (using $B = 2.3 \times 10^{-14}$ J) and no hysteretic behavior is predicted between the increasing and decreasing velocity path curves. The bed voidage curves displayed in Figure 4.2 show a decrease in the average gas volume fraction in the bed for $B = 2.3 \times 10^{-14}$ J due to the relatively strong adhesion.

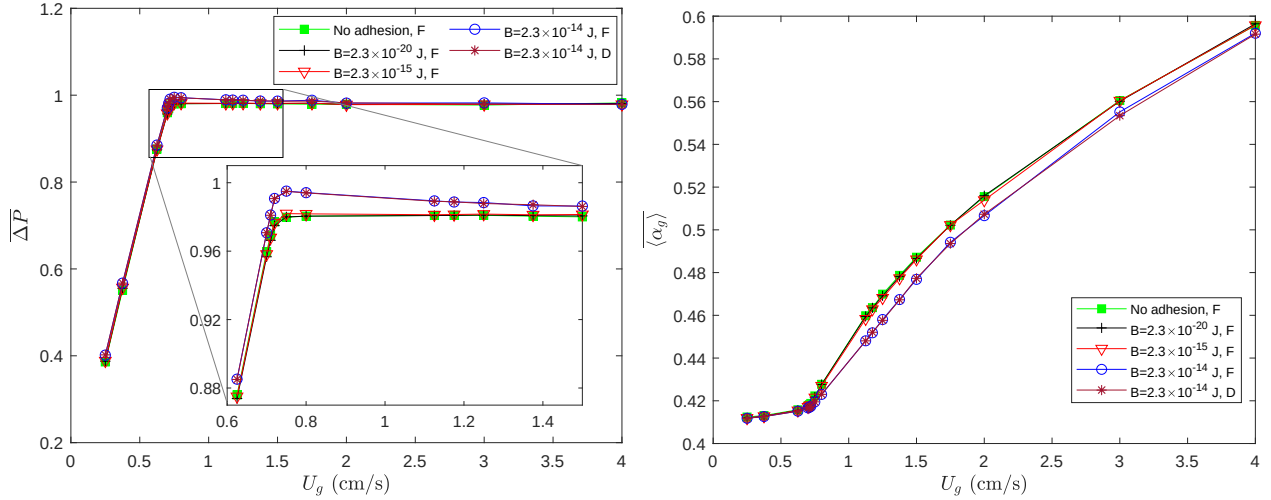


Figure 4.2 Normalized time-averaged overall bed pressure drop and time-spatial averaged gas volume fraction in the bed during fluidization and defluidization cycles with different B values in the adhesion pressure (Equation (4.19)). F represents a fluidization branch and D a defluidization branch in this and Figure 4.4. [9].

Based on the foregoing results, the adhesive contribution introduced by the kinetic theory model is insufficient to generate an overshoot in the bed pressure drop. This inability might be attributed to the binary and instantaneous collisions assumption used in the kinetic theory approach because fixed-bed flows are dominated by the influence of multiple and sustained contacts. The pressure-drop hysteresis between the fluidization and defluidization branches is not produced because the impact of deformation history is not taken into account in the kinetic theory adhesion model. In particular, the adhesive pressure is only a function of the particle volume fraction α_p , indicating that it is a symmetric closure. In the next section, we present a coordination-number-based approach suitable for quasi-static flow regimes.

4.2.3 Derivation of an adhesive pressure based on the coordination number

Here, we derive an adhesive pressure model by assuming that the dominant Van der Waals interaction occurs between particles in long-lasting contact characterized by the coordination number. The coordination number is defined as the mean number of particles in contact with

a given particle, which may be written as:

$$CN = 2 \frac{n_c}{n_p} \quad (4.25)$$

where n_c denotes the mean number of contacts per unit volume and n_p denotes the number of particles per unit volume. The factor 2 enters in Equation (4.25) because each contact is shared by two particles. The particle-particle stress tensor component due to the adhesive force may be computed as [151–153]:

$$\sigma_{ij}^{ad} = -\frac{1}{V} \sum_{c \in V} f_i^c b_j^c \quad (4.26)$$

where the sum is over all the contact points c in volume V . f_i^c represents the interaction force between two particles in contact at c and b_j^c represents the vector connecting the centers of these two particles if both centers are inside the volume V , or only the part in V if one of the centers is outside V . By using Equation (4.5), the adhesive contact force can be expressed as follows:

$$\mathbf{F}_{p^* \rightarrow p}^c = \frac{A}{6d_p} \frac{1}{(2u_0 + u_0^2)^2} \frac{1}{(1 + u_0)^3} \mathbf{k}^* \approx \frac{A}{6d_p} \frac{1}{4u_0^2} \mathbf{k}^* \quad (4.27)$$

where $u_0 = S_0/d_p$ is the minimum dimensionless separation distance between two particle surfaces and $\mathbf{k}^* = (\mathbf{x}^* - \mathbf{x}) / \|\mathbf{x}^* - \mathbf{x}\|$ is the unit vector along the line of centers of two interacting particles. Substituting Equation (4.27) into Equation (4.26) gives the following adhesive stress expression for homogeneous systems:

$$\sigma_{ij}^{ad} = \frac{1}{V} \sum_{c \in V} \frac{A}{24u_0^2} k_i^* k_j^* \quad (4.28)$$

The isotropic component of the adhesive stress given by Equation (4.28) is the adhesive pressure:

$$P_p^a = -\frac{\sigma_{ii}^{ad}}{3} = -\frac{n_c}{3} \frac{Ad_p^2}{24S_0^2} \quad (4.29)$$

Then, using Equations (4.29) and (4.25), the adhesive particle pressure can be expressed as:

$$P_p^a = -\frac{\alpha_p}{\pi d_p^2} CN \frac{Ad_p}{24S_0^2} \quad (4.30)$$

where CN is the coordination number.

4.2.4 Evaluation of the coordination-number-based adhesion model

Eulerian-Eulerian simulations were carried out using the parameter values in Table 4.2 to check the ability of the adhesive pressure model given by Equation (4.30) to create the pressure drop overshoot. These simulations are the same as those described in section 4.2.2, except that the coordination-number-based adhesive pressure model is utilized instead of the kinetic-theory-based one. In our tests, we used a constant coordination number of 4.77 corresponding to a fixed bed state and correlations between the coordination number and the solid volume fraction based on the CFD-DEM simulation results of Hou et al. [148]:

$$CN = 2 + 3.25\alpha_p^{0.4} \quad \text{for expanded beds} \quad (4.31)$$

$$CN = 4.87 \times 10^{-5} \frac{1 - (1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{11.6}} \quad \text{for fluidized beds} \quad (4.32)$$

These correlations were developed using simulations that account for the Van der Waals adhesion between particles. Figure 4.3 shows CN plotted as a function of α_p for expanded and fluidized bed states using Equations (4.31) and (4.32). In the expanded bed state, as the solid volume fraction decreases from the close-packing value (0.64) to zero, the coordination number slowly decreases until it reaches a minimum value of 2 corresponding to a chain-like structure, as demonstrated in Figure 4.3. On the other hand, the coordination number corresponding to the fluidized bed state decreases rapidly towards zero when the solid volume fraction decreases, as seen in Figure 4.3. The obtained bed pressure drop and mean gas

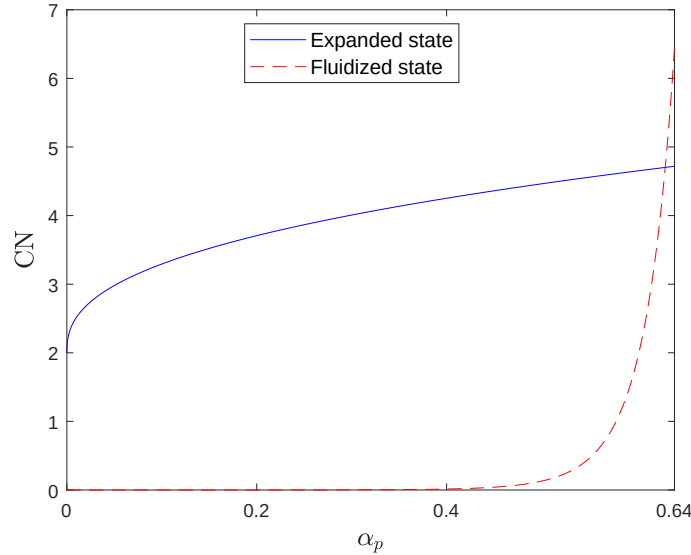


Figure 4.3 CN as a function of α_p for expanded and fluidized bed states.

volume fraction profiles are illustrated in Figure 4.4. As we can observe in the pressure drop versus superficial gas velocity plots, the constant fixed-bed coordination number and the expanded-bed correlation both generate overshoot, while the fluidized-bed correlation does not. Based on these results, we can infer that the coordination-number-based model provides an adhesive contribution large enough to produce an overshoot in the bed pressure drop.

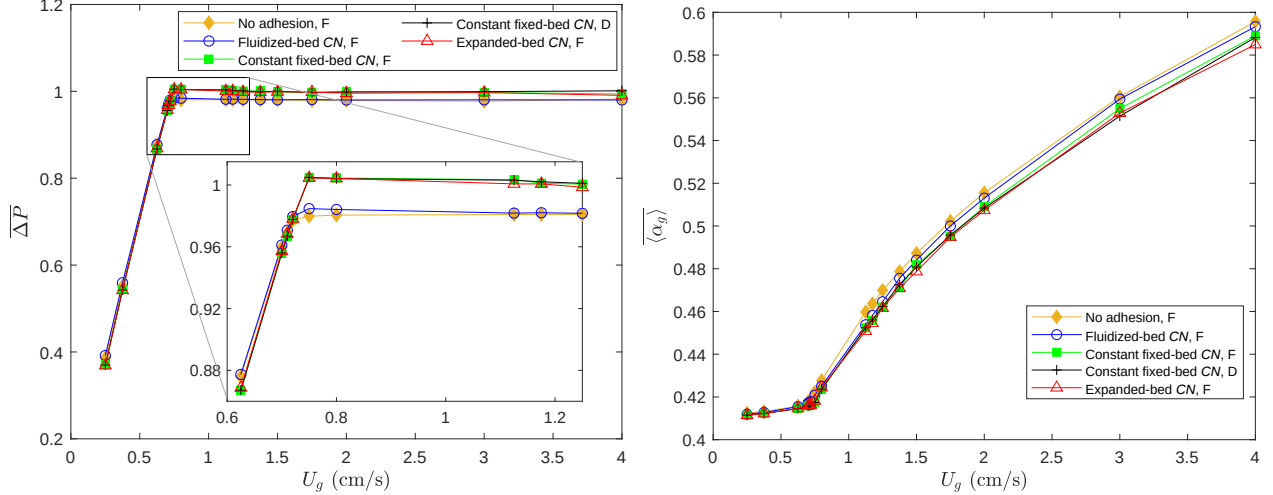


Figure 4.4 Normalized time-averaged overall bed pressure drop and time-spatial averaged gas volume fraction in the bed during fluidization and defluidization cycles without and with adhesion using the coordination-number-based model. [9].

The experimental bed voidage curves of Geldart A particles in Figure 4.1 demonstrate that at superficial gas velocities less than the minimum fluidization velocity U_{mf} , the bed voidage remains constant at ε_0 in the increasing velocity path. When the superficial gas velocity reaches U_{mf} , the forces exerted by the gas on the particles overcome the interparticle forces, particle-wall friction, and particles' weight, leading to the destruction of the contact network and an abrupt jump in the bed voidage from ε_0 to ε_{mf} . In contrast, in the decreasing velocity path, the bed voidage progressively decreases from ε_{mf} to ε_0 as the superficial gas velocity decreases from U_{mf} to zero. The simulation results in Figure 4.4 show a decrease in bed voidage owing to adhesion, but the hysteretic behavior between the fluidization and defluidization cycle curves observed experimentally is not predicted. To obtain this behavior, the role of Van der Waals interparticle force and particle-wall static friction should be dominant over that of hydrodynamic forces in the fixed bed state. Achieving this condition is influenced by the values of the various simulation model parameters. For example, the particle diameter in the experiments of Soleimani et al. [1] is $67 \mu\text{m}$, which is smaller than the particle diameter in our simulations ($100 \mu\text{m}$). In addition, the contact network formation and destruction (the coordination number evolution) should be taken into consideration in our two-fluid simulations to generate the hysteresis. Moreover, the effect of boundary condi-

tions (particle-wall friction) and dimensionality (quasi-2D to 3D) on the pressure overshoot should be explored. Considering the effect of static particle-wall friction on the pressure-drop overshoot in the two-fluid model could be the subject of future research. Accounting for this effect is essential to achieve a quantitative prediction because static wall friction may increase the overshoot intensity. However, the significance of this impact depends on the column diameter [71]. Regarding the effect of particle size, our simulations using the coordination-number-based model demonstrated that the diminution of the particle diameter notably increases the pressure overshoot intensity (data presented in Appendix D), which is consistent with experimental observations [118].

The number of interparticle contacts, and hence the radial distribution function, is influenced by adhesion. This could be investigated through DEM simulations. In the fixed-bed state, the dominant effect is for the frictional pressure and not the collisional pressure. Therefore, modifying the radial distribution function to consider the influence of adhesion may have a negligible effect on the overshoot obtained using the coordination number model. The kinetic theory adhesion model gives an adhesive contribution 6 orders of magnitude smaller than that of the coordination number model. This is because the kinetic theory assumptions, including the assumption that the radial distribution function is not modified by adhesion, are not valid.

4.3 Conclusion

In this research, two-fluid model simulations were performed with the aim of predicting the pressure-drop overshoot observed during fluidization of Geldart A particles. Two adhesive pressure models were suggested to account for the Van der Waals force among particles. The first model, which is based on the kinetic theory, gives an adhesion effect that is not strong enough to create the pressure drop overshoot. This model may be suitable for rapid granular flows, but it is not appropriate for quasi-static flows because it does not account for the long term and multiple particle-particle contacts. The second model, which is expressed in terms of the mean number of contacts per particle, makes use of CFD-DEM correlations that relate the coordination number to the solid volume fraction for various flow conditions. This model gives an adhesive contribution far larger than the one of the kinetic theory model and produces the overshoot in the bed pressure drop. The success of the aforementioned model appears to be attributable to the fact that it accounts for the multiple and sustained contacts. The hysteresis between the fluidization and defluidization branches was not predicted by any of the two adhesive pressure models.

A meso-scale numerical investigation is required to guide postulating a continuum evolution

equation for the coordination number or developing an Eulerian adhesive stress closure that accounts for the effect of deformation history and the transition between the different flow regimes (fixed, expanded and fluidized bed states) in order to predict the hysteresis in the bed pressure drop at the macro-scale.

Some researchers have previously claimed that the standard two-fluid model, which does not account for adhesion between particles, can correctly predict the fluidization behavior of Geldart A particles if a sufficiently high resolution is used. For example, Wang et al. [154] demonstrated that fluidized bed expansion can be accurately predicted (compared to discrete particle simulations) when the cell size is of the order of three particle diameters and the time step is small. However, they only studied the bed expansion at superficial gas velocities well above the minimum fluidization velocity, at which the coordination number and hence the adhesive contribution may be negligible. Our two-fluid simulations employ a small time step and a cell size of two times the particle diameter, which complies with the recommendation of Wang et al. [154]. The results of these simulations reveal that no overshoot is generated during the transition from fixed to fluidized bed without considering the effects of adhesion. Therefore, interparticle attractive forces may have a significant contribution to the hydrodynamic behavior observed in fluidized-bed experiments. Taking these adhesive interactions into account is critical for gaining a comprehensive understanding of the fluidization behavior of particles belonging to Geldart group A.

4.4 Acknowledgments

This project was provided with computing and storage resources by GENCI on the CSL/SKL partition of the Jean-Zay/Joliot-Curie supercomputer at IDRIS/TGCC thanks to grant A0142B06938, and by CALMIP through grant P1132. `neptune_cfd` is a multiphase CFD code developed in the framework of the NEPTUNE project, financially supported by EDF, CEA (Commissariat à l'Énergie Atomique), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and Framatome.

CHAPTER 5 ARTICLE 2 : MESO-SCALE NUMERICAL ANALYSIS OF THE ROLE OF VAN DER WAALS ADHESION AND STATIC FRICTION IN FLUIDIZED BEDS OF FINE SOLIDS

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Submitted to *Powder Technology* on September 25, 2024

Abstract This article explores the effect of Van der Waals force and static friction on the fluidization of fine solids using CFD-DEM simulations. The results show that both Van der Waals adhesion and static friction contribute to the pressure-drop hysteresis phenomenon. These results also demonstrate that to predict the homogeneous expansion of the bed across the range of velocities from the minimum required for fluidization to the minimum for bubbling, it is necessary to take into account the Van der Waals adhesion. The generated CFD-DEM dataset can guide the development of solid stress closures for two-fluid models to incorporate the effects of Van der Waals adhesion and static friction on fluidization hydrodynamics, allowing for the prediction of hysteresis in bed pressure drop at the macro-scale.

Keywords Gas–solid fluidized beds ; Van der Waals adhesion ; Static-dynamic friction ; Pressure-drop hysteresis ; Homogeneous fluidization ; CFD-DEM

5.1 Introduction

Fluidized and packed (fixed or moving) beds are used in several industrial processes and applications, including the chemical, pharmaceutical, food, and mining industries [17, 155–158]. Both fixed and fluidized beds have their own advantages and disadvantages [17, 112, 113]. Studying the hydrodynamics of these beds and developing numerical models able to predict the different transport phenomena occurring inside them can play a key role in their optimization and scale-up.

Several authors studied the role of friction and Van der Waals adhesion in fluidized beds. Dupuy et al. [99] showed through numerical simulations that friction hinders the dense packing of particles and plays a role in determining the minimum fluidization velocity. Zhang et al. [37] demonstrated, through Eulerian-Lagrangian simulations, that Van der Waals adhesion can lead to the aggregation of particles. Mutsers and Rietema [126] and Tsinontides and Jackson [127] hypothesized that the homogeneous fluidization observed in experiments with fine particles is caused by the adhesion and friction between these particles in contact.

Rietema and Piepers [128] attributed the overshoot in the pressure drop across a bed of fine solids to particle-particle Van der Waals adhesion, as well as frictional interactions between the particles and the wall. Srivastava and Sundaresan [125] linked the larger overshoot they observed in smaller columns to particle-wall frictional interactions.

The CFD-DEM (Computational Fluid Dynamics - Discrete Element Method) approach may be used to investigate fluid-solid flows in lab-scale fluidized beds containing typically the order of 10^6 particles [5, 77], whereas the two-fluid approach can be employed to simulate industrial-scale fluidized beds [6]. A main advantage of the CFD-DEM approach over the two-fluid model is its ability to account for multiple and long-duration particle contacts. The assumption of binary and instantaneous collisions and the lack of proper solid stress closures render the two-fluid model incapable of predicting several phenomena that occur in dense granular media, such as the Janssen effect in silos [134] and the pressure-drop hysteresis in fine-particle fluidized beds [1, 36, 118]. Numerical data from CFD-DEM simulations may be employed to develop particle stress closures for the two-fluid model, allowing it to handle very dense fluid-solid flows with increased accuracy.

Several researchers used mesoscopic simulation data from DEM or CFD-DEM to compute macroscopic quantities and develop continuum models. Dupuy et al. [76] developed a continuum model for the particle-wall contact shear stress through analysis of CFD-DEM simulations. Rothenburg and Krut [159] carried out and analyzed various DEM simulations of 2D granular arrangements of disks undergoing biaxial compression. Based on their analysis, they postulated a transport equation for the coordination number, which contains empirical parameters that indicate probabilities of contact formation and destruction. They found that the theoretical solution of this transport equation is in good agreement with the DEM simulation data. According to their investigation, variations in solid fraction cannot be described only in terms of coordination number but also in terms of anisotropy in contact orientations. Sun and Sundaresan [160] used DEM simulations as a basis to develop closures for the solid pressure and the macroscopic friction coefficient in simple shear flows. These authors proposed continuum transport equations for the coordination number and the fabric tensor, which are included in the aforementioned closures. The material parameters in their constitutive model were calibrated to produce the desired response given by the DEM data. Chialvo et al. [137] studied simple shear flows of noncohesive particles through DEM simulations. They investigated three different flow regimes: inertial (dilute), intermediate, and quasistatic, as well as the transitions between them. For each flow regime, they found an asymptotic power-law relation between the particle pressure and the shear rate scaled by powers of the distance to the jamming point (separating the inertial and quasistatic regimes). This jamming point is affected by particle-particle friction. They also proposed a function

that combines the previously mentioned asymptotic relationships, resulting in a continuous evolution of the solid pressure as a function of shear rate for the limits of the three flow regimes and the transitions between them. Luding [153] obtained macroscopic data such as bulk moduli, friction angle, and cohesion from DEM simulations of non-cohesive and cohesive particles subjected to a shear deformation. In his study, the macroscopic stress, stiffness, and fabric tensors were calculated. Gu et al. [141] modified the solid pressure and viscosity closures that are based on the kinetic theory to take adhesion into consideration. These modifications were guided by the results obtained from their CFD-DEM simulations. These researchers observed larger aggregates in a test with adhesion compared to a test without adhesion. Hou et al. [148] performed CFD-DEM simulations of fluidized beds with Geldart B and A particles accounting for the Van der Waals adhesion. Based on their mesoscopic data, they proposed correlations for the static, expanded, and fluidized bed states, which describe how the average number of contacts per particle varies with the particle volume fraction (macroscopic quantities). Vijayan et al. [161] used DEM to study the variation in the coordination number and contact anisotropy (fabric) for a 3D particle arrangement under uniaxial compression. They noticed a hysteresis between loading and unloading coordination number-strain curves. These authors defined three different flow regimes (quasi-static, dense, and collisional dilute) according to the value of the inertial number, which is expressed as a function of the compression strain rate and solid compressive pressure. They proposed a semi-empirical model that relates the contact anisotropy to the macroscopic stress.

Overall, Van der Waals and frictional interactions have a substantial effect on fluidization behavior. However, these interactions are not adequately modeled at the macroscale. Coupling mesoscopic and macroscopic scales is an effective strategy to address this issue. In this paper, we extract mesoscopic data from CFD-DEM simulations to guide the development of Eulerian solid stress closures for Van der Waals adhesion and friction. We implemented static-dynamic friction and Van der Waals adhesion models in the CFD-DEM code YALES2 [5]. Then, we used this code to perform Eulerian-Lagrangian simulations of fluidization and defluidization for Geldart A particles. From these simulations, we obtained information about the fluidization hydrodynamics and the structural and solid stress changes within the particle bed in the presence or absence of Van der Waals adhesion force. We show that both static friction and Van der Waals adhesion contribute to the pressure overshoot and that the homogeneous fluidization regime is only predicted when adhesion is present. Finally, we measure the source term in the coordination number transport equation. This source term is shown to be influenced by both the superficial gas velocity and Van der Waals adhesion force.

The paper is organised as follows: Section 5.2 briefly describes the modeling approach used

in this research and explains the implementation of static-dynamic friction and Van der Waals adhesion in DEM, Section 5.3 presents the fluidization and defluidization CFD-DEM simulations conducted in this study and discusses the results obtained, and Section 5.4 covers the calculation of the source term of the Eulerian transport equation for the coordination number from CFD-DEM simulations.

5.2 Numerical model

A computational framework has been developed by integrating the DEM for particle phase representation and the LES (Large-Eddy Simulation) method for gas phase representation within the YALES2 code [5]. This computational tool uses the finite volume method and is designed to solve the filtered Navier-Stokes equations at low Mach numbers for flows with turbulence and chemical reactions. The LES equations for the gas phase can be found in Dufresne et al. [5]. These equations account for the local volume fraction of the gas, which is computed using the particle centroid method [162].

The motion of a spherical particle p , encompassing both translational and rotational aspects, can be determined through the application of Newton's second law [5]:

$$d_t(\mathbf{x}_p) = \mathbf{u}_p, \quad (5.1)$$

$$m_p d_t(\mathbf{u}_p) = \mathbf{F}_p^e + \mathbf{F}_p^c, \quad (5.2)$$

$$I_p d_t(\boldsymbol{\omega}_p) = \mathbf{M}_p^d + \mathbf{M}_p^c + \mathbf{M}_p^r. \quad (5.3)$$

The variables I_p , m_p , $\mathbf{x}_p$, $\boldsymbol{\omega}_p$, and $\mathbf{u}_p$ denote respectively the moment of inertia, mass, position, angular velocity, and translation velocity of particle p . $\mathbf{F}_p^e$, $\mathbf{F}_p^c$, $\mathbf{M}_p^d$, $\mathbf{M}_p^c$, and $\mathbf{M}_p^r$ are respectively the overall external force acting upon particle p , the total contact force (due to inter-particle and particle-wall contacts), the torque of gas drag force, the torque of $\mathbf{F}_p^c$, and the torque due to rolling friction. The overall external force $\mathbf{F}_p^e$ encompasses the force of gravity $\mathbf{F}_p^g$ and the forces acting upon the solid by the gas, specifically the buoyancy force $\mathbf{F}_p^b$ and the drag force $\mathbf{F}_p^d$:

$$\mathbf{F}_p^e = \mathbf{F}_p^d + \mathbf{F}_p^b + \mathbf{F}_p^g. \quad (5.4)$$

Details about the modeling of the external force and the torques in Equations (5.2) and (5.3) can be found in the study by Nigmatova et al. [163] and in the thesis by Dufresne [78]. The contact forces are described in detail hereafter.

The Coulomb dynamic friction model relates the tangential and normal contact forces exerted

by particle q on particle p as follows:

$$\mathbf{f}_{q \rightarrow p, t}^c = -\mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\| \mathbf{t}_{pq}, \quad (5.5)$$

where μ_d is the dynamic (sliding) friction coefficient, $\mathbf{f}_{q \rightarrow p, n}^c$ is the normal contact force represented using a spring-dashpot system, and $\mathbf{t}_{pq}$ is the tangential unit vector defined as:

$$\mathbf{t}_{pq} = \begin{cases} \frac{\mathbf{u}_{pq, t}}{\|\mathbf{u}_{pq, t}\|}, & \text{if } \|\mathbf{u}_{pq, t}\| > 0, \\ 0, & \text{otherwise.} \end{cases} \quad (5.6)$$

In Equation (5.6), the instantaneous tangential relative velocity $\mathbf{u}_{pq, t}$ is defined as follows:

$$\mathbf{u}_{pq, t} = \mathbf{u}_{pq} - \mathbf{u}_{pq, n}, \quad (5.7)$$

where $\mathbf{u}_{pq} = \mathbf{u}_p - \mathbf{u}_q$ is the relative velocity, and $\mathbf{u}_{pq, n} = (\mathbf{u}_{pq} \cdot \mathbf{n}_{pq}) \mathbf{n}_{pq}$ is the normal component of the relative velocity. $\mathbf{n}_{pq}$ is the normal unit vector given by $\mathbf{n}_{pq} = (\mathbf{x}_q - \mathbf{x}_p) / \|\mathbf{x}_q - \mathbf{x}_p\|$, with $\mathbf{x}$ being the position vector of the particle center. When $\mathbf{u}_{pq, t}$ is zero, $\mathbf{t}_{pq}$ equals zero, and hence the tangential contact force $\mathbf{f}_{q \rightarrow p, t}^c$ is zero (Equation (5.5)). This indicates that the contact cannot support any tangential load when the particles are stationary. Thus, the dynamic friction model given by Equation (5.5), which is valid for rapid granular flows, is not suitable for fixed beds. To overcome this limitation, a model that accounts for both static and dynamic frictions was implemented in the massively parallel YALES2 code, as described in the next subsection.

5.2.1 Formulation and implementation of static-dynamic friction

Model formulation

In the static-dynamic friction model, the tangential contact force is composed of elastic (spring) and damping (dashpot) terms and is constrained by the Coulomb limit, as defined by the following equation [164]:

$$\mathbf{f}_{q \rightarrow p, t}^c = \begin{cases} \mathbf{f}_{q \rightarrow p, t}^*, & \text{if } \|\mathbf{f}_{q \rightarrow p, t}^*\| \leq \mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\|, \\ \mathbf{f}_{q \rightarrow p, t}^{\text{CL}}, & \text{if } \|\mathbf{f}_{q \rightarrow p, t}^*\| > \mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\|, \end{cases} \quad (5.8)$$

with

$$\mathbf{f}_{q \rightarrow p, t}^* = -k_t \boldsymbol{\delta}_{pq, t}^* - \gamma_t \mathbf{u}_{pq, t}, \quad (5.9)$$

and

$$\mathbf{f}_{q \rightarrow p, t}^{\text{CL}} = -k_t \boldsymbol{\delta}_{pq, t}^{\text{CL}} - \gamma_t \mathbf{u}_{pq, t} = \mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\| \mathbf{t}_{pq}, \quad (5.10)$$

where $\mathbf{f}_{q \rightarrow p, t}^*$ is the test force, k_t is the tangential spring stiffness, γ_t is the tangential viscous damping coefficient, and $\mathbf{t}_{pq} = \mathbf{f}_{q \rightarrow p, t}^* / \|\mathbf{f}_{q \rightarrow p, t}^*\|$ is the tangential unit vector. The superscript CL refers to the Coulomb limit. The tangential overlap $\boldsymbol{\delta}_{pq, t}$ depends on the contact history, as it cannot be determined instantaneously but must be accumulated over time and saturated to ensure that the Coulomb limit is never surpassed, as shown in the equation below:

$$\boldsymbol{\delta}_{pq, t} = \begin{cases} \boldsymbol{\delta}_{pq, t}^* & \text{if } \|\mathbf{f}_{q \rightarrow p, t}^*\| \leq \mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\|, \\ \boldsymbol{\delta}_{pq, t}^{\text{CL}} & \text{if } \|\mathbf{f}_{q \rightarrow p, t}^*\| > \mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\|, \end{cases} \quad (5.11)$$

with

$$\boldsymbol{\delta}_{pq, t}^* = \boldsymbol{\delta}_{pq, t}^{\text{prev}} \cdot \mathbf{H} + \Delta t_p \mathbf{u}_{pq, t}, \quad (5.12)$$

and

$$\boldsymbol{\delta}_{pq, t}^{\text{CL}} = \frac{1}{k_t} (-\mu_d \|\mathbf{f}_{q \rightarrow p, n}^c\| \mathbf{t}_{pq} - \gamma_t \mathbf{u}_{pq, t}), \quad (5.13)$$

where Δt_p is the particle time step, and $\boldsymbol{\delta}_{pq, t}^{\text{prev}}$ is the tangential overlap at the previous time step, which is rotated by a matrix $\mathbf{H}$ in order to be situated in the contact plane specified by the new normal unit vector [72]. The rotation matrix $\mathbf{H}$ is defined as:

$$\mathbf{H} = \begin{pmatrix} wb_x^2 + c & wb_x b_y - sb_z & wb_x b_z + sb_y \\ wb_x b_y + sb_z & wb_y^2 + c & wb_y b_z - sb_x \\ wb_x b_z - sb_y & wb_y b_z + sb_x & wb_z^2 + c \end{pmatrix}, \quad (5.14)$$

where $\mathbf{b}$, c , s , and w are given by:

$$\mathbf{b} = \frac{\mathbf{n}_{pq} \times \mathbf{n}_{pq}^{\text{prev}}}{\|\mathbf{n}_{pq} \times \mathbf{n}_{pq}^{\text{prev}}\|}, \quad c = \cos \theta, \quad s = \sin \theta, \quad w = 1 - c,$$

with θ defined as:

$$\theta = \arcsin(\|\mathbf{n}_{pq} \times \mathbf{n}_{pq}^{\text{prev}}\|),$$

where $\mathbf{n}_{pq}^{\text{prev}}$ is the normal unit vector at the previous time step. The tangential damping parameter γ_t can be formulated as follows:

$$\gamma_t = \frac{-2 \ln e_t}{\sqrt{\pi^2 + \ln^2 e_t}} \sqrt{k_t \frac{2}{7} m_{pq}}, \quad (5.15)$$

where e_t represents the tangential restitution coefficient. The static-dynamic model (Equation (5.8)) has greater computational and memory costs than the Coulomb dynamic model (Equation (5.5)). To account for static friction, the tangential overlap of each contact should be stored at each time step.

Model implementation

A multi-level domain decomposition method is employed in YALES2 [5, 165]. The grid cells are assembled into cell groups at a first level, and cell groups are distributed over processors at a second level [165]. In the third decomposition level, particles situated in a cell group are gathered in particle groups holding up to 500 particles each [5]. These decomposition levels aim at improving data locality, cache memory accesses, and load balancing.

A ghost particle method is used to treat contacts between particles that are not in the same processor region [5, 10]. In this method, a cell halo enclosing each processor region is employed to identify ghost particles [5]. The data of particles located in the cell halo are communicated among the involved processors to calculate the contact force.

Examining all the particles in the domain to determine the contacts with a given particle has a high computational cost, scaling as $\mathcal{O}(N_{tot}^2)$, where N_{tot} is the total number of particles. To deal with this problem, the linked-cell method is used, whose computational cost scales as $\mathcal{O}(N_{tot})$ [10, 78, 166, 167]. In this technique, a Cartesian grid of size larger than the particle diameter is overlaid on the main grid to identify the potential contact partners of each particle, as shown in Figure 5.1. The list of potential contact partners for a given particle is provided by looping over the 8 surrounding Cartesian grid cells plus the one in which the particle is located (26+1 grid cells in 3D) [10]. However, Newton's third law (action-reaction principle: $\mathbf{f}_{p \rightarrow q}^c = -\mathbf{f}_{q \rightarrow p}^c$) allows checking only half of these cells (4+1 cells in 2D) [166], and particles situated in these cells are identified as potential contact partners, as illustrated in Figure 5.1. During the calculation of the contact force, only the potential contact partners are checked. Once an overlap is detected between a certain particle and one of its potential contact partners, a contact force is computed.

Particles inside a given processor domain are distributed over various particle groups, as illustrated in Figure 5.2. In a particle group containing N_g particles, a given particle p has a local index $n_p^{loc} \in [1, N_g]$. This particle has also a unique global index $n_p^{glob} \in [1, N_{tot}]$, where N_{tot} is the total number of particles in the domain. The particle index that was used in the accumulation of the tangential overlap $\delta_{pq,t}$ (Equation (5.11)) is the global index because it does not change when the particle moves from one particle group to another or from one processor domain to another. When a particle moves from one CPU to another, the

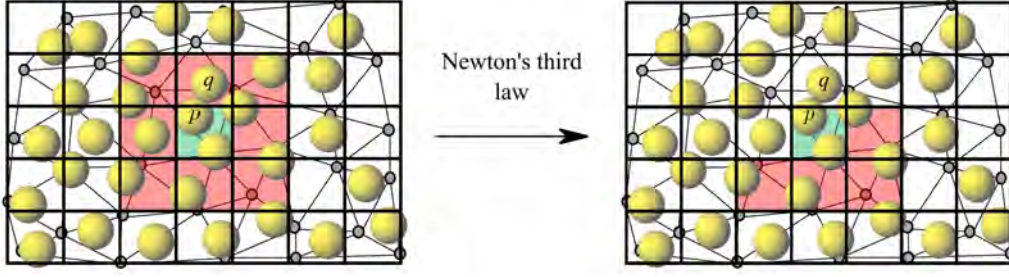


Figure 5.1 Linked-cell technique. $\bullet$: nodes of the main grid. --- : overlaid Cartesian grid. The particle of interest is located in the middle cell (green) and is indicated as p . The particles inside the middle cell or one of the lower neighboring cells (pink) are saved as potential contact partners of particle p . Adapted from [10].

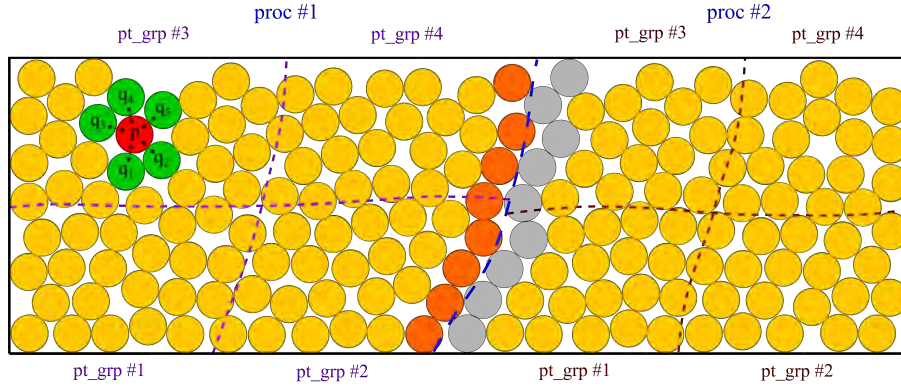


Figure 5.2 Particle distribution in a computational domain. --- : limit between processor domains. --- : limit between particle groups (pt_grp). $\bullet$: ghost particles of processor #2. $\bullet$: ghost particles of processor #1. A particle of interest, p , is in contact with 5 particles.

information about its contacts, based on global particle indices, is transferred along with the particle. The particle of interest p in Figure 5.2 is in contact with five q particles. Each of these (p, q) contact pairs has a distinct tangential overlap $\delta_{pq,t}$, which must be accumulated over time.

A two-step algorithm for determining the tangential overlap was implemented in YALES2. These two steps are described below.

First step: Insert a new pair in the list of contact pairs and accumulate the tangential overlap. This is achieved by:

- (1) Looping over the potential contact partners q of a given particle p at the current time step, or in other words, looping over potential contact pairs. The list of potential contact partners of a given particle is provided by the linked-cell method, as described previously.

- (2) Calculating the normal overlap at the current time step ($\delta_{pq,n} = r_p + r_q - \|\mathbf{x}_p - \mathbf{x}_q\|$, where r is the particle radius).
- (3) Inserting the pair (p, q) in the list of contact pairs if it is not already there (at the previous time step) and accumulating the tangential overlap $\delta_{pq,t}$, if particles p and q are in contact ($\delta_{pq,n} > 0$).

Second step: Erase an obsolete pair from the list of contact pairs. This is achieved by the following actions:

- (1) Looping over particles q that were in contact with a given particle p at the previous time step, or in other words, looping over already existing contact pairs.
- (2) Calculating the normal overlap at the current time step.
- (3) Erasing the pair (p, q) from the list of contact pairs if the particles p and q are no longer in contact ($\delta_{pq,n} \leq 0$).

Each particle situated at a processor boundary has two copies: a real and a ghost. The data of a certain duplicated particle, which are required to compute friction forces, are transmitted from the processor where it is real to the processor where it is ghost.

5.2.2 Formulation and implementation of Van der Waals force

The Van der Waals force was included in the DEM model by adding an adhesive force term, $\mathbf{F}_{q \rightarrow p}^{ad}$, to the particle equation of motion [146]:

$$\mathbf{F}_{q \rightarrow p}^{ad} = \frac{A}{6d_p} \frac{1}{(2u + u^2)^2} \frac{1}{(1 + u)^3} \mathbf{n}_{pq}. \quad (5.16)$$

Here, A denotes the Hamaker constant, $u = \|\mathbf{x}_q - \mathbf{x}_p\|/d_p - 1$ represents the dimensionless separation distance between the two particle surfaces, and $\mathbf{n}_{pq}$ signifies the normal unit vector. When the spheres are nearly touching, the force in Equation (5.16) can be written as:

$$\mathbf{F}_{q \rightarrow p}^{ad} = \frac{A}{6d_p} \frac{1}{(2u_0 + u_0^2)^2} \frac{1}{(1 + u_0)^3} \mathbf{n}_{pq} \approx \frac{A}{6d_p} \frac{1}{4u_0^2} \mathbf{n}_{pq} = \frac{Ad_p}{24S_0^2} \mathbf{n}_{pq}, \quad (5.17)$$

where $u_0 = S_0/d_p$ is the minimum dimensionless separation distance, and S_0 is the minimum cutoff distance between the surfaces of the two particles. The Van der Waals interaction diminishes quickly as u increases. Therefore, to simplify matters, we implemented the Van

der Waals force between two particles in the following manner:

$$\mathbf{F}_{q \rightarrow p}^{ad} = \begin{cases} \frac{Ad_p}{24S_0^2} \mathbf{n}_{pq}, & \text{if } \delta_{pq,n} > 0, \\ 0, & \text{otherwise.} \end{cases} \quad (5.18)$$

Additionally, we implemented the particle-wall Van der Waals force as [36]:

$$\mathbf{F}_{w \rightarrow p}^{ad} = \begin{cases} \frac{Ad_p}{12S_0^2} \mathbf{n}_{pw}, & \text{if } \delta_{pw,n} > 0, \\ 0, & \text{otherwise.} \end{cases} \quad (5.19)$$

In addition to the Hamaker model [31], there are several options for modeling Van der Waals forces in DEM, such as the Johnson-Kendall-Roberts (JKR) [168, 169], Derjaguin-Muller-Toporov (DMT) [170], modified Hamaker [171], square-well [36], and linear adhesion [172] models. Each of these models has its own assumptions and limitations. For simplicity, we chose the Hamaker model; however, more sophisticated models [171] may be used for enhanced accuracy.

5.2.3 Validation of friction and adhesion models

The static-dynamic friction model was implemented for both interparticle and particle-wall interactions and validated at both micro and macro scales. At the microscale, we found good agreement between the results of our simulations and those obtained using Walton's theoretical model [173] for both interparticle and particle-wall collisions. At the macroscale, we found a close match between the vertical solid stress profile in a silo obtained using the implemented static-dynamic friction model and that determined using Janssen's theoretical model [174], as well as between the mass flow rate of powder exiting a hopper obtained from our simulation and that calculated using Beverloo's empirical correlation [175]. The implementation of the interparticle and particle-wall Van der Waals adhesion forces was qualitatively validated at the microscale by predicting the effects of adhesion on rebound translational and rotational velocities, contact time, and maximum normal overlap [176, 177]. The results of the aforementioned validation tests are not presented in this paper since the focus of this study is to investigate the influence of friction and Van der Waals adhesion on fluidization hydrodynamics. Therefore, we only present the prediction of a pressure overshoot in a fluidized bed in the following section.

5.3 Fluidization and defluidization simulations

We conducted fluidization and defluidization CFD-DEM tests to analyze the impact of Van der Waals forces and static wall friction on pressure-drop hysteresis and to gather essential information for guiding the development of macroscopic solid stress models. These simulations, which are similar to those performed by Ye et al. [12], employ the parameters listed in Table 5.1.

Table 5.1 Parameters for the fluidization and defluidization simulations.

<i>Particle properties</i>		<i>Interparticle and particle-wall collisions</i>	
Diameter, d_p	75 μm	Normal spring stiffness, k_n	7 N/m
Density, ρ_p	1495 kg/m ³	Normal restitution coefficient, e_n	0.9
<i>Cuboid geometry</i>		Tangential spring stiffness, k_t	2 N/m
Width (x -direction), W	$40d_p$	Tangential restitution coefficient, e_t	0.9
Thickness (y -direction), T	$16d_p$	Dynamic friction coefficient, μ_d	0.2
Height (z -direction), H	$160d_p$	Maximum normal overlap, δ_n^{max}	$0.1d_p$
<i>Hexahedral mesh</i>		<i>Gas properties</i>	
Number of cells in the x -direction, N_c^x	12	Density, ρ_g	1.1979 kg/m ³
Number of cells in the y -direction, N_c^y	5	Viscosity, μ_g	1.8×10^{-5} Pa.s
Number of cells in the z -direction, N_c^z	48	<i>Advancement of gas</i>	
<i>Particle loading</i>		Time integration scheme	TFV4A [85]
Number of particles, N_{tot}	36,000	Spatial integration scheme	4th-order centered
<i>Time advancement of particles</i>		Courant number, CFL	0.01
Numerical scheme	Groot-Warren [82]	<i>Gas-particle interaction</i>	
Particle CFL number, CFL_s	1.5	Drag model	Gobin et al. [81]
Contact CFL number, CFL_s^c	0.05	<i>Interparticle and particle-wall adhesion</i>	
Number of sub-steps within the collision time, n_c	15	Minimum cutoff distance, S_0	4×10^{-10} m
		Hamaker constant, A	1.96×10^{-22} J

In the initial phase, we conducted particle settling under the influence of gravity ($g_z = -9.81$ m/s²). The particles used are categorized under Geldart group A, with their properties outlined in Table 5.1. The seeding region was positioned at a distance of d_p from the side walls within the z -range of 4 mm to 6.075 mm. Each cell was seeded with one particle along each dimension ($\Delta x, \Delta y, \Delta z$). Beginning at $t = 0$, we seeded 480 particles at intervals of 0.1 s until $t = 7.4$ s, with the simulation continuing for a total of 9 s. These particles experienced random translation velocities ranging from -0.1 to 0.1 m/s and random rotational velocities between -100 and $+100$ rad/s at seeding. For this study, we employed a zero rolling friction coefficient. Additionally, Van der Waals forces among particles and between particles and walls were taken into account during the settling process.

Subsequently, we used the formed static bed as the initial state for both fluidization and defluidization tests. Turbulence effects were neglected in these tests. All boundaries were treated as walls for particles. The bottom boundary served as the inlet for gas, and the top boundary functioned as the gas outlet, maintaining a pressure of 1 atm. A no-slip condition

was applied to the gas at the sidewalls. In these simulations, we vary the gas mass flow rate at the inlet using a step-wise approach. The mass flow rates are determined by the equation:

$$\dot{W} = \rho_g U_g S_b, \quad (5.20)$$

where U_g is the superficial gas velocity, and S_b is the cross-sectional area of the bed. Each superficial gas velocity (U_g) was maintained for a duration of $0.7 + H_b^0/U_g$ seconds, where $H_b^0 \approx 3.52$ mm represents the bed height at zero gas velocity. Time averages were computed over the last 0.3 seconds of each individual time interval during which a specific U_g value was sustained. The Hamaker constant value used in the test cases involving adhesion (refer to Table 5.1) yields an adhesion force $\mathbf{F}_{q \rightarrow p}^{ad}$ equal to $1.18m_p \mathbf{g}$. As given in Table 5.1, we used a very small CFL number (0.01) to improve numerical stability because the coupling between the gas and solid phases in YALES2 is explicit.

The time-averaged bed pressure drop was calculated using the formula:

$$\overline{\Delta P} = \frac{\sum_{k=1}^{N_r} \Delta P_k \Delta t_{g,k}}{\sum_{k=1}^{N_r} \Delta t_{g,k}}. \quad (5.21)$$

Here, Δt_g represents the gas time step, ΔP is the gas pressure drop between the inlet and 6.5 mm above the inlet, and N_r is the total number of gas time steps in the 0.3 s interval. Then, the normalized time-averaged bed pressure drop was determined as $\overline{\Delta P}/\Delta P_{eq}$, where ΔP_{eq} represents the pressure drop equivalent to the weight of the particles, which was computed as:

$$\Delta P_{eq} = \frac{m_b g}{S_b} = \frac{\pi d_p^3}{6} \frac{N_{tot} \rho_p g}{S_b} = 32.4 \text{ Pa}. \quad (5.22)$$

In this equation, m_b represents the mass of the particle bed, and N_{tot} represents the number of all the particles. Figure 5.3 illustrates the fluidization and defluidization pressure-drop curves for tests with and without adhesion effects (interparticle and particle-wall Van der Waals adhesion). The figure displays an overshoot in the bed pressure drop during fluidization, which is attributed to static wall friction in the case without adhesion. It also shows that the overshoot intensity increases when adhesion is present. Moreover, there is a hysteresis in pressure drop between the decreasing and increasing velocity path curves (defluidization and fluidization cycles, respectively).

A fluidization simulation that excluded both adhesion and particle-wall friction showed no overshoot. Another fluidization simulation, which accounted for interparticle adhesion but excluded particle-wall adhesion, demonstrated a smaller overshoot area compared to the

simulation that considered both interparticle and particle-wall adhesion. The data from these two simulations are presented in Appendix E.

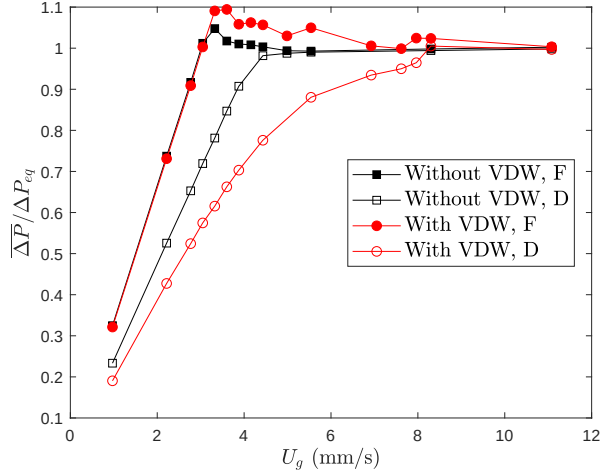


Figure 5.3 Normalized time-averaged overall bed pressure drop during fluidization and defluidization cycles without and with Van der Waals (VDW) adhesion. F represents a fluidization branch, and D represents a defluidization branch.

In our simulations, where all cells have the same volume, the time-spatial averaged solid volume fraction was computed as follows:

$$\overline{\langle \alpha_p \rangle} = \frac{\sum_{k=1}^{N_r} \langle \alpha_p \rangle_k \Delta t_{g,k}}{\sum_{k=1}^{N_r} \Delta t_{g,k}} = \frac{v_p \sum_{k=1}^{N_r} n_{sa,k} \Delta t_{g,k}}{v_{sa} \sum_{k=1}^{N_r} \Delta t_{g,k}}, \quad (5.23)$$

where v_p is the volume of one particle ($\pi d_p^3/6$), v_{sa} is the total volume below a designated height H_{sa} where spatial averaging was performed, and n_{sa} is the total number of particles situated below the height H_{sa} . This height is set at $H_{sa} = 14\Delta z = 3.5$ mm, which is approximately equal to the bed height when the gas velocity is zero. The bed voidage was then determined as follows: $\overline{\langle \alpha_g \rangle} = 1 - \overline{\langle \alpha_p \rangle}$.

The evolution of bed voidage during defluidization and fluidization cycles is plotted in Figure 5.4. In the fluidization branch, the bed voidage remains stable at around 0.38 until reaching the minimum fluidization velocity ($U_{mf} = 3.32$ mm/s), after which it begins to increase. The decreasing path curves do not return to the voidage of the settled bed, aligning with observations from experiments by Affleck et al. [118], particularly when the particle bed is tapped before fluidization. Additionally, defluidization curves differ between tests with and without adhesion, with adhesion resulting in a higher voidage for the static bed due

to hindered particle movement, consistent with findings in the fixed bed simulations by Mihajlovic et al. [177].

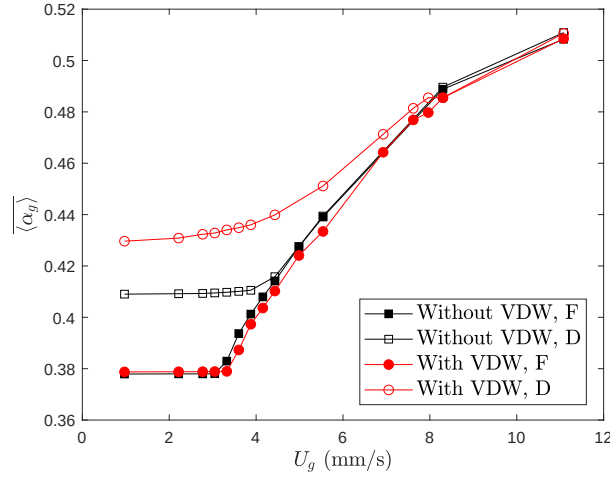


Figure 5.4 Bed voidage profiles during defluidization (D) and fluidization (F) cycles without and with Van der Waals (VDW) adhesion.

The minimum fluidization velocity calculated using the correlation proposed by Abrahamsen and Geldart [178], which is expressed as:

$$U_{mf} = 9 \times 10^{-4} (g [\rho_p - \rho_g])^{0.934} \frac{d_p^{1.8}}{\mu_g^{0.87} \rho_g^{0.066}}, \quad (5.24)$$

is approximately 3.5 mm/s. The simulation value of 3.32 mm/s is only about 5% lower than this estimate, indicating a very close agreement.

The time-spatial averaged coordination number was computed in the following manner:

$$\overline{\langle CN \rangle} = \frac{\sum_{k=1}^{N_r} \langle \alpha_p \rangle_k \langle CN \rangle_k \Delta t_{g,k}}{\sum_{k=1}^{N_r} \langle \alpha_p \rangle_k \Delta t_{g,k}} = \frac{\sum_{k=1}^{N_r} n_{sa,k} \langle CN \rangle_k \Delta t_{g,k}}{\sum_{k=1}^{N_r} n_{sa,k} \Delta t_{g,k}} = \frac{\sum_{k=1}^{N_r} \left(\sum_{i=1}^{n_{sa,k}} CN_i \right) \Delta t_{g,k}}{\sum_{k=1}^{N_r} n_{sa,k} \Delta t_{g,k}}. \quad (5.25)$$

The evolution of the coordination number during defluidization and fluidization cycles is presented in Figure 5.5. A hysteresis is observed for the average coordination number predictions between the decreasing and increasing gas velocity paths (below U_{mf}). In the absence of adhesion, the average coordination number decreases rapidly to nearly zero with the increase in superficial gas velocity (above U_{mf}) for both the defluidization and fluidization cycles. In contrast, in the presence of Van der Waals adhesion, the coordination number slowly decreases with the increase in superficial gas velocity (up to $U_g = 8.3$ mm/s). In the fluidization

and defluidization branches with adhesion, increasing the superficial gas velocity from 4.43 mm/s to 6.93 mm/s, for example, does not significantly decrease the coordination number despite an increase in the voidage (see Figure 5.4). This is a characteristic of the homogeneous fluidization regime. Therefore, the coordination number variations in Figure 5.5 reveal that predicting the homogeneous regime between the minimum fluidization and minimum bubbling velocities requires accounting for the Van der Waals adhesion. Some tests (shown in Appendix E) have demonstrated that suppressing Van der Waals adhesion between particles and walls does not alter the homogeneous fluidization regime and the overall coordination number trend.

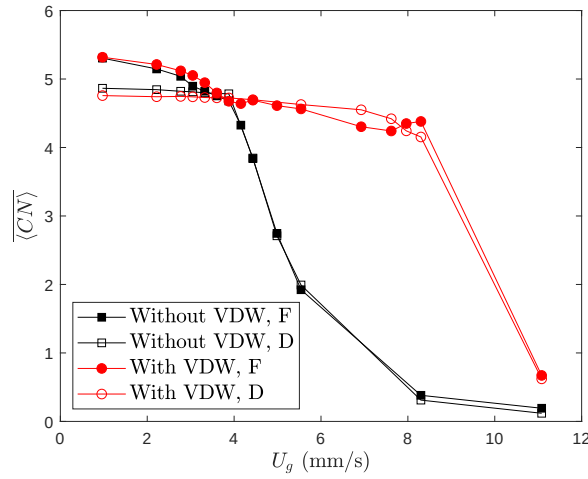


Figure 5.5 Evolution of the coordination number during defluidization (D) and fluidization (F) cycles, without and with Van der Waals (VDW) adhesion.

Additionally, the contact fabric tensor was computed as follows [152]:

$$R_{ij} = \frac{1}{N_{tot}} \sum_{k=1}^{N_{tot}} \sum_{c=1}^{c_k} n_{k,i}^c n_{k,j}^c, \quad (5.26)$$

where N_{tot} represents the number of particles in the bed ($N_{tot} = 36,000$ in our case), c_k denotes the count of contacts on particle k , and $\mathbf{n}_k^c$ indicates the unit branch vector that originates from the center of particle k and points towards a contact point c . The trace of this fabric tensor is equal to the average coordination number of all the particles. The fabric tensor, R_{ij} , is symmetric. The fabric component R_{zz} at a particular gas time step Δt_g was

calculated by averaging over the particle time steps as follows:

$$R_{zz} = \frac{1}{N_{tot}} \left(\frac{\sum_{j=1}^{N_{st}} (n_{1,z}^1 n_{1,z}^1 + \dots + n_{1,z}^{c_1} n_{1,z}^{c_1})_j \Delta t_{p,j}}{\sum_{j=1}^{N_{st}} \Delta t_{p,j}} + \dots + \frac{\sum_{j=1}^{N_{st}} (n_{N_{tot},z}^1 n_{N_{tot},z}^1 + \dots + n_{N_{tot},z}^{c_{N_{tot}}} n_{N_{tot},z}^{c_{N_{tot}}})_j \Delta t_{p,j}}{\sum_{j=1}^{N_{st}} \Delta t_{p,j}} \right). \quad (5.27)$$

Here, Δt_p is the particle time step, and N_{st} is the number of sub-steps (particle time steps) in a given gas time step. The time-averaged R_{zz} was then computed as:

$$\overline{R_{zz}} = \frac{\sum_{k=1}^{N_r} R_{zz,k} \Delta t_{g,k}}{\sum_{k=1}^{N_r} \Delta t_{g,k}}. \quad (5.28)$$

The other fabric tensor components were determined similarly to how $\overline{R_{zz}}$ was calculated.

Figure 5.6 shows the diagonal components of the fabric tensor as a function of the superficial gas velocity during defluidization and fluidization cycles, without and with adhesion. The R_{zz} component of the fabric tensor indicates the degree of alignment of contacts within the particle bed (orientation of the unit branch vector) along the z -axis. As observed in Figure 5.6, the fabric component $\overline{R_{zz}}$ exhibits higher values in the fixed bed state compared to the fabric components $\overline{R_{xx}}$ and $\overline{R_{yy}}$, indicating that more contacts are oriented in the z direction than in the x and y directions. In the fixed bed state, the variation in these diagonal components with the gas velocity is relatively small, indicating that the contact orientations in the x , y , and z directions remain nearly unchanged. At high gas velocities, the fabric diagonal components decrease significantly and reach very small values as contacts are lost. In the presence of adhesion, the fabric diagonal components maintain high values at higher gas velocities compared to the case without adhesion. This implies that adhesion inhibits changes in contact orientations and the disintegration of the contact network.

The macroscopic collisional stress tensor in an averaging volume V can be expressed as [152, 153, 179]:

$$\sigma_{ij} = -\frac{1}{V} \sum_{k=1}^{n_s} \sum_{c=1}^{c_k} l_{k,i}^c f_{k,j}^c \quad (5.29)$$

where n_s is the number of particles whose centers lie within the volume V , c_k is the number of contacts on particle k , $\mathbf{l}_k^c$ is the branch vector from the center of particle k to a contact

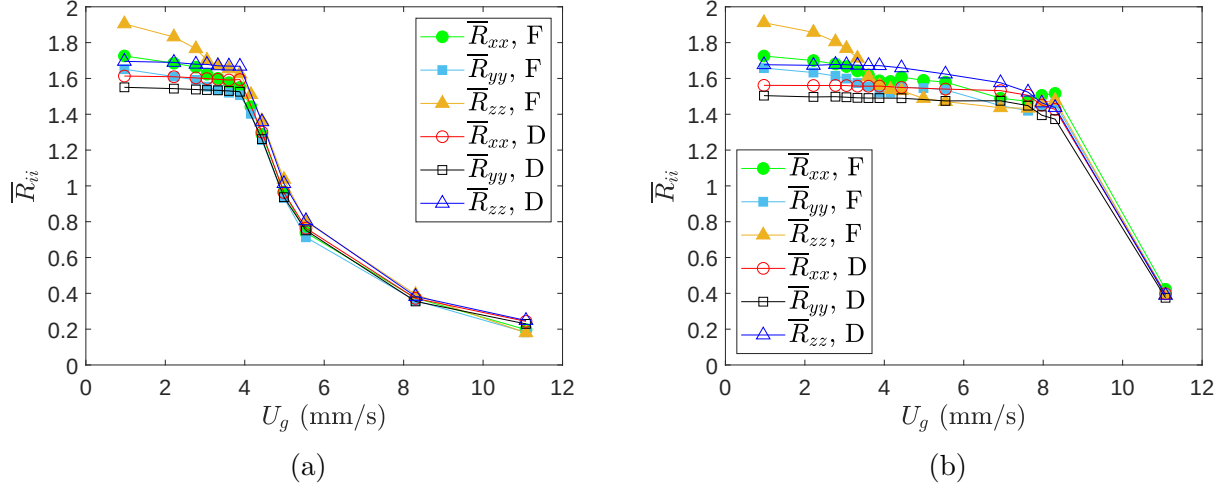


Figure 5.6 Variation of the time-averaged diagonal components of the fabric tensor with the superficial gas velocity during defluidization (D) and fluidization (F) cycles for test cases: (a) without Van der Waals adhesion, and (b) with Van der Waals adhesion.

point c , and $\mathbf{f}_k^c$ is the contact force acting on particle k . For a particle p in contact with a particle q at a point c , the branch vector $\mathbf{l}_p^c$ is given by:

$$\mathbf{l}_p^c = \left(\frac{d_p}{2} - \frac{\delta_{pq,n}}{2} \right) \mathbf{n}_{pq}. \quad (5.30)$$

The computational domain was divided into 32 slices, each with a thickness of $\Delta z = 5d_p$, as illustrated in Figure 5.7. The collisional stress was calculated for each slice.

The time-averaged σ_{zz} , for instance, was calculated as follows:

$$\overline{\sigma_{zz}} = \frac{\sum_{k=1}^{N_r} \sigma_{zz,k} \Delta t_{g,k}}{\sum_{k=1}^{N_r} \Delta t_{g,k}}, \quad (5.31)$$

where $\sigma_{zz,k}$ is the collisional stress zz -component at a given gas time step $\Delta t_{g,k}$, calculated

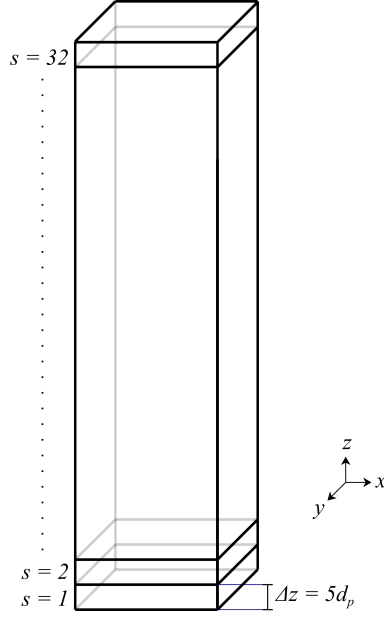


Figure 5.7 Division of the cuboid into slices. s denotes the slice number. Each slice has a thickness $\Delta z = 5d_p$.

by averaging over the particle time steps as follows:

$$\sigma_{zz} = -\frac{1}{V} \left(\frac{\sum_{j=1}^{N_{st}} \overbrace{(l_{1,z}^1 f_{1,z}^1 + \dots + l_{1,z}^{c_1} f_{1,z}^{c_1})_j}^{\text{particle 1}} \Delta t_{p,j}}{\sum_{j=1}^{N_{st}} \Delta t_{p,j}} + \dots + \frac{\sum_{j=1}^{N_{st}} \overbrace{(l_{n_s,z}^1 f_{n_s,z}^1 + \dots + l_{n_s,z}^{c_{n_s}} f_{n_s,z}^{c_{n_s}})_j}^{\text{particle } n_s} \Delta t_{p,j}}{\sum_{j=1}^{N_{st}} \Delta t_{p,j}} \right). \quad (5.32)$$

where n_s is the number of particles located inside a given slice of volume V . The contribution of particle-wall interactions was not included in the computation of the stress given by Equation (5.32). The time-averaged repulsive solid pressure was then determined as:

$$\overline{P}_p^r = \frac{1}{3} (\overline{\sigma_{xx}} + \overline{\sigma_{yy}} + \overline{\sigma_{zz}}). \quad (5.33)$$

The time-averaged adhesive solid pressure $\overline{P}_p^a$ was computed similarly to the repulsive solid pressure $\overline{P}_p^r$, but using the Van der Waals force instead of the collision force. The effective

solid pressure is the sum of the repulsive and adhesive solid pressures:

$$\overline{P}_p^e = \overline{P}_p^r + \overline{P}_p^a. \quad (5.34)$$

Figure 5.8 shows the variation of repulsive solid pressure with depth for different superficial gas velocities, with each curve belonging to either the fluidization or defluidization branch. These data are from a test case without adhesion. As observed, at the lowest gas velocity of 0.97 mm/s, where the bed is fixed, the repulsive solid pressure increases with depth. Additionally, the repulsive solid pressure decreases as the gas velocity increases because the contact network between the particles is disrupted. At a gas velocity of 4.43 mm/s, the repulsive solid pressure approaches zero due to the expansion of the bed. Furthermore, there is a noticeable difference in the repulsive solid pressure values between the defluidization and fluidization curves, for example, at gas velocities of 0.97, 2.22, and 2.77 mm/s, where the defluidization curves exhibit lower repulsive pressure values. This is consistent with the higher voidage values observed at these velocities during defluidization compared to fluidization. In the defluidization cycle, a reduction in gas velocity from 3.88 to 3.05 mm/s leads to an increase in repulsive pressure due to the compression of the bed. This results in higher repulsive pressures during defluidization compared to fluidization, specifically in the lower regions of the bed. The transition from higher repulsive pressures during defluidization in comparison with fluidization to the opposite occurs at a gas velocity of 3.05 mm/s, at which the bed voidage starts to increase in the fluidization branch (refer to Figure 5.4).

Figures 5.9, 5.10, and 5.11 illustrate the repulsive, adhesive, and effective solid pressures during defluidization and fluidization cycles with Van der Waals adhesion. In Figure 5.9, within the fluidization branch at a velocity of 3.05 mm/s, for example, the repulsive pressure is higher compared to the case without adhesion (see Figure 5.8). This increase is due to adhesion inhibiting the expansion of the bed. The shift from higher repulsive pressures during defluidization compared to fluidization to the opposite happens at a gas velocity of 3.32 mm/s, where the bed voidage begins to rise in the fluidization branch (see Figure 5.4).

In Figure 5.10, we observe that the adhesive solid pressure during defluidization generally exhibits a lower magnitude compared to that during fluidization. This is consistent with the higher bed voidage and lower coordination number during defluidization compared to fluidization because the Van der Waals force is applied at contact. Additionally, as the superficial gas velocity increases along the fluidization branch, the magnitude of adhesive pressure decreases due to the declining coordination number. Unlike repulsive pressure, adhesive pressure does not vary significantly with depth due to the uniform coordination number distribution within the bed and the constant magnitude of the applied Van der

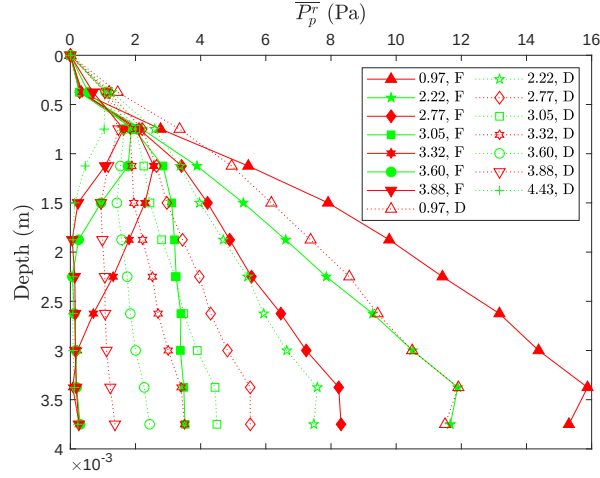


Figure 5.8 Variation of time-averaged repulsive particle pressure with depth during deflu-idization (D) and fluidization (F) cycles without Van der Waals adhesion. The numbers in the legends of this figure and Figures 5.9, 5.10, and 5.11 are the superficial gas velocity values in mm/s.

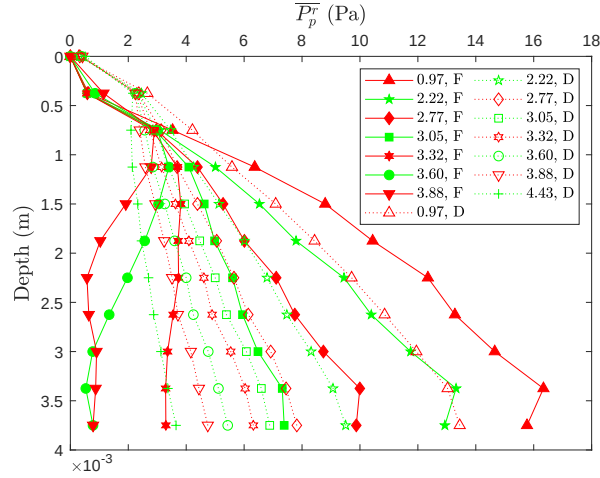


Figure 5.9 Variation of time-averaged repulsive particle pressure with depth during deflu-idization (D) and fluidization (F) cycles with Van der Waals adhesion.

Waals forces.

In Figure 5.11, we note that the effective pressure values are lower than the repulsive pressure values indicated in Figure 5.9 due to the negative adhesion contribution, as per Equation (5.34).

The particle-wall contact forces were calculated in each slice. For instance, the z -component

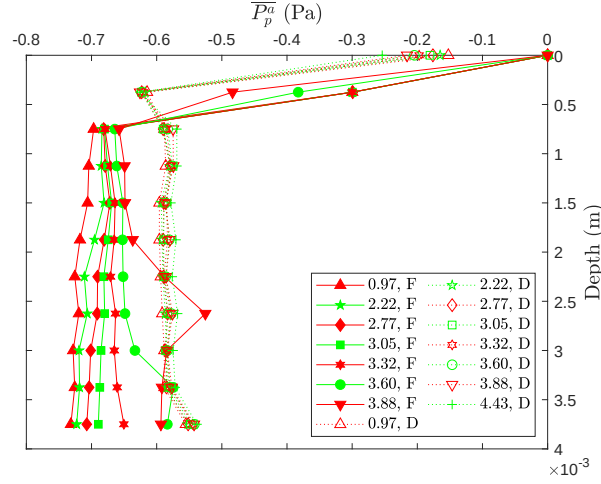


Figure 5.10 Variation of time-averaged adhesive particle pressure with depth during deflu-idization (D) and fluidization (F) cycles.

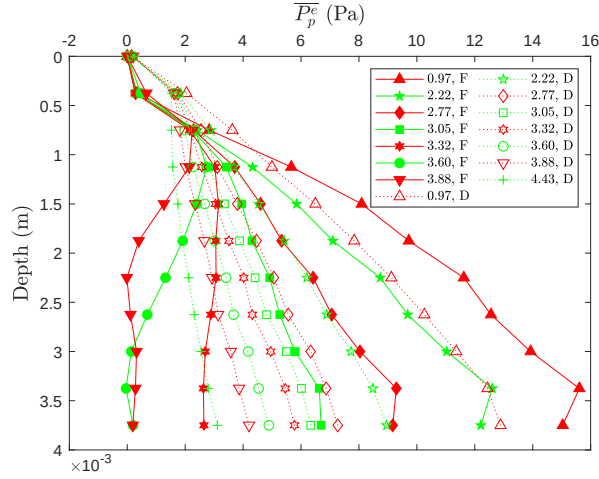


Figure 5.11 Variation of time-averaged effective particle pressure with depth during deflu-idization (D) and fluidization (F) cycles with Van der Waals adhesion.

of the particle-wall contact force at a particular gas time step was determined by averaging over the particle time steps as follows:

$$f_{w \rightarrow p, z}^a = \frac{\sum_{j=1}^{N_{st}} f_{w \rightarrow p, z} |_j \Delta t_{p, j}}{\sum_{j=1}^{N_{st}} \Delta t_{p, j}} = \frac{\sum_{j=1}^{N_{st}} f_{w \rightarrow p, z} |_j \Delta t_{p, j}}{\Delta t_g}, \quad (5.35)$$

where $f_{w \rightarrow p, z} |_j$ represents the z -component of the contact force applied by all walls w to

particle p at the particle time step $\Delta t_{p,j}$, and Δt_g is the gas time step. When adhesion is present, $\mathbf{f}_{w \rightarrow p}$ is the sum of repulsive contact force (modeled by spring-dashpot systems in both the tangential and normal directions) and adhesive contact force (Van der Waals force in the normal direction). The sum of the contact force over all particles with centers located within slice s was determined as follows:

$$F_{w \rightarrow p, z}^s = \sum_{n_s} f_{w \rightarrow p, z}^a, \quad (5.36)$$

where n_s denotes the number of particles in the slice s at Δt_g . The time average of $F_{w \rightarrow p, z}^s$ was then calculated as follows:

$$\bar{F}_{w \rightarrow p, z}^s = \frac{\sum_{k=1}^{N_r} F_{w \rightarrow p, z}^s|_k \Delta t_{g, k}}{\sum_{k=1}^{N_r} \Delta t_{g, k}}, \quad (5.37)$$

where N_r is the total number of gas time steps in the averaging time interval. To obtain the time-averaged particle-wall shear stress $\bar{\sigma}_{pw}^s$, we divided $\bar{F}_{w \rightarrow p, z}^s$ by the wall surface area S_w , which is given by:

$$S_w = 2W\Delta z + 2T\Delta z = 560d_p^2. \quad (5.38)$$

Here, $\Delta z = 5d_p$ represents the thickness of the slice s . W and T refer to the width and thickness of the cuboid, as specified in Table 5.1.

Figure 5.12 depicts the variation of time-averaged particle-wall shear stress with depth during defluidization (D) and fluidization (F) cycles in the absence of Van der Waals adhesion. In defluidization, the shear stress is positive, whereas it is negative during fluidization. During the defluidization cycle, as gas velocity decreases, the wall friction opposes the downward movement of particles, resulting in a positive shear stress (in the positive z direction). Conversely, during the fluidization cycle, as gas velocity increases, wall friction counteracts the upward movement of particles, leading to a negative shear stress (in the negative z direction). Loezos et al. [139] employed a positive sign for the particle-wall friction term in a particle force balance model during defluidization, while a negative sign was used during fluidization. Furthermore, Figure 5.12 shows that as the superficial gas velocity rises, the magnitude of the particle-wall shear stress diminishes. This occurs because the increase in gas velocity leads to a reduction in the number of contacts, particularly between particles near the walls.

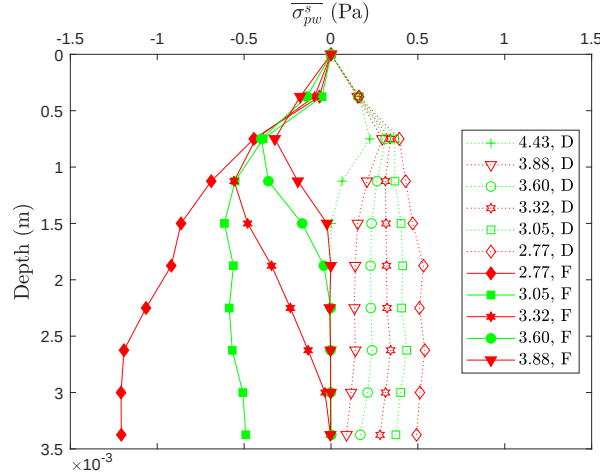


Figure 5.12 Variation of time-averaged particle-wall shear stress with depth during defluidization (D) and fluidization (F) cycles without Van der Waals adhesion. The numbers in the legend are the superficial gas velocity values in mm/s.

5.4 Computation of the coordination number source term

In our previous study [180], we proposed an adhesive pressure model based on the coordination number within the Eulerian-Eulerian framework. This model successfully predicted an overshoot in the bed pressure drop; however, it could not predict the hysteresis in the pressure drop due to the lack of a model for the coordination number evolution. To determine this evolution at the macro-scale, it is essential to propose a transport equation for the coordination number. The first step in this process is to measure the source term of this transport equation. This measurement is crucial for developing and validating an expression for the source term, which can then be utilized in two-fluid simulations. In this section, we compute the coordination number source term from our CFD-DEM simulations using two methods: the direct Lagrangian method and the mesoscopic Eulerian method, which are detailed in the following subsections.

5.4.1 Direct Lagrangian method

The Lagrangian equation of the coordination number CN following a given particle can be written as:

$$\frac{dCN}{dt} = S_{CN}, \quad (5.39)$$

where d/dt is the time derivative along the particle trajectory, and S_{CN} is a source term. The corresponding Eulerian equation can be written for uniform particle mass as follows:

$$\frac{D}{Dt}(n_p \langle CN \rangle) = n_p \left\langle \frac{dCN}{dt} \right\rangle, \quad (5.40)$$

where n_p denotes the particle number density, and $\langle CN \rangle$ stands for the ensemble average of the coordination number. The term on the left-hand side of Equation (5.40) can be expressed as:

$$\frac{D}{Dt}(n_p \langle CN \rangle) = \frac{\partial}{\partial t}(n_p \langle CN \rangle) + \frac{\partial}{\partial x_i}(n_p U_{p,i} \langle CN \rangle) + \frac{\partial}{\partial x_i}(n_p \langle u'_{p,i} CN \rangle). \quad (5.41)$$

Here, $U_{p,i} = \langle u_{p,i} \rangle$ represents the average particle velocity, and $u'_{p,i}$ denotes the uncorrelated random particle velocity. The term on the right-hand side of Equation (5.40) represents the source term and can be calculated directly from the Lagrangian simulation:

$$n_p \langle S_{CN} \rangle = n_p \left\langle \frac{dCN}{dt} \right\rangle = \frac{1}{V_c} \sum_{k=1}^{N_p^c} \frac{dCN_k}{dt}, \quad (5.42)$$

where V_c stands for the volume of a given cell, and N_p^c refers to the number of particles whose centers are inside this cell. With the direct Lagrangian method, Equation (5.42) is used to compute the source term from CFD-DEM simulations. The time derivative in Equation (5.42) was calculated for a specific particle k with a backward difference:

$$\left. \frac{dCN_k}{dt} \right|_n = \frac{CN_k|_n - CN_k|_{n-1}}{\Delta t_g}, \quad (5.43)$$

where n and $n-1$ represent the current and previous states, respectively, and Δt_g stands for the gas time step.

5.4.2 Mesoscopic Eulerian method

We assume that the last term in Equation (5.41) is negligible. Then, we can write the following:

$$\frac{D}{Dt}(n_p \langle CN \rangle) = \frac{\partial}{\partial t}(n_p \langle CN \rangle) + \frac{\partial}{\partial x_i}(n_p U_{p,i} \langle CN \rangle) = n_p \langle S_{CN} \rangle. \quad (5.44)$$

In this equation, it is assumed that the mean coordination number $\langle CN \rangle$ is convected with the local average velocity (correlated mesoscopic velocity) of the particles $U_{p,i}$, and that no diffusive transport takes place. Using Equation (5.44), the source term can be expressed as:

$$n_p \langle S_{CN} \rangle = \frac{1}{v_p} \left[\frac{\partial}{\partial t}(\alpha_p \langle CN \rangle) + \frac{\partial}{\partial x_i}(\alpha_p U_{p,i} \langle CN \rangle) \right], \quad (5.45)$$

where $v_p = \pi d_p^3/6$ denotes the volume of one particle. The partial derivatives in Equation (5.45) can be computed from the calculated Eulerian variables. The mean coordination number in a given cell was determined as follows:

$$\langle CN \rangle = \frac{1}{N_p^c} \sum_{k=1}^{N_p^c} CN_k, \quad (5.46)$$

where N_p^c is the number of particles in the cell and CN_k is the coordination number of particle k . Similarly, the mean particle velocity in a particular cell was calculated as:

$$U_{p,i} = \frac{1}{N_p^c} \sum_{k=1}^{N_p^c} u_{k,i}, \quad (5.47)$$

where $u_{k,i}$ is the velocity of particle k . The solid volume fraction for a specific cell was obtained as follows:

$$\alpha_p = \frac{N_p^c v_p}{V_c}, \quad (5.48)$$

where V_c is the volume of the cell.

The time derivative in Equation (5.45) was computed for a specific cell with a backward difference:

$$\left. \frac{\partial}{\partial t} (\alpha_p \langle CN \rangle) \right|_n = \frac{(\alpha_p \langle CN \rangle)|_n - (\alpha_p \langle CN \rangle)|_{n-1}}{\Delta t_g}, \quad (5.49)$$

where n and $n-1$ represent the current and previous states, respectively, and Δt_g stands for the gas time step.

The divergence in Equation (5.45) was calculated by employing the Gauss-Ostrogradsky theorem. This theorem is given by:

$$\iint_S Q_i n_i dS = \iiint_V \frac{\partial Q_i}{\partial x_i} dV, \quad (5.50)$$

where V refers to the volume bounded by a surface S , Q_i represents a vector field, and n_i stands for the unit vector normal to S and oriented outward. Assuming that the spatial variation of $\partial Q_i / \partial x_i$ is negligible inside the volume V , the integral over V in Equation (5.50) can be expressed as:

$$\iiint_V \frac{\partial Q_i}{\partial x_i} dV = \frac{\partial Q_i}{\partial x_i} V. \quad (5.51)$$

Assuming that the spatial variation of $Q_i n_i$ is negligible inside each face (part of the surface

S), the integral over S in Equation (5.50) can be formulated as:

$$\iint_S Q_i n_i dS = \sum_{j=1}^{N_f} \int_{S_j} Q_i n_i dS = \sum_{j=1}^{N_f} Q_{i,j} n_{i,j} S_j, \quad (5.52)$$

where N_f is the number of faces comprising the closed surface S , and S_j is the surface area of face j . Substituting Equations (5.51) and (5.52) into Equation (5.50) gives:

$$\sum_{j=1}^{N_f} Q_{i,j} n_{i,j} S_j = \frac{\partial Q_i}{\partial x_i} V. \quad (5.53)$$

Then, the divergence of Q_i can be calculated in the following way:

$$\frac{\partial Q_i}{\partial x_i} = \frac{1}{V} \sum_{j=1}^{N_f} Q_{i,j} n_{i,j} S_j. \quad (5.54)$$

We used the face-to-element connectivity in YALES2, which enabled us to consider two adjacent cells and compute the flux between them (flux across a face). The value of $\alpha_p U_{p,i} \langle CN \rangle$ at a face j between two adjacent cells c_1 and c_2 was determined as follows:

$$(\alpha_p U_{p,i} \langle CN \rangle)_j = \frac{1}{2} \left[(\alpha_p U_{p,i} \langle CN \rangle)_{c_1} + (\alpha_p U_{p,i} \langle CN \rangle)_{c_2} \right]. \quad (5.55)$$

The divergence of $\alpha_p U_{p,i} \langle CN \rangle$ for a particular cell with volume V_c and N_f^c faces was computed as follows (see Equation (5.54)):

$$\frac{\partial}{\partial x_i} (\alpha_p U_{p,i} \langle CN \rangle) = \frac{1}{V_c} \sum_{j=1}^{N_f^c} (\alpha_p U_{p,i} \langle CN \rangle)_j n_{i,j} S_j, \quad (5.56)$$

where $(\alpha_p U_{p,i} \langle CN \rangle)_j$ was obtained from Equation (5.55). With the mesoscopic Eulerian method, the source term is calculated using Equation (5.45), where the time derivative and divergence terms are computed using Equations (5.49) and (5.56).

5.4.3 Results

Figure 5.13 displays the distributions of the coordination number source term at a superficial gas velocity of 11.08 mm/s, obtained using the direct Lagrangian and mesoscopic Eulerian methods. The two distributions are identical, indicating consistency between the two methods. The positive source term values imply an increase in the coordination number, while the negative source term values imply a decrease in the coordination number.

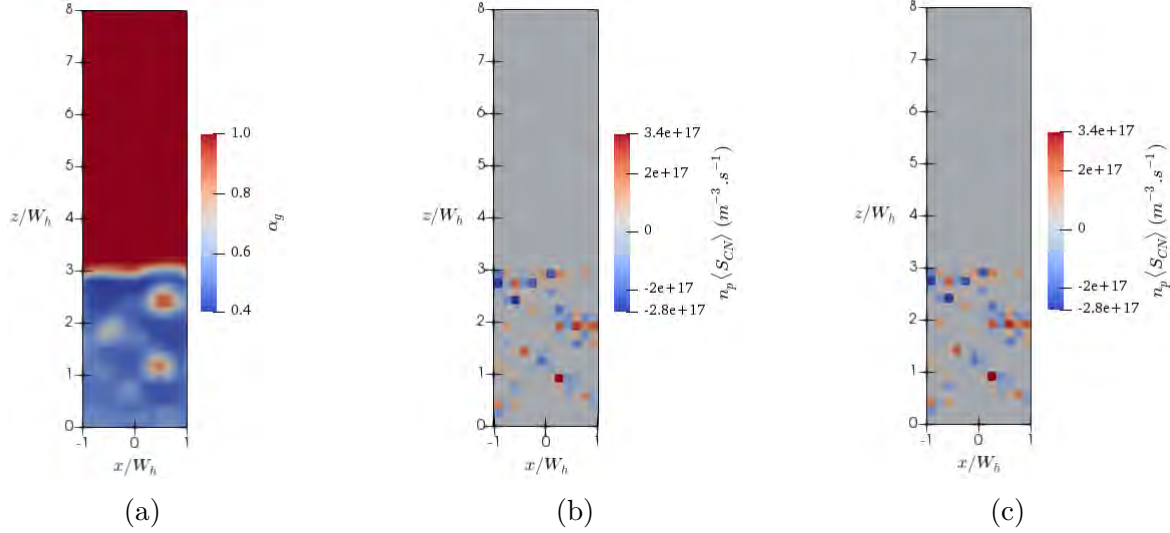


Figure 5.13 Computation of the coordination number source term at $U_g = 11.08$ mm/s: instantaneous distributions of (a) gas volume fraction, (b) coordination number source term computed using the direct Lagrangian method, and (c) coordination number source term computed using the mesoscopic Eulerian method. W_h represents half the width of the cuboid.

Figure 5.14 illustrates the distribution of the coordination number source term, computed using the direct Lagrangian method, for various inlet gas velocities during the fluidization cycle with adhesion. In the fixed bed regime, the coordination number source term is zero everywhere, indicating no change in the coordination number. In the expanded bed regime (homogeneous fluidization), the source term is non-zero in very few cells, and at certain times, it is zero in all cells. To demonstrate this regime adequately, we provide a representative source term distribution in Figure 5.14b. This distribution shows that there are slight variations in the coordination number in the homogeneous fluidization regime. In the bubbling bed regime, the local magnitudes of the source term are higher due to significant variations in the coordination number.

Figure 5.15 shows the distributions of the coordination number source term at a superficial gas velocity of 5.54 mm/s for tests conducted with and without adhesion. Both Figures 5.15a and 5.15b represent the same time instant. As observed, the local magnitudes of the coordination number source term in the absence of adhesion (no homogeneous fluidization regime) are significantly larger than those in the presence of adhesion (homogeneous fluidization). These distributions reveal that the coordination number varies considerably in the absence of adhesion compared to when adhesion is present.

The obtained measurements of the source term are essential for developing and validating a

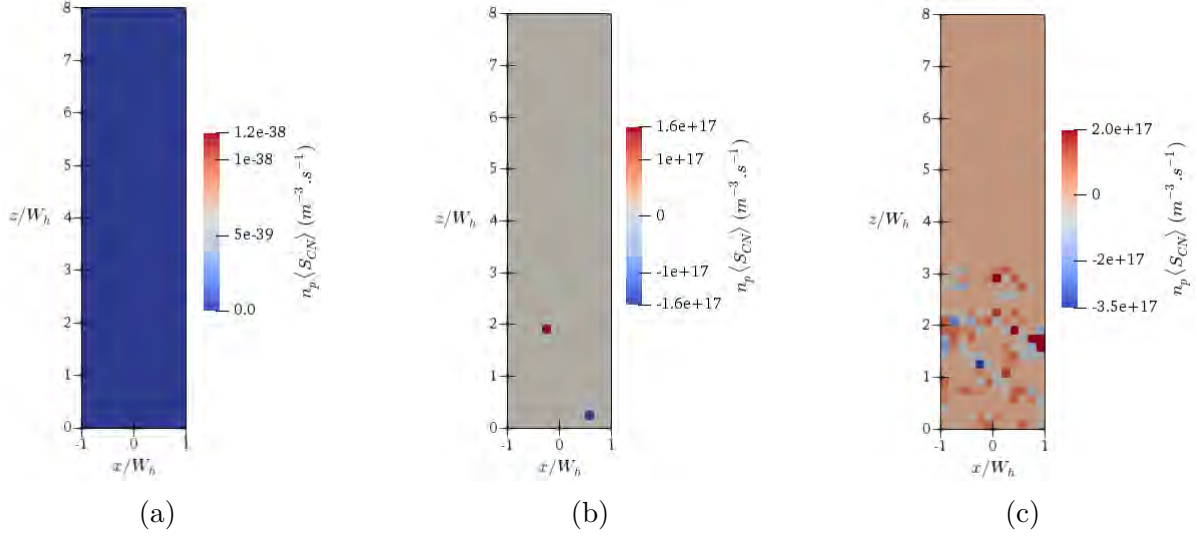


Figure 5.14 Instantaneous distribution of the coordination number source term in the presence of adhesion at different superficial gas velocity values: (a) 0.97 mm/s (fixed bed), (b) 5.54 mm/s (expanded bed), and (c) 11.08 mm/s (bubbling bed).

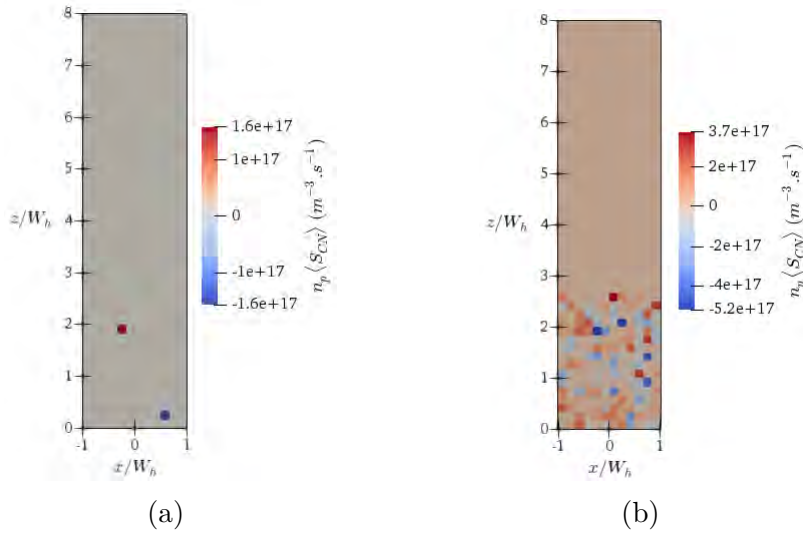


Figure 5.15 Comparison of coordination number source term at a superficial gas velocity of 5.54 mm/s : (a) with vs. (b) without Van der Waals adhesion.

Eulerian model for it. The developed source term expression can then be used in two-fluid simulations to determine the evolution of the coordination number and predict the hysteresis in the bed pressure drop at the macroscale.

5.5 Conclusion

In this study, CFD-DEM simulations were conducted to predict the pressure-drop hysteresis phenomenon observed in fluidized beds of fine solids and to gather information for developing closure models for two-fluid simulations. Since the Coulomb dynamic friction model is suitable for fluidized beds but not for static beds, we implemented and employed a static-dynamic friction model that is appropriate for all flow regimes in our meso-scale simulations. Additionally, we accounted for Van der Waals adhesion.

In a fluidization test case without adhesion, an overshoot attributed to static wall friction was predicted. With adhesion, the intensity of the overshoot increased. A hysteresis in the pressure drop across the fine particle bed was observed. Furthermore, our results reveal that predicting the homogeneous bed expansion between the minimum fluidization and minimum bubbling velocities necessitates accounting for Van der Waals adhesion.

We extracted new numerical data from our fluidization and defluidization CFD-DEM simulations. In addition, we measured the source term of the coordination number transport equation. All these data may be utilized to guide the development of and validate Eulerian models for adhesion and friction, enabling the prediction of hysteresis in the bed pressure drop at the macroscopic scale.

The coordination number source term is affected by the superficial gas velocity and Van der Waals forces. In contrast to the case without Van der Waals adhesion, the presence of adhesion prevents significant variations in the coordination number when the superficial gas velocity is increased to a value between the minimum fluidization velocity and the bubbling threshold. The coordination number source term may be formulated using an expression that relaxes the coordination number towards its equilibrium value. This equilibrium value, corresponding to a specific flow regime (fixed, expanded, or fluidized), may be defined based on the local value of the solid volume fraction. The relaxation time also needs to be determined. The measurements from CFD-DEM simulations conducted in this study represent an important step towards developing a continuum transport equation for the coordination number and predicting pressure hysteresis using Eulerian-Eulerian simulations. This hysteresis should first be compared with that obtained from CFD-DEM simulations and then with that observed in experiments to evaluate the accuracy of the Eulerian model. This could be the focus of future research.

Our fluidization and defluidization simulations did not use spring stiffness values obtained from real material properties, specifically Young's modulus and Poisson's ratio. Using these properties would result in a much higher spring stiffness value, leading to a considerably

smaller contact duration and particle time step, which significantly increases the computational cost. A potential solution to reduce computational cost would be to implement the modified adhesion model suggested by Gu et al. [171], which allows the use of lower spring stiffness values than reality without affecting accuracy.

5.6 Acknowledgments

The authors gratefully acknowledge the CORIA laboratory and the YALES2 community for providing the YALES2 code (CNRS deposit by Vincent Moureau, Ghislain Lartigue, and Pierre Benard). The authors would also like to acknowledge Dr. Yann Dufresne and Dr. Ainur Nigmatova for their valuable discussions on CFD-DEM modeling of fluid-particle flows. This project was provided with computing and storage resources by GENCI on the CSL/SKL partition of the Jean-Zay/Joliot-Curie supercomputer at IDRIS/TGCC thanks to grant A0142B06938, and by CALMIP through grant P1132.

CHAPTER 6 CFD-DEM VALIDATION AND COORDINATION NUMBER SOURCE TERM FORMULATION

6.1 Introduction

In this chapter, DEM tests are performed to validate the static-dynamic friction and Van der Waals adhesion models. The static-dynamic friction model is tested using both micro-scale and macro-scale methods. Micro-scale tests include particle-wall and particle-particle collisions, compared with Walton theory. Macro-scale tests involve the Janssen effect in a silo, compared with Janssen theory. The validation of the Van der Waals force is qualitative and based on micro-scale particle-wall and particle-particle collision tests. Additionally, the validation tests include silo discharge tests compared with the Beverloo correlation and angle of repose tests to examine the influence of dynamic and rolling friction coefficients. Next, preliminary two-fluid simulations are conducted with a coordination number transport equation to predict hysteresis in the bed pressure drop. Moreover, the coordination number source term is measured from CFD-DEM simulations, and a relaxation expression for it is postulated. In addition, numerical stability is enhanced by introducing a stability condition for explicit gas-particle coupling and proposing a penalization approach to achieve semi-implicit coupling.

This chapter is organized as follows: Section 6.2 presents the results of DEM validation tests, Section 6.3 introduces a preliminary formulation of the source term in the coordination number transport equation, and Section 6.4 discusses the coupling between gas and particles.

6.2 DEM validation

6.2.1 Validation of the static-dynamic friction model

Before proceeding with the validation tests of the static-dynamic friction model, we provide additional details about its implementation, complementing the information presented in the previous chapter. The arrays used to accumulate the tangential overlap are as follows:

- (a) Number of potential contact partners of a given particle: $PN(1 : N_g)$.
- (b) Local indices of potential contact partners: $C_p^{loc}(1 : 30, 1 : N_g)$. The first dimension of this array (30), which corresponds to the number of potential contact partners of a given particle, is enlarged when needed.
- (c) Global index of a given particle in a particle group (global index from a local index):

- $J_p^{glob}(1 : N_g)$.
- (d) Coordination number: $CN(1 : N_g)$.
 - (e) Global indices of potential contact partners: $C_p^{glob}(1 : 30, 1 : N_g)$. The first dimension of this array (30) is enlarged when needed. This array represents potential or candidate contact pairs.
 - (f) Global indices of particles in contact (contact pairs): $I_p^{glob}(1 : 12, 1 : N_g)$. The first dimension of this array is chosen as the maximum possible coordination number in the case of non-overlapping spheres ($CN_{max} = 12$) [181]. In our tests, 12 was sufficient. As a precautionary measure, a code line is added that causes an intentional crash if the number of contacts per particle exceeds 12 and advises the user to increase the first dimension of I_p^{glob} and the tangential overlap arrays mentioned below to an appropriate value.
 - (g) x , y , and z components of the tangential overlap between particles in contact: $\delta_{t,x}(1 : 12, 1 : N_g)$, $\delta_{t,y}(1 : 12, 1 : N_g)$, and $\delta_{t,z}(1 : 12, 1 : N_g)$.

The insertion of a (p, q) contact pair into the list of contact pairs is performed as follows:

$$I_p^{glob}(CN(n_p^{loc}) + 1, n_p^{loc}) = J_p^{glob}(C_p^{loc}(k, n_p^{loc})) \quad (6.1)$$

$$\delta_{t,x}(CN(n_p^{loc}) + 1, n_p^{loc}) = 0 \quad (6.2)$$

$$\delta_{t,y}(CN(n_p^{loc}) + 1, n_p^{loc}) = 0 \quad (6.3)$$

$$\delta_{t,z}(CN(n_p^{loc}) + 1, n_p^{loc}) = 0 \quad (6.4)$$

$$CN(n_p^{loc}) = CN(n_p^{loc}) + 1 \quad (6.5)$$

where $k \in \{1, 2, \dots, PN(n_p^{loc})\}$ is an index used to access the potential contact partners of p . By Equation (6.1), the global index of a potential contact partner q ($C_p^{loc}(k, n_p^{loc}) = n_q^{loc}$) is added to the list containing the global indices of the particles in contact with particle p , given that the condition $\delta_{pq,n} > 0$ is satisfied. By Equations (6.2), (6.3), and (6.4), the tangential overlap between particle p and particle q is initialized to zero. According to Equation (6.5), the number of particles in contact with p is increased by 1. Each contact pair is stored twice: for instance, concerning the global indices of particles in contact, the global index of q is added to the I_p^{glob} of p , and at the same time, the global index of p is added to the I_q^{glob} of q . This action is motivated by the fact that by only looking at half the space to find the potential contact partners, a given contact is only encountered once in the loop over all particles, but it is not known beforehand for which of the two particles of the contact. For example, in Figure 6.1, at time t , p can see q , but q can't see p . However, at time $t + \Delta t_p$, q

can see p but not vice versa.

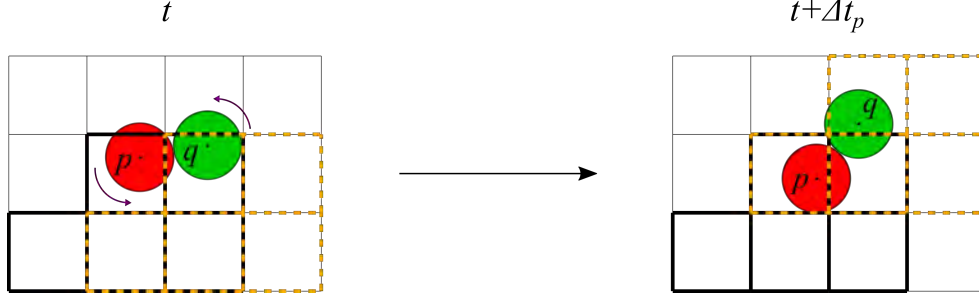


Figure 6.1 One-way detection of a contact partner. The contact pair (p, q) is rotating. —: linked-cell grid. —: cells seen by p . - - -: cells seen by q .

The removal of a (p, q) pair from the list of contact pairs is achieved by copying the last element of the global index and tangential overlap arrays to their respective erase positions, as shown in the following equations:

$$I_p^{glob}(k_c, n_p^{loc}) = I_p^{glob}(CN(n_p^{loc}), n_p^{loc}) \quad (6.6)$$

$$\delta_{t,x}(k_c, n_p^{loc}) = \delta_{t,x}(CN(n_p^{loc}), n_p^{loc}) \quad (6.7)$$

$$\delta_{t,y}(k_c, n_p^{loc}) = \delta_{t,y}(CN(n_p^{loc}), n_p^{loc}) \quad (6.8)$$

$$\delta_{t,z}(k_c, n_p^{loc}) = \delta_{t,z}(CN(n_p^{loc}), n_p^{loc}) \quad (6.9)$$

and decreasing the number of particles in contact with p as follows:

$$CN(n_p^{loc}) = CN(n_p^{loc}) - 1 \quad (6.10)$$

where $k_c \in \{1, 2, \dots, CN(n_p^{loc})\}$ is an index used to access the particles in contact with p at the previous time step, and CN is the coordination number at the previous time step. This erase procedure is illustrated in Figure 6.2. The two copies of a given contact pair are erased: for example, in terms of global indices of particles in contact, the global index of q is erased from the I_p^{glob} of p , and simultaneously, the global index of p is erased from the I_q^{glob} of q .

Each particle situated at a processor boundary has two copies: a real and a ghost. The data of a certain duplicated particle are transmitted from the processor where it is real to the processor where it is a ghost. In addition to previously exchanged information between processors, such as particle position and velocity, data of ghost particles required to compute friction forces, namely I_p^{glob} , $\delta_{t,x}$, $\delta_{t,y}$, $\delta_{t,z}$, CN , J_p^{glob} , $\mathbf{x}_p^{\text{prev}}$, and Δt_p , are transmitted between processors. The cell size used in the linked-cell method is 1.25 times the particle diameter,

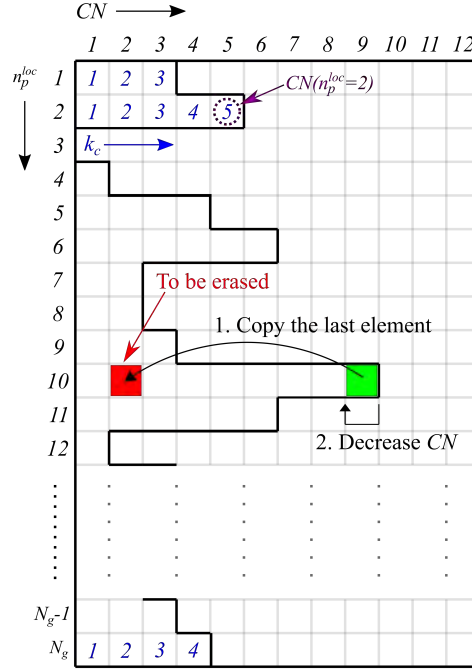


Figure 6.2 Erasing a contact pair. For $n_p^{loc} = 10$, the erase position is at $k_c = 2$. The maximum coordination number is set at 12.

which ensures that the particle remains a potential contact partner when it is no longer in contact, allowing the erasure of the contact pair. The relative error in the sum of contact forces per particle between one-time-step restarts of a packed particle bed using different numbers of processors is verified to be negligible.

In the presence of periodicity, a given particle can be real and ghost at the same time for a given processor if the two periodic boundaries belong to the processor domain boundary. Our algorithm uses global indices to identify contact pairs, which causes an issue in the presence of periodicity because a single particle with a given global index can have two local indices: one is a real particle index and the other is a ghost particle index. The static-dynamic friction model has been implemented in YALES2 for particle-particle and particle-planar wall interactions. Extending the implementation to handle cases with periodic boundaries and/or non-planar walls could be the subject of future work.

In order to validate the model implementation, we performed micro- and macro-scale tests: particle-wall collision, particle-particle collision, and Janssen effect.

Particle-wall collision

Here we compare the rebound angles predicted using the implemented static-dynamic friction model to those predicted by Walton's theoretical model [173] for particle-wall dry collisions at different incidence angles. An oblique particle-wall collision is depicted schematically in Figure 6.3. The values of the parameters used in our particle-wall collision simulations are

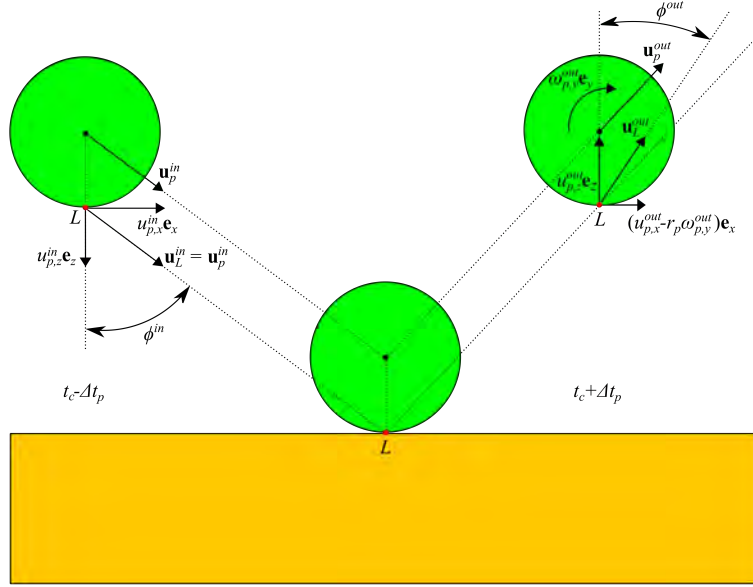


Figure 6.3 Particle-wall collision. t_c is the contact time, and Δt_p is the particle time step. The superscripts *in* and *out* refer to incidence and rebound parameters, respectively; for example, ϕ^{in} and ϕ^{out} are the incidence and rebound angles. $\mathbf{u}_p$ is the translational particle velocity, $\boldsymbol{\omega}_p$ is the particle angular velocity, and r_p is the particle radius. L denotes the point at the bottom of the particle, and $\mathbf{u}_L$ denotes the velocity of this point.

listed in Table 6.1. These simulations are similar to those carried out by Costa et al. [164]. In our simulations, the initial particle's angular velocity, rolling friction torque, and gravity are all set to zero. The numerical scheme of Groot and Warren [82] is used for particle time advancement. According to Walton's model [173], the non-dimensional rebound angle, $\psi^{out} = \tan(\phi^{out})$, is given by the following equation:

$$\psi^{out} = \begin{cases} -e_t \psi^{in}, & \text{for } \psi^{in} \leq \psi_{tr}^{in} \text{ (sticking),} \\ \psi^{in} - \mu_d \left(1 + \frac{1}{K^2}\right) (1 + e_n), & \text{for } \psi^{in} > \psi_{tr}^{in} \text{ (sliding),} \end{cases} \quad (6.11)$$

with

$$\psi_{tr}^{in} = \mu_d \left(1 + \frac{1}{K^2}\right) \frac{1 + e_n}{1 + e_t}, \quad (6.12)$$

Table 6.1 Parameters for the simulations of particle-wall collisions.

Parameter	Value
Particle diameter, d_p	2.5 mm
Particle density, ρ_p	2540 kg/m ³
Normal spring stiffness, k_n	2279 N/m
Normal restitution coefficient, e_n	0.97
Tangential spring stiffness, k_t	710 N/m
Tangential restitution coefficient, e_t	0.39
Dynamic friction coefficient, μ_d	0.1
Magnitude of the initial particle's translational velocity, u_{p0}	0.0025 m/s
Particle time step, Δt_p	2×10^{-5} s

where $\psi^{in} = \tan(\phi^{in})$ is the non-dimensional incidence angle, and K^2 equals 2/5. The value of ψ_{tr}^{in} obtained by substituting the values of μ_d , e_n , and e_t (given in Table 6.1) in Equation (6.12) is 0.496. In our simulations, the non-dimensional incidence and rebound angles are calculated from the velocities at the bottom point L (see Figure 6.3) as follows:

$$\psi^{in} = -\frac{u_{p,x}^{in} - r_p \omega_{p,y}^{in}}{u_{p,z}^{in}} \quad (6.13)$$

$$\psi^{out} = \frac{u_{p,x}^{out} - r_p \omega_{p,y}^{out}}{u_{p,z}^{out}} \quad (6.14)$$

where $\omega_{p,y}^{in} = 0$ in our case. When the positive term $r_p \omega_{p,y}^{out}$ becomes greater than $u_{p,x}^{out}$, the sign of ψ^{out} shifts from positive to negative. As shown in Figure 6.4, the non-dimensional rebound angles predicted by our simulations are in good agreement with those obtained using Walton's model. The theoretical rebound angular velocity determined from the conservation of angular momentum between before and after collision is expressed as:

$$\omega_{p,y}^{out} = \begin{cases} \omega_{p,y}^{in} + \frac{5}{2r_p} \left(\frac{K^2}{K^2 + 1} \right) (1 + e_t) u_{p,x}^{in}, & \text{for } \psi^{in} \leq \psi_{tr}^{in}, \\ \omega_{p,y}^{in} - \frac{5\mu_d}{2r_p} (1 + e_n) u_{p,z}^{in}, & \text{for } \psi^{in} > \psi_{tr}^{in}. \end{cases} \quad (6.15)$$

In our tests, $\omega_{p,y}^{in} = 0$. Figure 6.5 demonstrates that the agreement between simulation and theory for rebound angular velocity is good. The theoretical rotational restitution coefficient is given by the following equation [173]:

$$\beta = \begin{cases} e_t, & \text{if } \beta^* \geq e_t \text{ (sticking),} \\ \beta^*, & \text{if } \beta^* < e_t \text{ (sliding),} \end{cases} \quad (6.16)$$

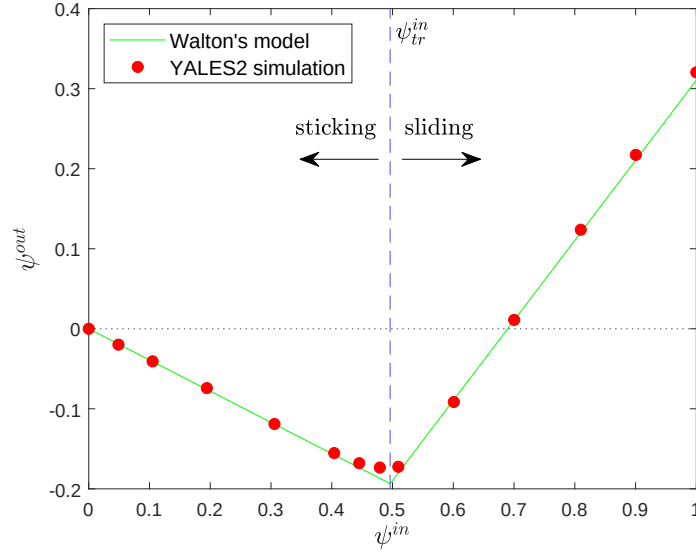


Figure 6.4 Rebound angles of a particle colliding with a wall at different incidence angles. Comparison of simulation results with Walton's model predictions.

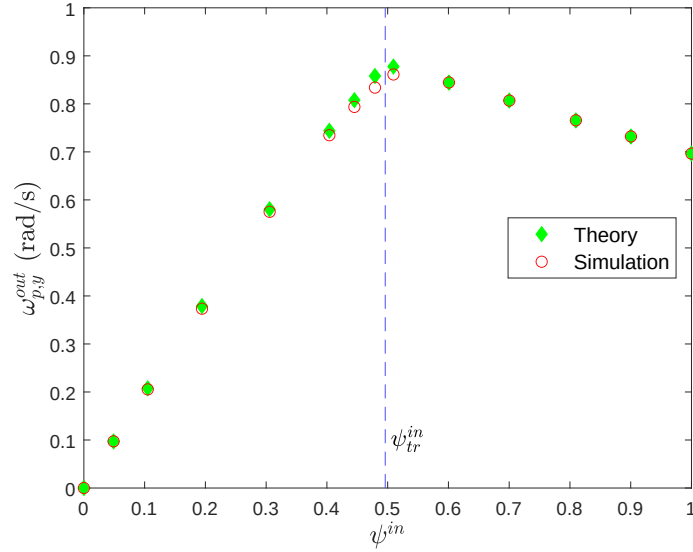


Figure 6.5 Rebound angular velocity of a particle colliding with a wall at various incidence angles. Comparison between YALES2 simulation and theory.

with

$$\beta^* = -1 + \mu_d (1 + e_n) \left(1 + \frac{1}{K^2} \right) \frac{|u_{p,z}^{in}|}{u_{p,x}^{in}}. \quad (6.17)$$

In our simulations, the rotational restitution coefficient is obtained from the tangential velocities of the point L (see Figure 6.3) before and after collision as follows:

$$\beta = -\frac{u_{p,x}^{out} - r_p \omega_{p,y}^{out}}{u_{p,x}^{in}}. \quad (6.18)$$

Figure 6.6 shows that the values of the rotational restitution coefficient obtained from YALES2 simulations agree with those determined theoretically.

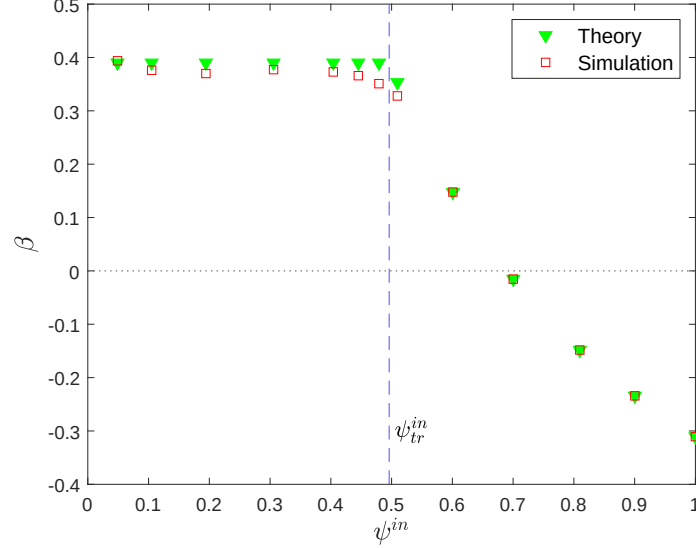


Figure 6.6 Rotational restitution coefficient as a function of non-dimensional incidence angle for particle-wall collisions. Comparison between simulation predictions and theoretical calculations.

Particle-particle collision

A schematic representation of a particle-particle collision is shown in Figure 6.7. As seen in Figure 6.7, a new coordinate system (x'', y, z'') is defined with the z'' axis oriented by the normal unit vector along the line of centers of two interacting particles, $\mathbf{n}_{pq}$, and the x'' axis oriented by the tangential unit vector, $\mathbf{t}_{pq}$. Then, the unit vectors in the directions of the z'' and x'' axes can be expressed in the old coordinate system as:

$$\mathbf{e}_{z''} = \mathbf{n}_{pq} = \begin{pmatrix} n_x \\ 0 \\ n_z \end{pmatrix} \quad (6.19)$$

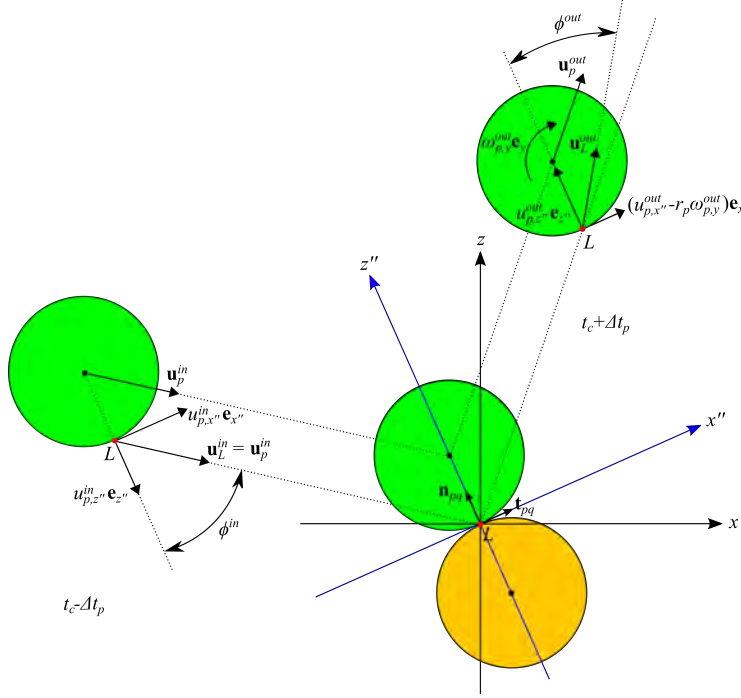


Figure 6.7 Particle-particle collision.

$$\mathbf{e}_{x''} = \mathbf{t}_{pq} = \begin{pmatrix} t_x \\ 0 \\ t_z \end{pmatrix} = \begin{pmatrix} n_z \\ 0 \\ -n_x \end{pmatrix} \quad (6.20)$$

The particle velocity can be transformed into the new coordinate system as follows:

$$u_{p,x''} = \frac{n_z u_{p,x} - n_x u_{p,z}}{n_z^2 + n_x^2} \quad (6.21)$$

$$u_{p,z''} = \frac{u_{p,x} - n_z u_{p,x''}}{n_x} \quad (6.22)$$

The simulation parameters for particle-particle collisions are the same as those used for particle-wall collisions (Table 6.1). In our simulations, a moving particle p collides with a stationary target particle q , which begins moving following the collision. The illustration in Figure 6.7 represents the scenario where the target particle remains at rest after collision, which is not the case in our simulations. The incidence angle is varied by changing the initial z position of the particle p while keeping the same direction of its initial velocity. The non-dimensional incidence and rebound angles are calculated in our simulations as follows:

$$\psi^{in} = -\frac{u_{p,x''}^{in}}{u_{p,z''}^{in}} \quad (6.23)$$

$$\psi^{out} = \frac{u_{q,x''}^{out} - u_{p,x''}^{out} + r_q \omega_{q,y}^{out} + r_p \omega_{p,y}^{out}}{u_{q,z''}^{out} - u_{p,z''}^{out}} \quad (6.24)$$

where particles p and q are identical and $\omega_{p,y}^{in}$ equals zero in our tests. As shown in Figure 6.8, the non-dimensional rebound angles for particle-particle collisions obtained from our DEM simulations are in good agreement with those calculated using Walton's theoretical model (Equation (6.11)).

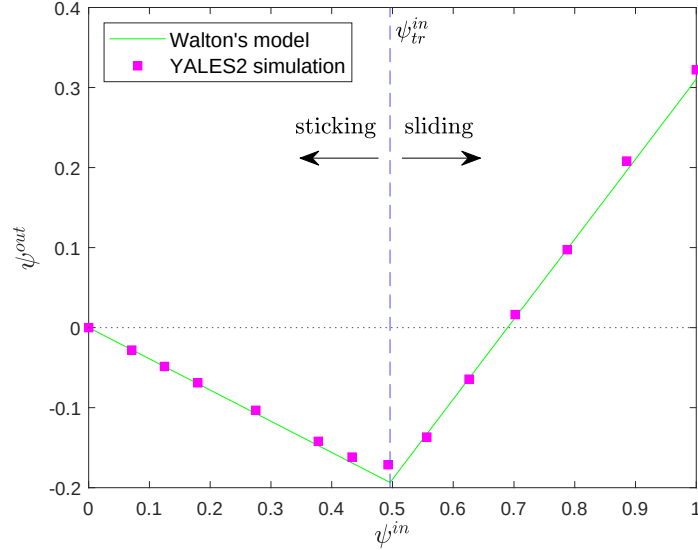


Figure 6.8 Rebound angles of a particle colliding with another particle at various incidence angles. Comparison between YALES2 simulation results and Walton's model calculations.

Janssen effect

Here we compare the vertical solid stress profile predicted by a DEM simulation to that predicted by Janssen's theoretical model [174] for a static bed of soft spheres. In the absence of wall friction, the vertical solid stress increases linearly with depth, similar to how hydrostatic pressure evolves in a liquid. In the presence of wall friction, the vertical solid stress increases linearly up to a certain depth before saturating owing to the shear stress at the sidewalls. The Coulomb dynamic friction model is unsuitable for predicting the Janssen effect (a zero fraction of the solid's weight is supported by the sidewalls because the static wall friction is absent), and the implemented static-dynamic friction model should be used instead.

The parameters used in the simulation are shown in Table 6.2. One layer of non-overlapping particles is seeded at 0.7 m above the bottom of the cuboid. This layer consists of 36 particles, which are seeded every 3000 iterations until the total number of particles given in Table 6.2 is reached. The particles are seeded with random translational and rotational velocities and

Table 6.2 Parameters for the Janssen effect simulation.

Parameter	Value
Cuboid bed height, H	0.8 m
Size of the square cross-section of the cuboid bed, W	0.03 m
Particle diameter, d_p	2.24 mm
Particle density, ρ_p	2500 kg/m ³
Number of particles, N_{tot}	44,460
Interparticle normal spring stiffness, k_n	243 N/m
Interparticle normal restitution coefficient, e_n	0.94
Interparticle tangential spring stiffness, k_t	243 N/m
Interparticle tangential restitution coefficient, e_t	0.94
Interparticle dynamic friction coefficient, μ_d	0.3
Interparticle rolling friction coefficient, μ_r	0.003
Particle-wall normal spring stiffness, k_n^w	243 N/m
Particle-wall normal restitution coefficient, e_n^w	0.9
Particle-wall tangential spring stiffness, k_t^w	243 N/m
Particle-wall tangential restitution coefficient, e_t^w	0.9
Particle-wall dynamic friction coefficient, μ_d^w	0.3
Particle-wall rolling friction coefficient, μ_r^w	0.003
Gravitational acceleration applied in the z -direction, g_z	-9.81 m/s ²
Particle time step, Δt_p	1×10^{-5} s

allowed to settle under gravity. It is worth noting that the filling method had an effect on the vertical solid stress profile; loading all of the particles at once caused stress buildup in particular sections of the bed. For particle time advancement, the Groot and Warren numerical scheme [82] is employed.

The macroscopic collisional stress tensor may be computed using Equation (5.29). The contribution of the particle-wall interactions is not included in the computation of the stress tensor defined in Equation (5.29). The computational domain is divided into slices, as illustrated in Figure 6.9, and the collisional stress is calculated for each slice. The stress tensor component σ_{zz} , for example, is computed according to Equation (5.29) as follows:

$$\sigma_{zz} = -\frac{1}{V} \left(\underbrace{l_{1,z}^1 f_{1,z}^1 + \cdots + l_{1,z}^{c_1} f_{1,z}^{c_1}}_{\text{particle 1}} + \cdots + \underbrace{l_{n_s,z}^1 f_{n_s,z}^1 + \cdots + l_{n_s,z}^{c_{n_s}} f_{n_s,z}^{c_{n_s}}}_{\text{particle } n_s} \right) \quad (6.25)$$

where n_s is the number of particles located inside a given slice of volume V . According to Janssen's theory [174], the vertical solid stress in a cuboid bed of square cross-section is given by:

$$\sigma_{zz} = \rho_p \langle \alpha_p \rangle g \lambda \left(1 - e^{-\zeta/\lambda} \right), \quad (6.26)$$

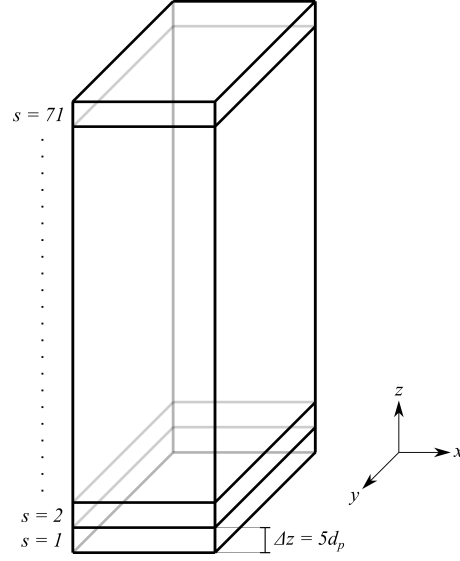


Figure 6.9 Division of the cuboid into slices for Janssen effect tests. s denotes the slice number. Each slice has a thickness $\Delta z = 5d_p$.

with

$$\lambda = \frac{W}{4\mu_d^w S_r}, \quad (6.27)$$

where $\langle\alpha_p\rangle$ is the spatially averaged particle volume fraction, g is the gravitational acceleration, ζ is the depth, W is the width of the bed cross-section, μ_d^w is the wall friction coefficient, and $S_r = \sigma_{xx}/\sigma_{zz} = \sigma_{yy}/\sigma_{zz}$ is the Janssen coefficient. Figure 6.10 shows the collisional stress ratios obtained from our DEM simulation. The value of S_r in Equation (6.27), which is taken as the average of all σ_{xx}/σ_{zz} and σ_{yy}/σ_{zz} points with depths greater than 0.1 m (see Figure 6.10), is 0.53. Figure 6.11 displays profiles of instantaneous vertical stress produced by the YALES2 simulation (Equation (6.25)), vertical stress computed using Janssen's model (Equation (6.26)), and hydrostatic stress. The hydrostatic stress is calculated as follows:

$$\sigma_{zz} = \rho_p \langle\alpha_p\rangle g \zeta. \quad (6.28)$$

As seen in Figure 6.11, the solid stress profile obtained using the implemented static-dynamic friction model accords with Janssen's theory. Due to the influence of static wall friction, the particle stress saturates at a level lower than the hydrostatic stress. Figure 6.12 demonstrates the effect of the dynamic wall friction coefficient used in the DEM simulation on the vertical stress profile. As can be seen, when the wall friction coefficient is larger, the vertical stress saturates at a lower level. Figure 6.13 illustrates the effect of the bed width on the vertical stress profile. As we can see, increasing the bed width reduces the effect of static wall friction

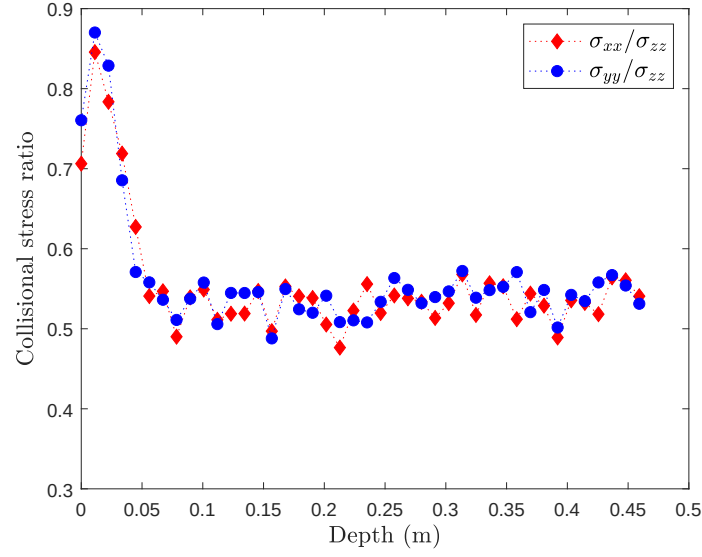


Figure 6.10 Collisional stress ratio vs. depth in a static bed of soft particles.

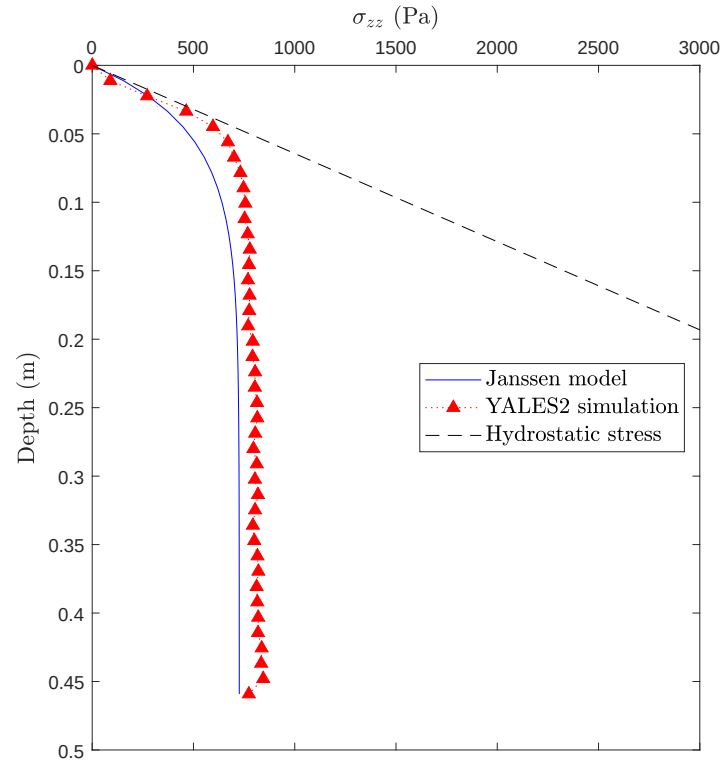


Figure 6.11 Vertical solid stress as a function of depth. Comparison of Janssen theory, DEM simulation, and hydrostatic stress.

on the vertical solid stress.

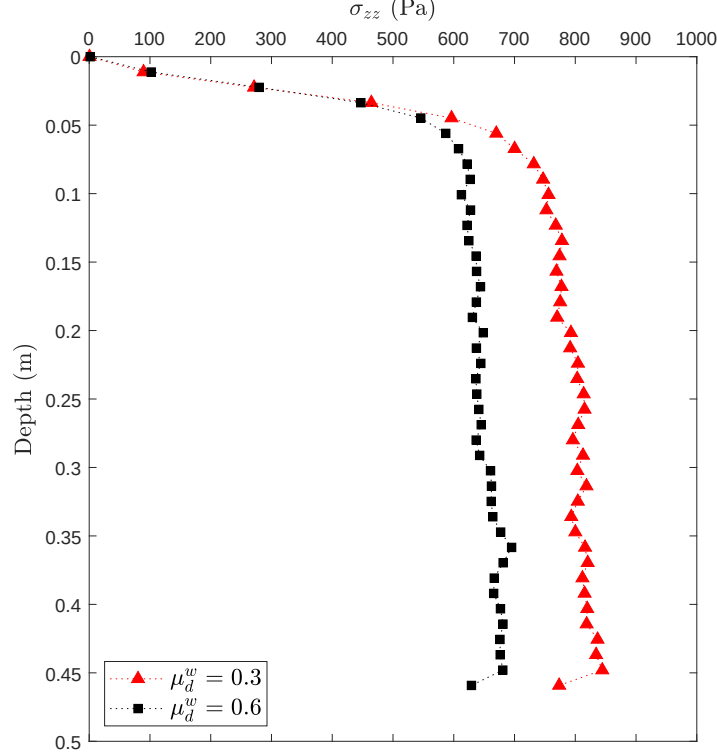


Figure 6.12 Effect of the wall friction coefficient on the vertical solid stress profile.

6.2.2 Validation of the Van der Waals adhesion model

The implementation of the Van der Waals force in DEM was presented previously in Section 5.2.2.

Particle-particle collision

We perform particle-particle collision tests to qualitatively verify the implementation of the Van der Waals force in YALES2. These tests are similar to those in [176, 177] and are illustrated in Figure 6.14. The parameters used in these simulations are given in Table 6.3. The Groot and Warren scheme [82] is used for particle time advancement. The particle time step is chosen very small (see Table 6.3) to guarantee accurate resolution of particle-particle interaction in the presence of adhesion. There is no rolling friction or gravitational force considered in these simulations. The base value of the Hamaker constant specified in Table 6.3 gives an adhesion force that is five times the force of gravity acting on the particle ($\mathbf{F}_{q \rightarrow p}^{ad} = 5m_p \mathbf{g}$).

First, we explore the impact of the Hamaker constant on various parameters, including rebound translational and rotational velocities, contact time, and maximum normal overlap,

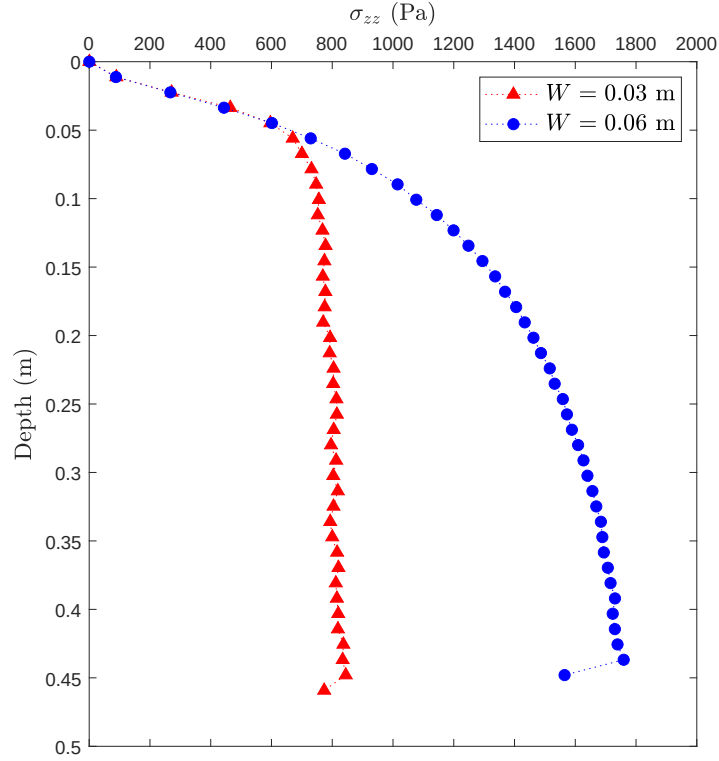


Figure 6.13 Effect of the bed width on the vertical solid stress profile using $\mu_d^w = 0.3$.

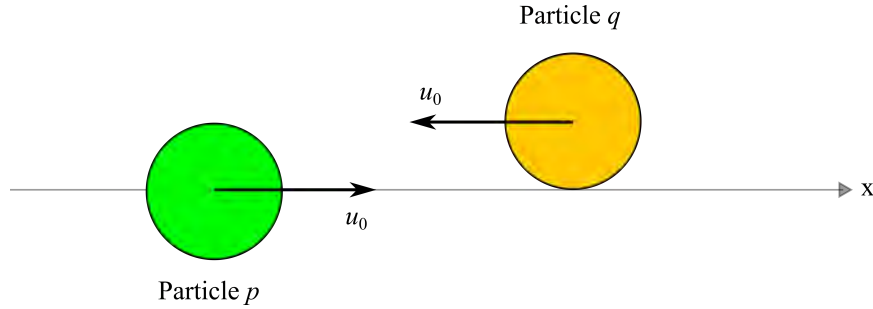


Figure 6.14 Collision between two identical spheres. u_0 is the initial particle's translational velocity.

as illustrated in Figure 6.15. This figure shows that the curves without adhesion coincide with the curves using a Hamaker constant of 6.225×10^{-20} J, which is attributed to the significant inertia of the simulated particles. Increasing the Hamaker constant to 3.4×10^{-16} J decreases the rebound translational velocity and increases the rebound rotational velocity, which is consistent with the findings of Kosinski and Hoffmann [176]. Figures 6.15c and 6.15d indicate that augmenting the Hamaker constant to 3.4×10^{-16} J extends the contact time and increases the maximum normal overlap due to increased adhesion. Figure 6.15 demonstrates

Table 6.3 Simulation parameters for interparticle collisions with Van der Waals adhesion.

Parameter	Value
Particle diameter, d_p	500 μm
Particle density, ρ_p	2525 kg/m^3
Base value of the normal spring stiffness, k_n	77199 N/m
Normal restitution coefficient, e_n	0.9
Base value of the tangential spring stiffness, k_t	22054 N/m
Tangential restitution coefficient, e_t	0.9
Dynamic friction coefficient, μ_d	0.1
Particle time step, Δt_p	6.6×10^{-8} s
Minimum cutoff distance, S_0	4×10^{-10} m
Base value of the Hamaker constant, A	6.225×10^{-20} J

that as the impact translational velocity rises, the maximum normal overlap and the rebound translational and rotational velocities increase due to increased kinetic energy. The contact time decreases with the increase in impact translational velocity for $A = 3.4 \times 10^{-16}$ J, while remaining approximately constant for the case without adhesion.

Then, we examine the influence of spring stiffness on the rebound translational and rotational velocities, contact time, and maximum normal overlap for interparticle collisions using $A = 6.225 \times 10^{-20}$ J, as shown in Figure 6.16. Since e_n is equal to e_t (see Table 6.3), we employ the relationship $k_t = 2k_n/7$ [182]. Consequently, with k_n values of 77,199 and 975,746 N/m (see Figure 6.16), corresponding k_t values of 22,054 and 278,784 N/m are used, respectively. Using the specified Hamaker constant value, the increase in spring stiffness exhibits a negligible impact on the rebound translational and rotational velocities. Conversely, the contact time and maximum normal overlap decrease with increasing spring stiffness.

Next, we analyze the effect of spring stiffness on the rebound translational and rotational velocities, contact duration, and maximum normal overlap using a Hamaker constant of 3.4×10^{-16} J, as depicted in Figure 6.17. With this value of the Hamaker constant, increasing the spring stiffness results in higher rebound translational velocity and lower rebound rotational velocity. The contact time is inversely proportional to the spring stiffness, as shown in Figure 6.17c. The maximum normal overlap decreases with the increase in spring stiffness, as illustrated in Figure 6.17d. The effect of increasing the spring stiffness, which serves as an energy reservoir and represents repulsion, is opposite to the effect of increasing the Hamaker constant, which represents adhesion (see Figures 6.15 and 6.17).

The normal overlap as a function of time during interparticle collisions is depicted in Figure 6.18 for an impact translational velocity of 0.45 m/s, with varying spring stiffness and

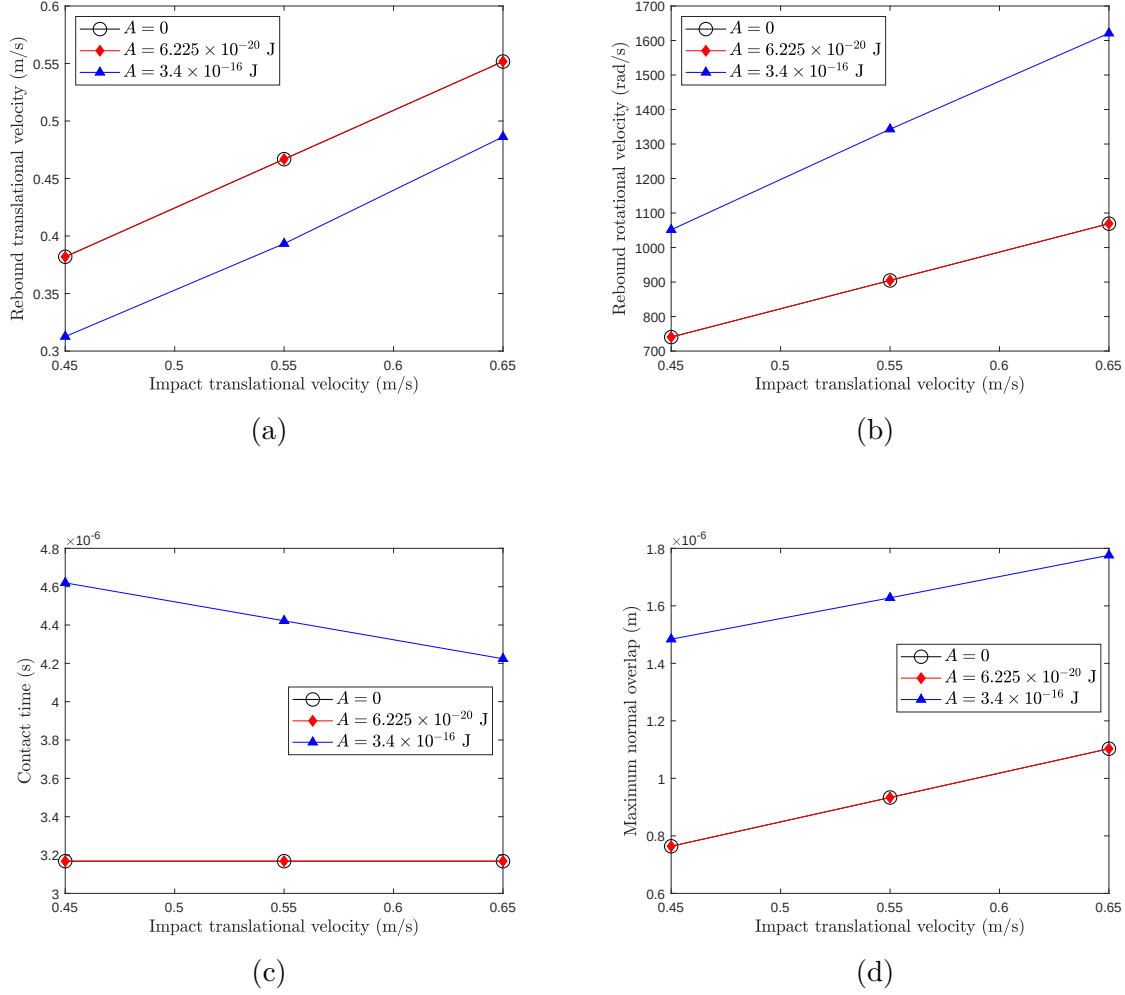


Figure 6.15 Impact of the Hamaker constant on interparticle collisions: (a) rebound translational velocity, (b) rebound rotational velocity, (c) contact time, and (d) maximum normal overlap.

Hamaker constant values. The tangential spring stiffness used in these tests is $k_t = 2k_n/7$. In Figure 6.18, it is evident that increasing the Hamaker constant to 3.4×10^{-16} J leads to a higher maximum normal overlap and longer collision time. On the contrary, when the spring stiffness is increased for a given Hamaker constant value, the collision time and maximum normal overlap decrease.

Particle-wall collision

In addition to the particle-particle collision tests, we conduct particle-wall collision simulations with adhesion. The parameters for particle-wall collisions match those outlined in

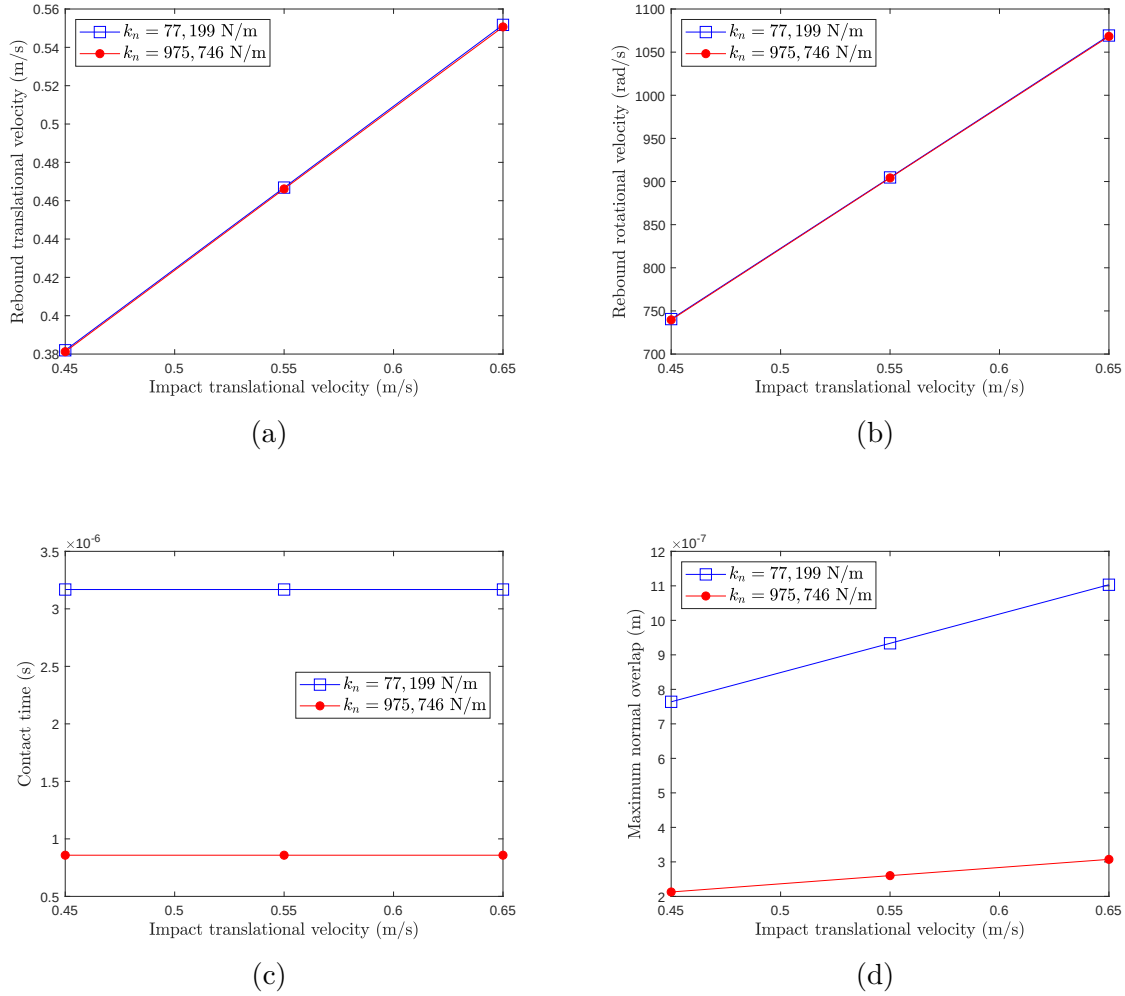


Figure 6.16 Effect of the spring stiffness on interparticle collisions using $A = 6.225 \times 10^{-20} \text{ J}$: (a) rebound translational velocity, (b) rebound rotational velocity, (c) contact time, and (d) maximum normal overlap.

Table 6.3 for particle-particle collisions. Our simulations for particle-wall collisions use an impact translational velocity of 0.45 m/s and an angle of incidence of 45° . Figure 6.19 depicts the normal overlap over time in these particle-wall collisions, with different values for spring stiffness and Hamaker constant. The trends observed in this figure mirror those seen for particle-particle collisions.

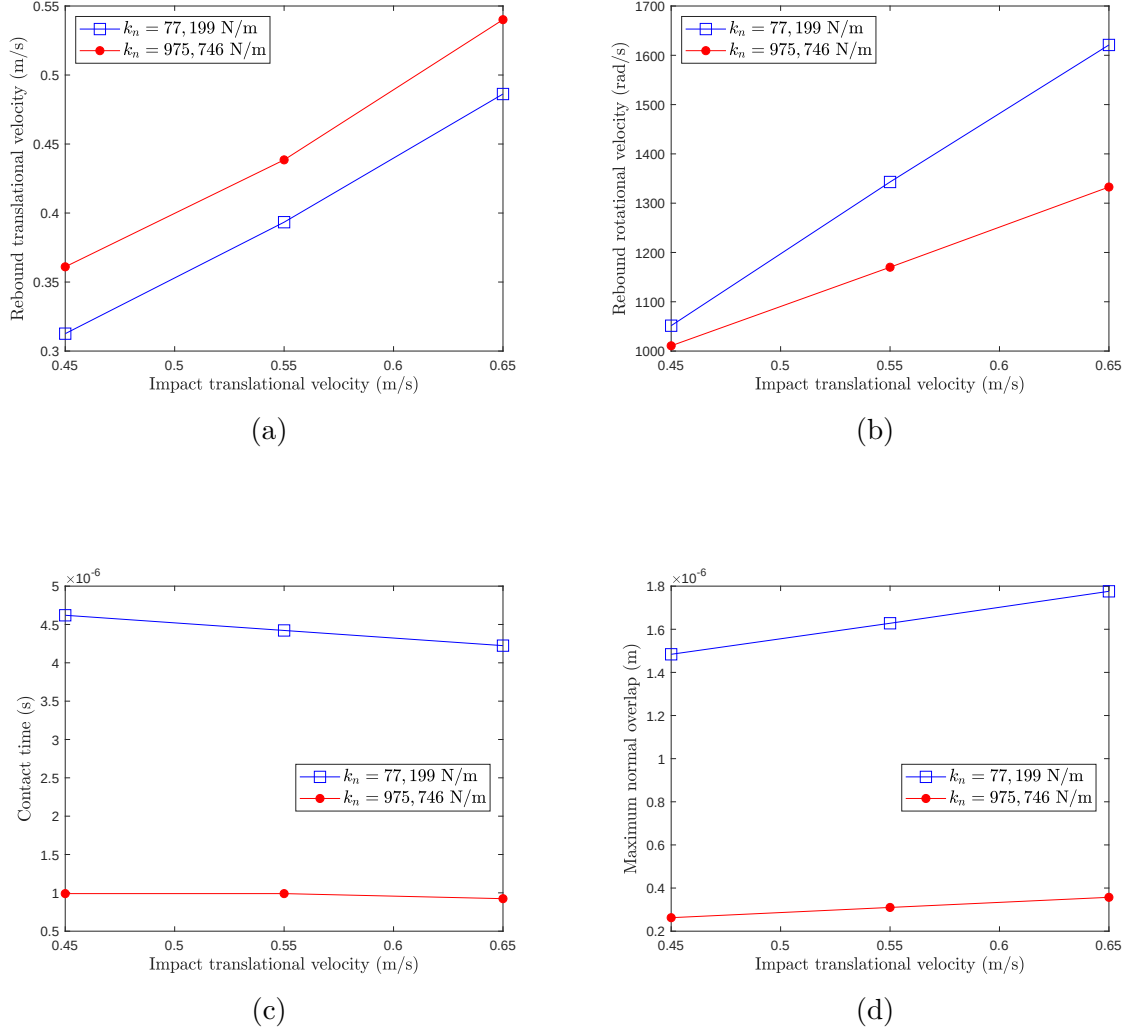


Figure 6.17 Effect of the spring stiffness on interparticle collisions using $A = 3.4 \times 10^{-16} \text{ J}$: (a) rebound translational velocity, (b) rebound rotational velocity, (c) contact time, and (d) maximum normal overlap.

6.2.3 Additional DEM validation tests

Particle rolling on a wall

In this test, we examine the effects of rolling and dynamic friction on a particle rolling on a wall. The rolling friction torque is modeled as follows [183–185]:

$$\mathbf{M}_p^r = -\mu_r \|\mathbf{f}_{q \rightarrow p,n}^c\| r_{pq} \frac{\boldsymbol{\omega}_{pq}}{\|\boldsymbol{\omega}_{pq}\|}. \quad (6.29)$$

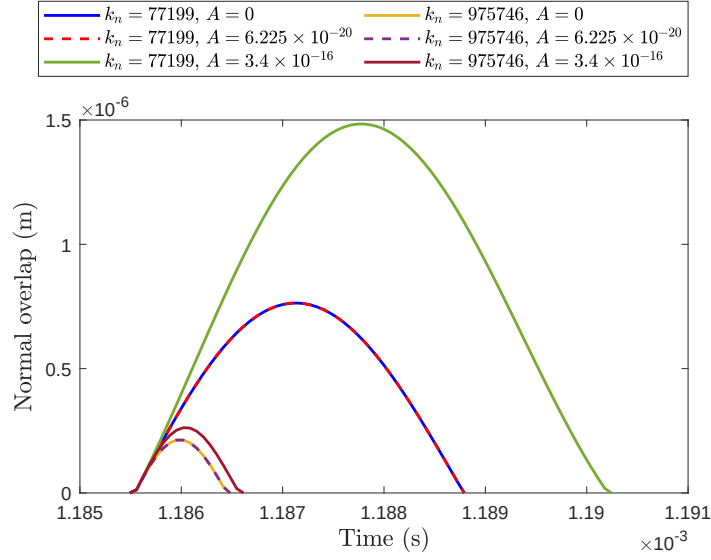


Figure 6.18 Normal overlap as a function of time during particle-particle collisions with an impact translational velocity of 0.45 m/s.

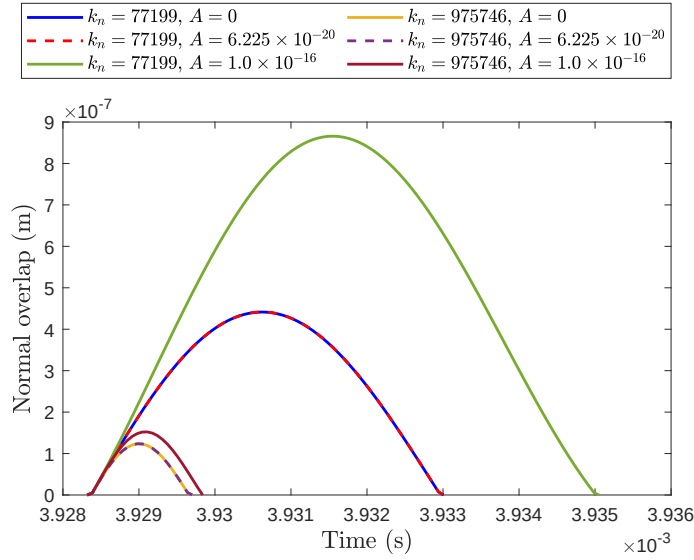


Figure 6.19 Normal overlap as a function of time during particle-wall collisions with an impact translational velocity of 0.45 m/s and an angle of incidence equal to 45° .

Here, μ_r represents the coefficient of rolling friction, $\omega_{pq} = \omega_p - \omega_q$ denotes the relative angular velocity, and $r_{pq} = (1/r_p + 1/r_q)^{-1}$ stands for the effective radius. The simulation parameters employed are presented in Table 6.4. A particle with zero initial velocity was first allowed to settle on the wall under the influence of gravity (9.81 m/s^2). After the particle

Table 6.4 Parameters for the simulation of a particle rolling on a wall.

Parameter	Value
Particle diameter, d_p	2.5 mm
Particle density, ρ_p	2540 kg/m ³
Normal spring stiffness, k_n	2279 N/m
Normal restitution coefficient, e_n	0.97
Tangential spring stiffness, k_t	710 N/m
Tangential restitution coefficient, e_t	0.39
Particle time step, Δt_p	2×10^{-5} s

settled, it was initially given a translational velocity parallel to the wall with a magnitude of 0.1 m/s and a zero rotational velocity.

Figure 6.20 displays the distance traveled by the particle as a function of time for different values of the dynamic and rolling friction coefficients. As seen, the particle travels a specific distance and then stops. The distance traveled by the particle decreases as the rolling or dynamic friction coefficient increases. This is because friction acts against the particle's movement.

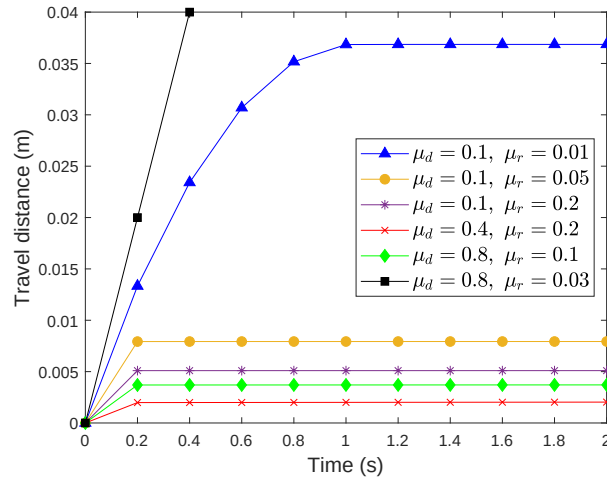


Figure 6.20 Distance traveled by a particle rolling on a wall as a function of time for different values of the dynamic and rolling friction coefficients (μ_d and μ_r , respectively).

Angle of repose

Several authors have utilized the angle of repose method to evaluate interparticle interactions [184, 186–188]. In this section, we perform angle of repose DEM tests using the ledge and

funnel methods to study the effects of dynamic and rolling friction coefficients on the angle of repose.

Ledge method The simulation parameters for the angle of repose tests using the ledge method are detailed in Table 6.5.

Table 6.5 Simulation parameters for the angle of repose using the ledge method.

Parameter	Value
Cuboid bed height, H	0.6 m
Size of the square cross-section of the cuboid bed, W	0.2 m
Particle diameter, d_p	5.756 mm
Particle density, ρ_p	3000 kg/m ³
Number of particles, N_{tot}	29,524
Interparticle normal spring stiffness, k_n	11121.33 N/m
Interparticle normal restitution coefficient, e_n	0.15
Interparticle tangential spring stiffness, k_t	11121.33 N/m
Interparticle tangential restitution coefficient, e_t	0.15
Interparticle dynamic friction coefficient, μ_d	0.5 (base value)
Interparticle rolling friction coefficient, μ_r	0.3 (base value)
Particle-wall normal spring stiffness, k_n^w	11121.33 N/m
Particle-wall normal restitution coefficient, e_n^w	0.15
Particle-wall tangential spring stiffness, k_t^w	11121.33 N/m
Particle-wall tangential restitution coefficient, e_t^w	0.15
Particle-wall dynamic friction coefficient, μ_d^w	0.5
Particle-wall rolling friction coefficient, μ_r^w	0.3
Gravitational acceleration applied in the z -direction, g_z	-9.81 m/s ²
Particle time step, Δt_p	2×10^{-5} s

The particles were seeded and permitted to settle under gravity during the first 4 seconds. Subsequently, the right wall was set as an outlet for the particles to form a slope over 6 seconds. The numerical scheme used for particle time advancement is the Groot and Warren scheme [82]. The rolling friction model employed is the Beer and Johnston model [183], which is given by Equation 6.29.

First, we studied the influence of the interparticle dynamic friction coefficient on the angle of repose while maintaining a fixed interparticle rolling friction coefficient of 0.3. Figure 6.21 illustrates the variation of the angle of repose with the interparticle dynamic friction coefficient. As observed, a higher dynamic friction coefficient results in a higher angle of repose. Figure 6.22 depicts the slopes formed at various dynamic friction coefficient values. This figure demonstrates that steeper slopes form at higher dynamic friction coefficients.

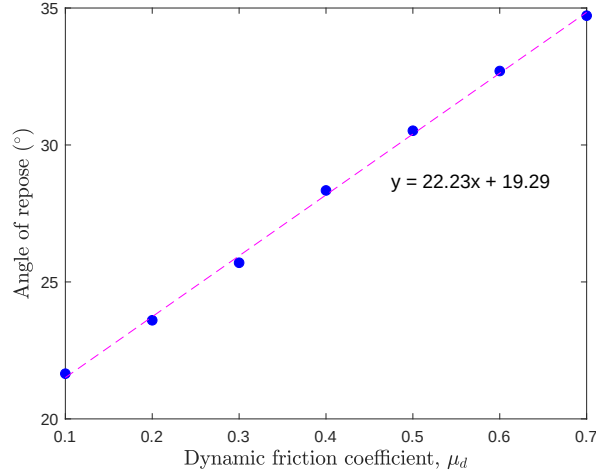


Figure 6.21 Variation of angle of repose with interparticle dynamic friction coefficient using the ledge method.

Next, we examined the influence of the interparticle rolling friction coefficient on the angle

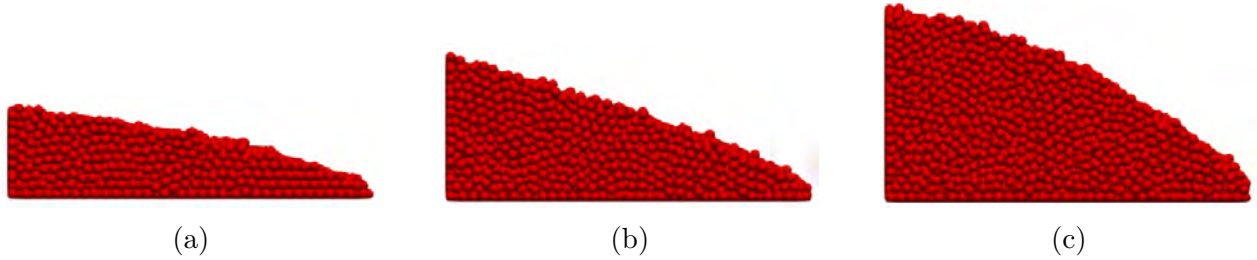


Figure 6.22 Slopes created using the ledge method with different values of the interparticle dynamic friction coefficient: (a) $\mu_d = 0$, (b) $\mu_d = 0.1$, and (c) $\mu_d = 0.3$.

of repose while maintaining a fixed interparticle dynamic friction coefficient of 0.5. These tests varied only the rolling friction between particles, while the particle-wall rolling friction coefficient remained fixed at 0.3. As shown in Figure 6.23, increasing the interparticle rolling friction coefficient leads to a higher angle of repose. The regression line's slope in Figure 6.23 is higher than that in Figure 6.21. This indicates that the rolling friction coefficient has a more pronounced effect on the angle of repose than the dynamic friction coefficient. Figure 6.24 depicts slopes formed at different values of the interparticle rolling friction coefficient. As shown in this figure, a higher rolling friction coefficient results in a steeper slope.

Funnel method The parameters used in the simulations of the angle of repose using the funnel method are provided in Table 6.6. The geometry and mesh used in these simulations

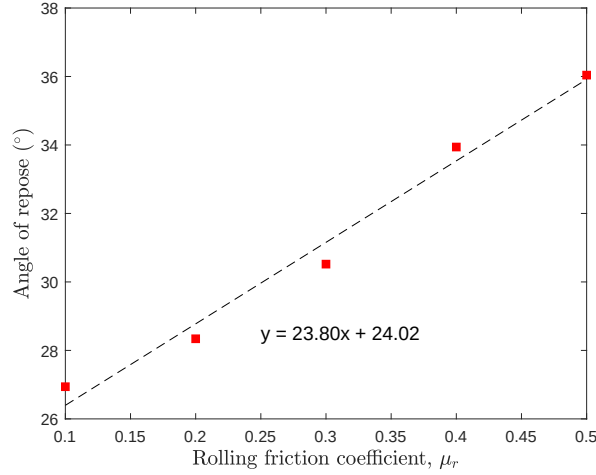


Figure 6.23 Variation of angle of repose with interparticle rolling friction coefficient using the ledge method.

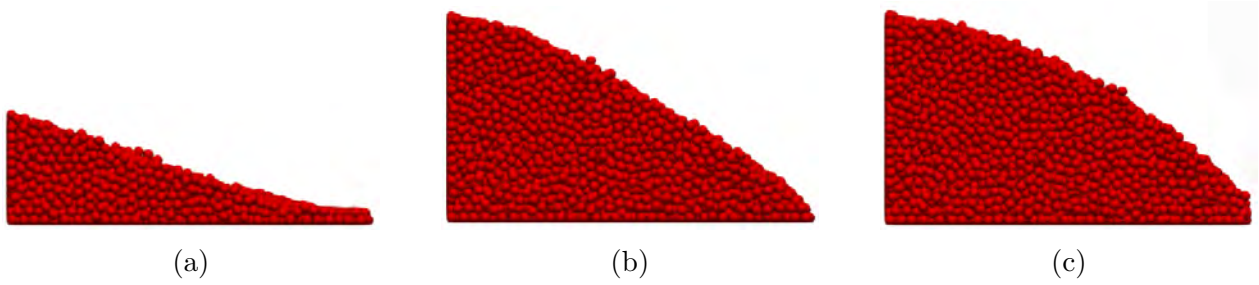


Figure 6.24 Slopes created using the ledge method with different values of the interparticle rolling friction coefficient: (a) $\mu_r = 0$, (b) $\mu_r = 0.1$, and (c) $\mu_r = 0.3$.

are illustrated in Figure 6.25. The particles were seeded in the upper region of the geometry and allowed to fall under gravity to the lower region. The numerical scheme employed for particle time advancement is the Groot and Warren scheme [82]. The rolling friction model used is the Beer and Johnston model [183]. For particle-wall interactions, the Coulomb dynamic friction model was employed with $\mu_d^w = 0.5$. The simulation time is 7.5 seconds.

First, we studied the effect of the interparticle dynamic friction coefficient on the angle of repose using an interparticle rolling friction coefficient of 0.3. The angle of repose was determined as the average of the right and left angles of the heap. Figure 6.26 displays how the angle of repose varies with the interparticle dynamic friction coefficient, and Figure 6.27 depicts heaps formed at different values of the interparticle dynamic friction coefficient. These figures demonstrate that as the interparticle dynamic friction coefficient increases, so does the angle of repose.

Table 6.6 Simulation parameters for the angle of repose using the funnel method.

Parameter	Value
Particle diameter, d_p	5.756 mm
Particle density, ρ_p	3000 kg/m ³
Number of particles, N_{tot}	2,800
Interparticle normal spring stiffness, k_n	11121.33 N/m
Interparticle normal restitution coefficient, e_n	0.15
Interparticle tangential spring stiffness, k_t	11121.33 N/m
Interparticle tangential restitution coefficient, e_t	0.15
Interparticle dynamic friction coefficient, μ_d	0.5 (base value)
Interparticle rolling friction coefficient, μ_r	0.3 (base value)
Particle-wall normal spring stiffness, k_n^w	11121.33 N/m
Particle-wall normal restitution coefficient, e_n^w	0.15
Particle-wall dynamic friction coefficient, μ_d^w	0.5
Particle-wall rolling friction coefficient, μ_r^w	0.3
Gravitational acceleration applied in the y -direction, g_y	-9.81 m/s ²
Particle time step, Δt_p	2×10^{-5} s

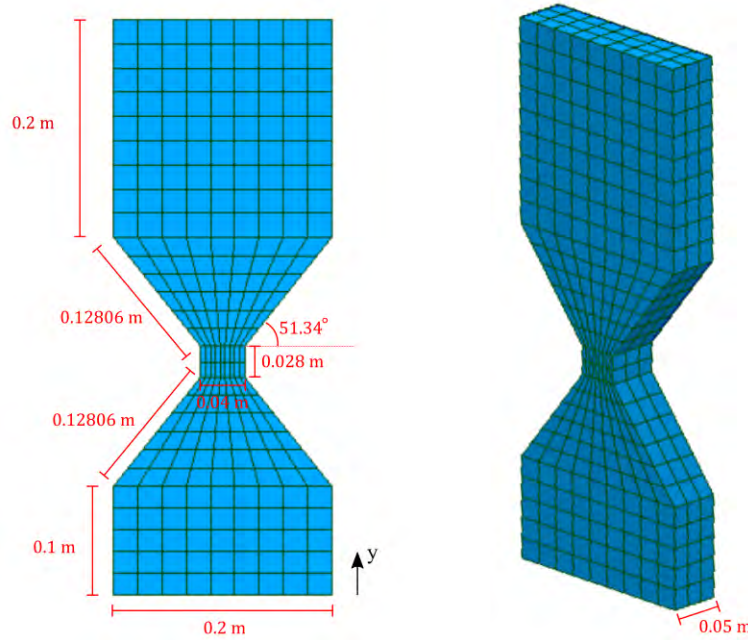


Figure 6.25 Mesh 2D and 3D views for angle of repose simulations using the funnel method.

Figure 6.28 illustrates how the angle of repose varies with the interparticle rolling friction coefficient, and Figure 6.29 shows heaps formed at various values of the interparticle rolling friction coefficient. These figures show that as the interparticle rolling friction coefficient increases, the angle of repose increases. The slope of the regression line in Figure 6.28 is

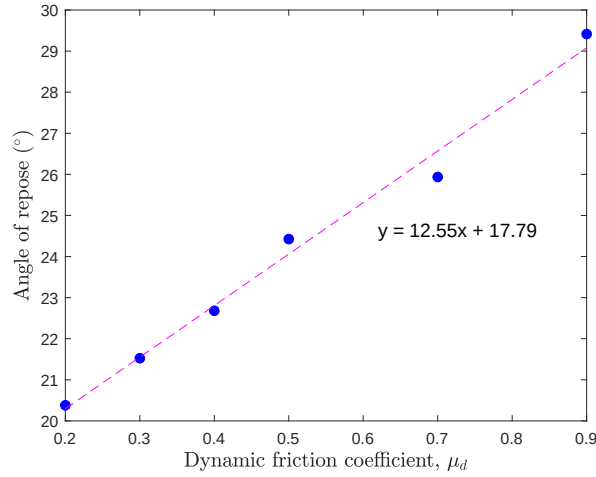


Figure 6.26 Variation of angle of repose with interparticle dynamic friction coefficient using the funnel method.

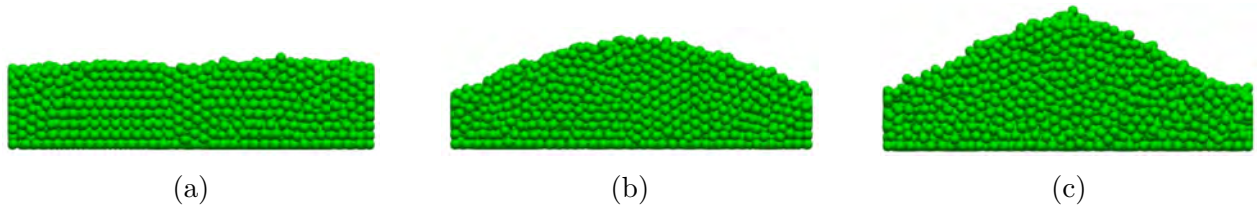


Figure 6.27 Slopes created using the funnel method with different values of the interparticle dynamic friction coefficient: (a) $\mu_d = 0$, (b) $\mu_d = 0.2$, and (c) $\mu_d = 0.7$.

higher than that of the regression line in Figure 6.26. This suggests that the impact of the rolling friction coefficient on the angle of repose is greater than that of the dynamic friction coefficient.

Hopper discharge

Several researchers have studied the influence of interparticle friction on the rate of discharge from hoppers and silos [175, 189, 190]. The parameters for the hopper discharge simulation are detailed in Table 6.7.

The geometry and mesh used in this simulation are illustrated in Figure 6.30. The total time of the simulation is 9 seconds. From 0 to 4 seconds, particles were seeded in batches (3,040 particles every 26,000 iterations) and allowed to settle under gravity in the upper part of the geometry. During this filling stage, an additional wall was positioned at a height of 0.162216 meters to close the opening in the middle of the geometry. Subsequently, from 4 to 9

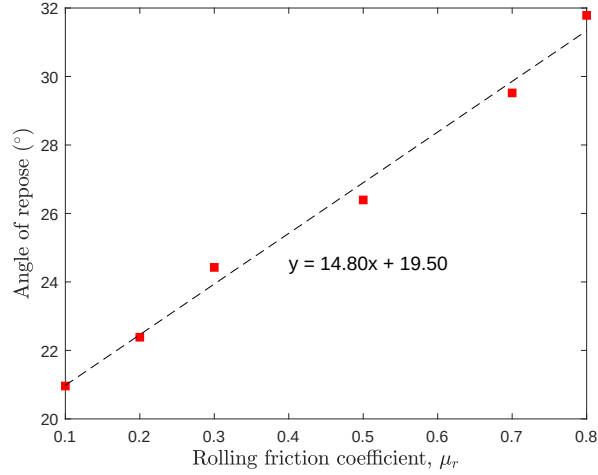


Figure 6.28 Variation of angle of repose with interparticle rolling friction coefficient using the funnel method.

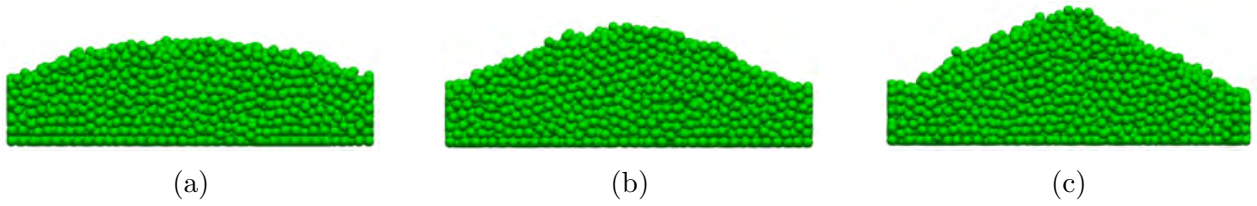


Figure 6.29 Slopes created using the funnel method with different values of the interparticle rolling friction coefficient: (a) $\mu_r = 0$, (b) $\mu_r = 0.1$, and (c) $\mu_r = 0.3$.

seconds, the hopper was discharged by removing this additional wall. The numerical scheme employed for particle time advancement is the Groot and Warren scheme [82]. The rolling friction model used is the Beer and Johnston model [183]. For particle-wall interactions, the Coulomb dynamic friction model was employed with $\mu_d^w = 0.2$.

Figure 6.31 shows the coordination number distribution after filling and during the discharge of the hopper. There is a homogeneous distribution of the coordination number in the settled bed, with an average coordination number of around 5. During the hopper discharge, the falling particles have a coordination number of zero.

Figure 6.32 demonstrates the number of particles remaining in the upper part of the geometry (N_p) as a function of time (t). It shows the decrease in the number of particles in the hopper during the discharge phase.

The total mass of particles in the hopper before the discharge is $M_b = m_p N_{tot} = 0.626$ kg, where m_p denotes the mass of a single particle. The segment of the $t - N_p$ curve between 4.12

Table 6.7 Parameters for the hopper discharge simulation.

Parameter	Value
Particle diameter, d_p	2.24 mm
Particle density, ρ_p	2500 kg/m ³
Number of particles, N_{tot}	42,560
Interparticle normal spring stiffness, k_n	243 N/m
Interparticle normal restitution coefficient, e_n	0.94
Interparticle tangential spring stiffness, k_t	243 N/m
Interparticle tangential restitution coefficient, e_t	0.94
Interparticle dynamic friction coefficient, μ_d	0.2
Interparticle rolling friction coefficient, μ_r	0.09
Particle-wall normal spring stiffness, k_n^w	243 N/m
Particle-wall normal restitution coefficient, e_n^w	0.9
Particle-wall dynamic friction coefficient, μ_d^w	0.2
Particle-wall rolling friction coefficient, μ_r^w	0.09
Gravitational acceleration applied in the z -direction, g_z	-9.81 m/s ²
Particle time step, Δt_p	1×10^{-5} s

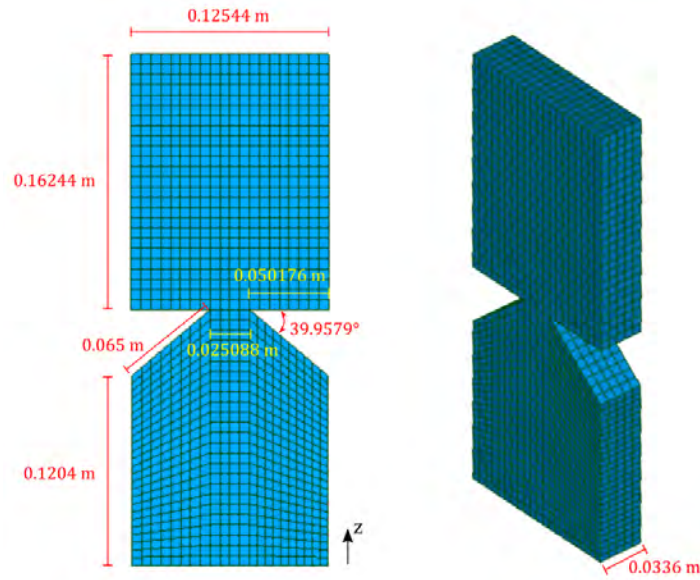


Figure 6.30 Mesh 2D and 3D views for the hopper discharge simulation.

and 5 seconds (see Figure 6.32) was fitted using a first-order polynomial function, with a_c representing its slope. Then, the mass flow rate of powder exiting the hopper was calculated in the following way:

$$\dot{M} = a_c m_p = 0.483 \text{ kg/s.} \quad (6.30)$$

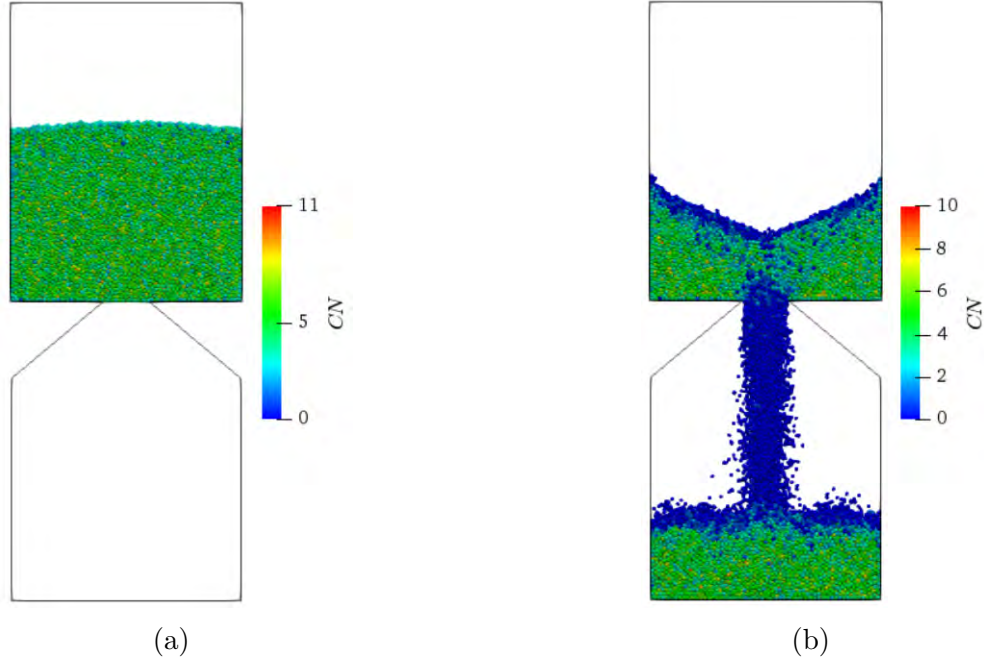


Figure 6.31 Coordination number distribution: (a) in the filled hopper at $t = 4.0$ s, and (b) during hopper discharge at $t = 4.7$ s.

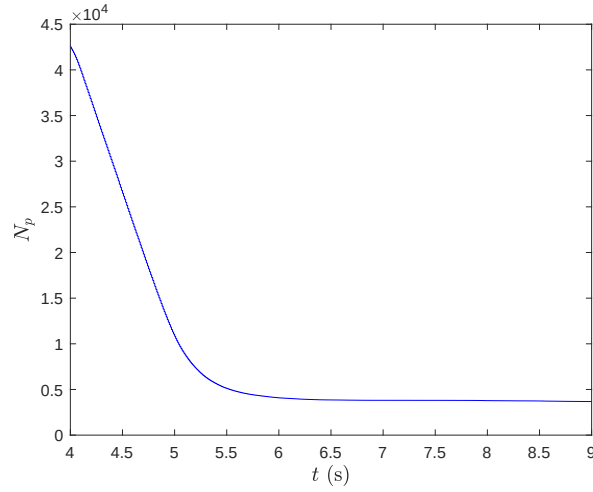


Figure 6.32 Number of particles remaining in the hopper as a function of time during the discharge stage.

The Beverloo correlation for a rectangular hopper is [175]:

$$\dot{M} = 1.03g^{1/2}\rho_b(L_e - C_h d_p)(W_e - C_h d_p)^{3/2}. \quad (6.31)$$

Here, ρ_b represents the bulk density of the bed, L_e stands for the length of the hopper opening, W_e denotes the width of the hopper opening, and C_h signifies the Beverloo constant, which has a value of 1.5 for particles of spherical shape [190]. The static bulk density was obtained as follows:

$$\rho_b = \frac{M_b}{V_b} = \frac{m_p N_{tot}}{W_b T_b H_b}, \quad (6.32)$$

where V_b denotes the total volume of the bed, W_b signifies the width of the bed, T_b stands for the thickness of the bed, and H_b represents the height of the bed. While we used the static bulk density in the Beverloo correlation, it is proposed to employ the flowing bulk density [175]. For the definition of the flowing bulk density, refer to the study by Artega and Tuzun [189]. By substituting the values of all parameters into the Beverloo correlation (Equation 6.31), we determined $\dot{M}$ to be 0.486 kg/s. This value closely matches the one obtained from our simulation, which was 0.483 kg/s.

Simulation of particle-particle collisions using real material properties

We conducted particle-particle collision tests using the actual material properties of the particles. These simulations are similar to those performed by Stevens and Hrenya [11]. The parameters of our tests are provided in Table 6.8.

Table 6.8 Parameters for simulations of particle-particle collisions using real material properties.

Parameter	Value
Particle diameter, d_p	25.4 mm
Particle density, ρ_p	8030 kg/m ³
Normal spring stiffness, k_n	5.16×10^7 N/m
Normal restitution coefficient, e_n	0.879
Particle time step, Δt_p	3×10^{-8} s

The collision tests performed are depicted in Figure 6.33. In these simulations, gravity, adhesion, tangential contact force, and rolling friction were all set to zero.

We employed a linear Hookean contact model, which was previously described. The normal spring stiffness in this model is determined from the real material properties (Young's modulus and Poisson ratio) by the following equation [167, 191]:

$$k_n = \frac{16}{15} E_{pq} \sqrt{r_{pq}} \left[\frac{15 m_{pq} u_{n,\max}^2}{16 E_{pq} \sqrt{r_{pq}}} \right]^{1/5}, \quad (6.33)$$

where $u_{n,\max}$ is a typical maximum normal velocity of impact, m_{pq} represents the effective

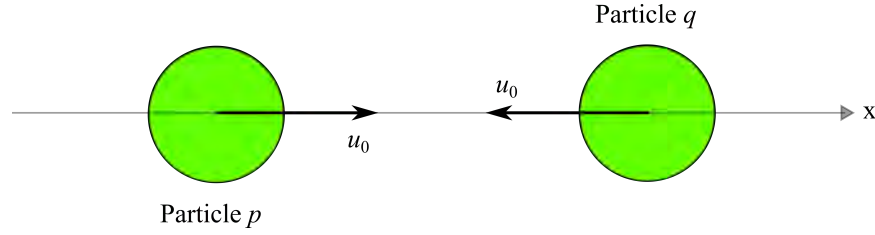


Figure 6.33 Head-on collision between a pair of identical spheres. u_0 is the initial particle's translational velocity.

mass, r_{pq} stands for the effective radius, and E_{pq} denotes the effective Young's modulus given by:

$$E_{pq} = \left[\frac{1 - \nu_p^2}{E_p} + \frac{1 - \nu_q^2}{E_q} \right]^{-1}, \quad (6.34)$$

where E represents the Young's modulus of the particle, and ν denotes the Poisson ratio of the particle. In our tests, we used stainless steel particles with $E = 1.93 \times 10^{11}$ N/m² and $\nu = 0.35$ [11]. Using these values and $u_{n,max} = 1.18$ m/s in Equation 6.33, we obtained $k_n = 5.16 \times 10^7$ N/m.

The normal restitution coefficient was calculated as:

$$e_n = -\frac{u_r^{out}}{u_r^{in}} = -\frac{u_p^{out} - u_q^{out}}{u_p^{in} - u_q^{in}}, \quad (6.35)$$

where u_r^{out} represents the rebound relative velocity between the two colliding particles, and u_r^{in} denotes the impact relative velocity between them. Figure 6.34 presents the normal restitution coefficient and contact duration as functions of impact relative velocity obtained using YALES2 for the stainless steel particles, alongside the results obtained by Stevens and Hrenya [11]. As observed, our results are nearly identical to those of Stevens and Hrenya [11]. Both the normal restitution coefficient and contact duration exhibit constancy across varying impact relative velocities. However, experimental data in the literature reveal that the normal restitution coefficient varies with the impact relative velocity [11], contrary to the predictions of the linear Hookean contact model. Future work could involve implementing non-linear contact models to better align with the observed experimental trends.

Figure 6.35 presents a comparison of our results for the normal contact force as a function of normal overlap with those obtained by Stevens and Hrenya [11] at an impact relative velocity $u_r^{in} = 0.84$ m/s ($u_p^{in} = 0.42$ m/s and $u_q^{in} = -0.42$ m/s). Our results closely align with theirs.

We have also studied the effect of the normal spring stiffness on the contact duration at an impact relative velocity of 0.84 m/s. Decreasing the value of the normal spring stiffness from

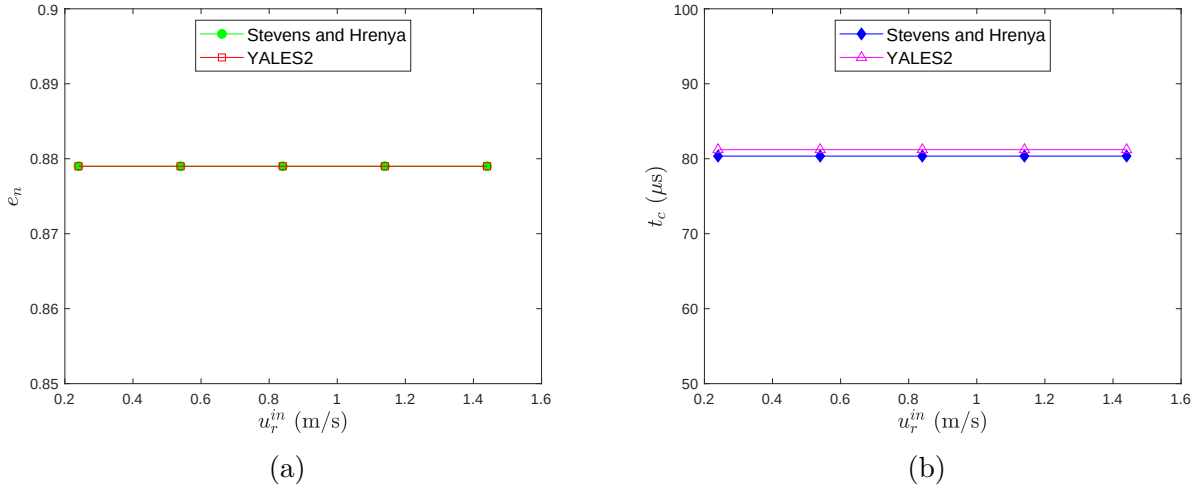


Figure 6.34 Comparison of interparticle collision simulation results: YALES2 vs. Stevens and Hrenya [11]. (a) Normal restitution coefficient as a function of impact relative velocity. (b) Contact duration as a function of impact relative velocity.

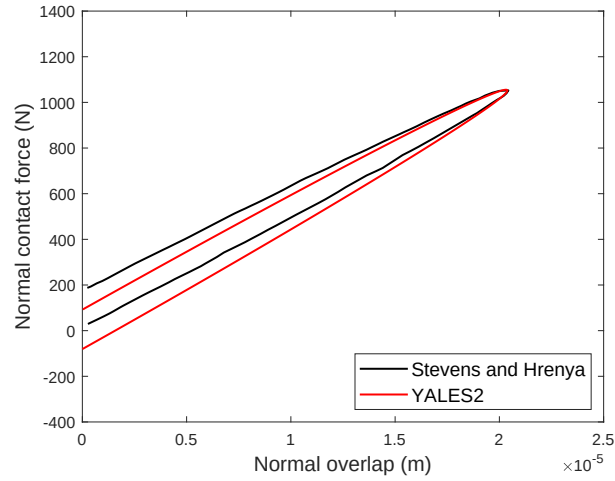


Figure 6.35 Comparison of normal contact force vs. normal overlap between the YALES2 simulation and the Stevens and Hrenya simulation [11] at an impact relative velocity of 0.84 m/s.

5.16×10^7 N/m (the value obtained from the real material properties) to 5.16×10^4 N/m resulted in an increase in the contact duration from 81.21 μ s to 2569.08 μ s.

6.3 Formulation of the coordination number source term

6.3.1 Preliminary two-fluid simulations with a coordination number transport equation

We performed fluidization and defluidization two-fluid simulations with a coordination number transport equation. These simulations are similar to the experiments conducted by Soleimani et al. [1]. In their experiments, glass beads belonging to the Geldart *A* group, with a diameter $d_p = 67 \mu\text{m}$ and a density $\rho_p = 2595 \text{ kg/m}^3$, were fluidized by air at 20°C . This gas has a density $\rho_g = 1.2 \text{ kg/m}^3$ and a viscosity that is determined as follows [192]:

$$\mu_g = 1.46 \times 10^{-6} \frac{T^{1.504}}{T + 120} = 1.8 \times 10^{-5} \text{ Pa.s}, \quad (6.36)$$

where T denotes the temperature in Kelvin. The column employed in their experiments had a diameter of 5.25 cm. The initial fixed-bed height was 15 cm, and the initial solid volume fraction was 0.554.

In our simulations, we used the parameters listed in Table 6.9. The coordination number was

Table 6.9 Parameters for two-fluid simulations with a coordination number transport equation.

Parameter	Value
Particle diameter, d_p	67 μm
Particle density, ρ_p	2595 kg/m^3
Particle-particle normal restitution coefficient, e_c	0.9
Gas density, ρ_g	1.2 kg/m^3
Gas viscosity, μ_g	$1.8 \times 10^{-5} \text{ Pa.s}$
Cuboid bed size, $L_x \times L_y \times L_z$	$5.25 \times 0.525 \times 21 \text{ cm}^3$
Cell size, $\Delta x = \Delta y = \Delta z$	0.0525 cm
Initial particle bed height, H_{ini}	15 cm
Initial particle volume fraction, $\alpha_{p,ini}$	0.554
Frictional pressure constant, Fr	0.05 Pa
Frictional pressure constant, n	2
Frictional pressure constant, m	5
Threshold solid volume fraction for friction, $\alpha_{p,min}$	0.5
Close-packing solid volume fraction, $\alpha_{p,max}$	0.64
Minimum surface separation distance, S_0	$4 \times 10^{-10} \text{ m}$
Hamaker constant, A	$7.21 \times 10^{-20} \text{ J}$
Maximum Courant number, CFL_{max}	0.1

initialized to 4.77 inside the bed (below the initial bed height of 15 cm) and to zero above

the bed. A zero coordination number was imposed at all boundaries (Dirichlet condition). A no-slip boundary condition was used for the particles at the walls.

The coordination number transport equation was expressed as follows:

$$\frac{\partial}{\partial t} (\alpha_p \rho_p CN) + \frac{\partial}{\partial x_i} (\alpha_p \rho_p U_{p,i} CN) = S_{CN}, \quad (6.37)$$

where CN denotes the mean coordination number in a given cell, $U_{p,i}$ signifies the average velocity of the particles in the cell, and S_{CN} represents the source term. In this equation, it is assumed that CN is convected with $U_{p,i}$, and that no diffusive transport takes place. The source term was written as:

$$S_{CN} = c_s \alpha_p \rho_p |D_p| (CN_r - CN), \quad (6.38)$$

where c_s is a constant, CN_r represents the coordination number associated with a particular flow regime (static or fluidized bed), and D_p denotes the strain rate tensor of the particles. This formula for the source term is chosen to relax the coordination number towards the equilibrium value CN_r . The modulus of D_p is given by:

$$|D_p| = \sqrt{\frac{1}{2} D_p^T : D_p}, \quad (6.39)$$

with

$$\begin{aligned} D_p^T : D_p = & \left(\frac{\partial U_{p,x}}{\partial x} \right)^2 + \left(\frac{\partial U_{p,y}}{\partial y} \right)^2 + \left(\frac{\partial U_{p,z}}{\partial z} \right)^2 \\ & + \frac{1}{2} \left(\frac{\partial U_{p,x}}{\partial y} + \frac{\partial U_{p,y}}{\partial x} \right)^2 + \frac{1}{2} \left(\frac{\partial U_{p,x}}{\partial z} + \frac{\partial U_{p,z}}{\partial x} \right)^2 + \frac{1}{2} \left(\frac{\partial U_{p,y}}{\partial z} + \frac{\partial U_{p,z}}{\partial y} \right)^2. \end{aligned} \quad (6.40)$$

A transition solid volume fraction $\alpha_{p,tr}$, corresponding to the minimum fluidization condition, was employed to determine CN_r as outlined below:

$$CN_r = \begin{cases} 4.77, & \text{if } \alpha_p > \alpha_{p,tr}, \\ 4.87 \times 10^{-5} \frac{1 - (1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{11.6}}, & \text{else.} \end{cases} \quad (6.41)$$

In this equation, we use a constant coordination number corresponding to the fixed-bed state [148] if α_p is greater than $\alpha_{p,tr}$, and a CFD-DEM correlation for the fluidized-bed state [148] if α_p is less than or equal to $\alpha_{p,tr}$.

We investigated the impact of the constant c_s on the pressure drop, coordination number, and

voidage profiles during defluidization and fluidization cycles using $\alpha_{p,tr} = 0.55$. Additionally, we explored the influence of $\alpha_{p,tr}$ on these profiles using $c_s = 5.6$.

Figure 6.36 illustrates the effects of c_s and $\alpha_{p,tr}$ on the pressure drop profiles. As seen in this figure, there is a hysteresis between the defluidization and fluidization branches. This hysteresis was not predicted before implementing the transport equation for the coordination number. Figure 6.36a demonstrates that the hysteresis area between the defluidization and fluidization curves increases as c_s decreases. A decrease in c_s means an increase in relaxation time. Figure 6.36b shows that decreasing the value of $\alpha_{p,tr}$ increases the hysteresis area. A decrease in $\alpha_{p,tr}$ enlarges the α_p range for which the constant fixed-bed coordination number ($CN_r = 4.77$) is applied.

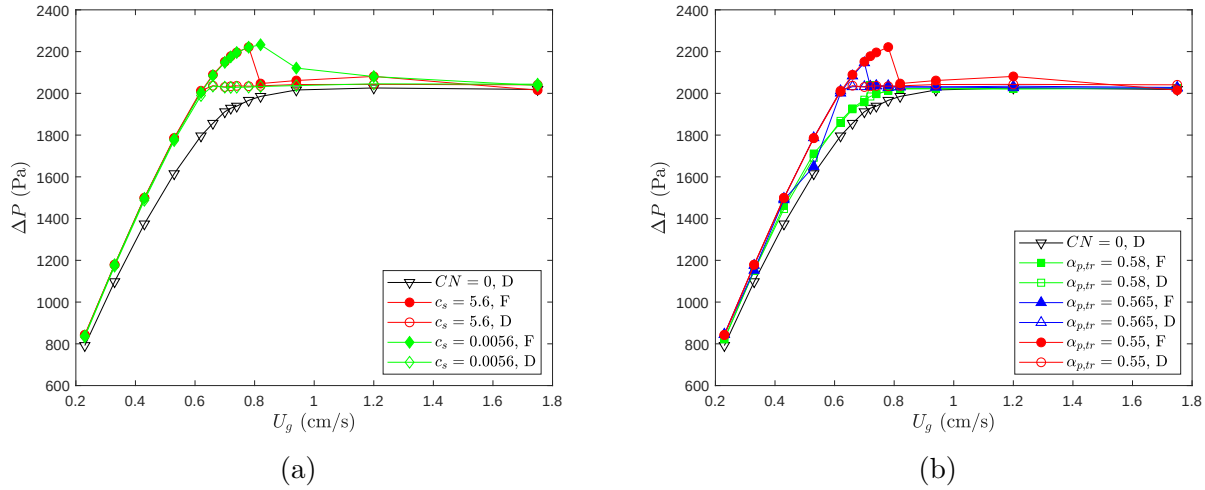


Figure 6.36 Effects of (a) c_s and (b) $\alpha_{p,tr}$ on the instantaneous pressure drop profiles. F represents a fluidization branch, and D represents a defluidization branch.

Figure 6.37 demonstrates the impacts of c_s and $\alpha_{p,tr}$ on the coordination number profiles. Figure 6.37a shows that the coordination number does not substantially change with an increase in superficial gas velocity. This figure also displays a hysteresis in the coordination number between the decreasing and increasing gas velocity paths. For example, for $c_s = 0.0056$, the coordination number in the fluidization branch is higher than in the defluidization branch. The hysteresis is larger for $c_s = 0.0056$ than for $c_s = 5.6$ because a lower c_s implies a higher relaxation time. The hysteresis in the coordination number leads to the hysteresis in the pressure drop. Figure 6.37b shows that for $\alpha_{p,tr} = 0.55$ and $\alpha_{p,tr} = 0.565$, the coordination number does not change substantially. However, for $\alpha_{p,tr} = 0.58$, the coordination number decreases from around 4 to 0.5 with the increase in superficial gas velocity. This occurs because, for $\alpha_{p,tr} = 0.58$, there is a smaller α_p range for which the constant

fixed-bed coordination number ($CN_r = 4.77$) is used.

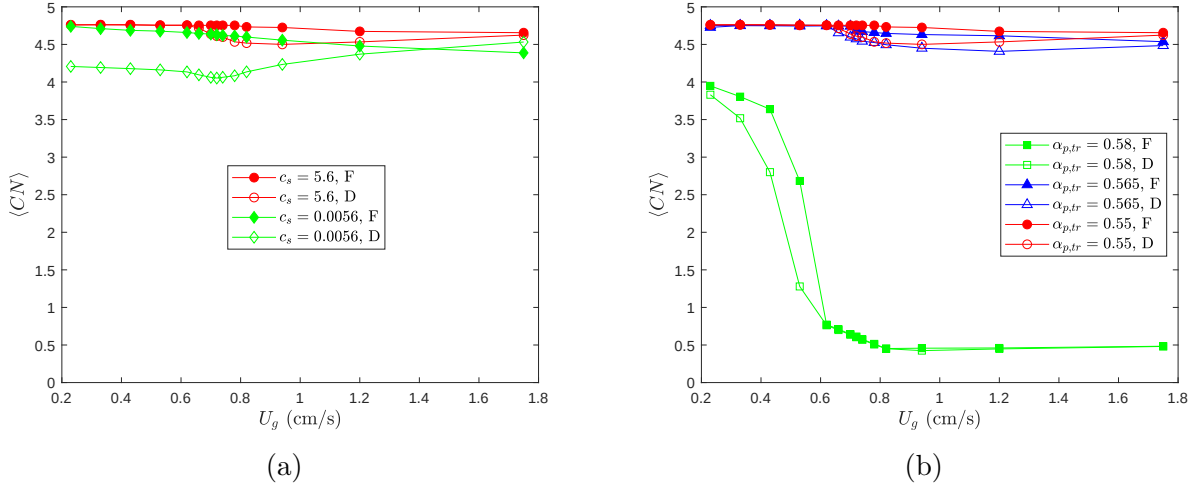


Figure 6.37 Effects of (a) c_s and (b) $\alpha_{p,tr}$ on the instantaneous spatially-averaged coordination number profiles.

Figure 6.38 illustrates the effects of c_s and $\alpha_{p,tr}$ on the profiles of bed voidage. This figure shows that the voidage is lower with adhesion compared to without adhesion ($CN = 0$). The analysis of Figures 6.38a and 6.38b is similar to that of the coordination number profiles. For instance, in Figure 6.38b, using $\alpha_{p,tr} = 0.58$, higher voidage values were reached compared to $\alpha_{p,tr} = 0.55$ and $\alpha_{p,tr} = 0.565$. This observation aligns with the lower coordination number values for $\alpha_{p,tr} = 0.58$.

Figure 6.39 depicts the influence of $\alpha_{p,tr}$ on both the strain rate tensor of the particles and the coordination number source term. Figure 6.39a demonstrates that for $\alpha_{p,tr} = 0.55$, the modulus of the strain rate tensor is higher in the defluidization branch compared to the fluidization branch. This figure also shows that the modulus of the strain rate tensor increases with the increase in gas velocity. The strain rate tensor reflects the deformation of the particle phase. The instantaneous spatial-averaged source term shown in Figure 6.39b was calculated by substituting the values of the instantaneous spatial-averaged parameters into Equation 6.38. In this figure, negative values of the source term are observed for $\alpha_{p,tr}$ equal to 0.58. This indicates a decrease in the coordination number towards the equilibrium value given by the fluidized bed correlation.

Although we were able to predict a hysteresis in the pressure drop using the proposed source term expression, the results indicate an issue with this proposition. Besides reflecting the deformation of the particle phase, there is no robust justification for including $|D_p|$ in the

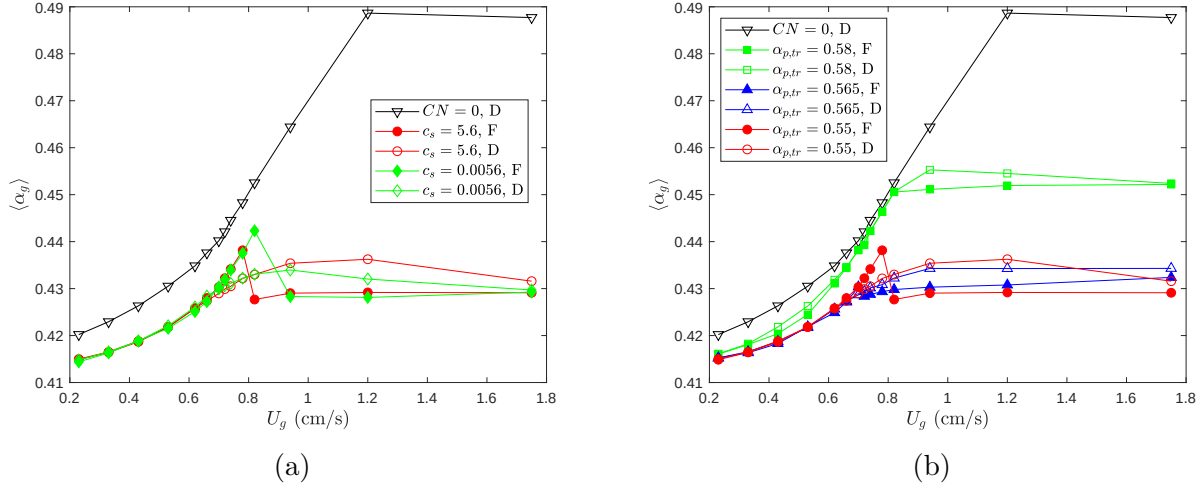


Figure 6.38 Effects of (a) c_s and (b) $\alpha_{p,tr}$ on the instantaneous spatially-averaged gas volume fraction profiles.

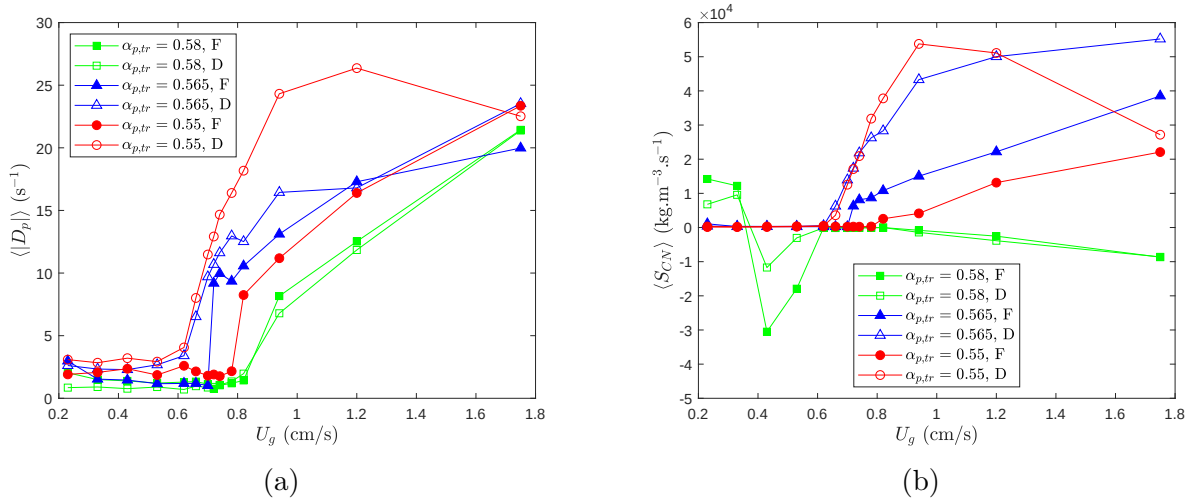


Figure 6.39 Effect of $\alpha_{p,tr}$ on (a) the spatial-averaged modulus of the strain rate tensor of the particles and (b) the spatial-averaged coordination number source term profiles.

expression of the source term. The formulation of this term should be based on CFD-DEM measurements, and the evolution of the coordination number should be verified by CFD-DEM results. In the following section, we will measure the coordination number source term from CFD-DEM simulations.

6.3.2 Coordination number transport equation guided by CFD-DEM

We conducted CFD-DEM simulations at low and high gas velocities to compute the coordination number source term. Details of the methods used for this computation are provided in the previous chapter. These simulations were analogous to the experiments performed by Soleimani et al. [1], but employed significantly smaller geometry and fewer particles due to the high computational cost associated with the CFD-DEM approach. The parameters used in these simulations are detailed in Table 6.10.

Table 6.10 Parameters for the simulations used to measure the source term in the coordination number transport equation.

<i>Particle properties</i>		<i>Interparticle collisions</i>	
Diameter, d_p	67 μm	Normal spring stiffness, k_n	210 N/m
Density, ρ_p	2595 kg/m ³	Normal restitution coefficient, e_n	0.9
<i>Cuboid geometry</i>		Tangential spring stiffness, k_t	60 N/m
Width (x -direction), W	$40d_p$	Tangential restitution coefficient, e_t	0.9
Thickness (y -direction), T	$16d_p$	Dynamic friction coefficient, μ_d	0.2
Height (z -direction), H	$160d_p$	Rolling friction coefficient, μ_r	0.01
<i>Hexahedral mesh</i>		Maximum normal overlap, δ_n^{max}	$0.1d_p$
Number of cells in the x -direction, N_c^x	12	<i>Particle-wall collisions</i>	
Number of cells in the y -direction, N_c^y	5	Normal spring stiffness, $k_{w,n}$	210 N/m
Number of cells in the z -direction, N_c^z	48	Normal restitution coefficient, $e_{w,n}$	0.9
<i>Particle loading</i>		Maximum normal overlap, $\delta_{w,n}^{max}$	$0.1d_p$
Number of particles, N_{tot}	36,000	<i>Gas properties</i>	
<i>Time advancement of particles</i>		Density, ρ_g	1.2 kg/m ³
Numerical scheme	Groot-Warren [82]	Viscosity, μ_g	1.8×10^{-5} Pa.s
Particle CFL number, CFL_s	1.5	<i>Advancement of gas</i>	
Contact CFL number, CFL_s^c	0.05	Time integration scheme	TFV4A [85]
Number of sub-steps within the collision time, n_c	15	Spatial integration scheme	4th-order centered
		Courant number, CFL	0.1
		<i>Gas-particle interaction</i>	
		Drag model	Gobin et al. [81]

In the initial phase, we performed particle settling under gravity ($g_z = -9.81$ m/s²) without the presence of gas, using solely DEM. The particles, classified under Geldart group A, have properties listed in Table 6.10. The seeding region was located at a distance of d_p from the sidewalls, spanning a z -range of $15\Delta z = 3.35$ mm to $45\Delta z = 10.05$ mm. Each cell was seeded with one particle per dimension ($\Delta x, \Delta y, \Delta z$). Starting at $t = 0$, 1800 particles were seeded every 0.1 seconds until $t = 1.9$ seconds, with the simulation running for a total of 2.5 seconds. The particles were assigned random translational velocities between -0.1 and 0.1 m/s and random rotational velocities between -100 and $+100$ rad/s at seeding. Because e_n is equal to e_t , we use $k_t = 2k_n/7$ as shown in Table 6.10. A rolling friction coefficient of 0.01, as reported and used by Frankowski and Morgeneyer [193] for smooth spherical glass beads,

was employed for particle-particle interactions. Zero particle-wall friction was used, and Van der Waals adhesion was not considered in these simulations.

Afterward, the static bed formed was utilized as the initial state for a test at a superficial gas velocity of 3.089 cm/s (approximately $4.3U_{mf}$) to fluidize the bed and remove any stresses that had arisen within the bed during settling. Initially, the gas velocity was set to zero everywhere for this test, which lasted 2 seconds. Following this, we set the gas velocity at the inlet to zero for 1 second. The final state from this simulation was used as the starting point for our low and high gas velocity tests ($U_g = 0.226$ cm/s $\approx 0.317U_{mf}$ and $U_g = 3.089$ cm/s $\approx 4.3U_{mf}$, respectively) to measure the coordination number source term. Turbulence effects were neglected in these tests, and all boundaries were treated as walls for particles. The bottom boundary functioned as the gas inlet, while the top boundary acted as the gas outlet, maintaining a pressure of 1 atm. A no-slip condition was applied to the gas at the sidewalls. In these simulations, which lasted 1 second, we imposed the gas velocity at the inlet using a Dirichlet boundary condition. For the linked-cell method, the cell size was set to $1.25d_p$. We used 40 processors and a boundary halo enclosing each processor region of $1.5d_p$ for the ghost particle method. Each cell group consisted of 300 cells. Zero spatial filtering operations (for the gas volume fraction and the interphase momentum transfer [5]) were employed. The number of cells used in each direction (see Table 6.10) results in $\Delta x = \Delta z \approx 3.33d_p$ and $\Delta y = 3.2d_p$. These sizes are greater than the critical cell size of $3d_p$, thus ensuring that the potential instabilities and discontinuities associated with the particle centroid method are avoided [80].

We conducted tests at both low and high gas velocities ($U_g = 0.226$ cm/s $\approx 0.317U_{mf}$ and $U_g = 3.089$ cm/s $\approx 4.3U_{mf}$, respectively) to measure the coordination number source term, as mentioned earlier. Figure 6.40 illustrates the coordination number for each particle in the bed at the low and high gas velocities. In the static bed state, the coordination number exhibits a homogeneous distribution, with an average value of nearly 5. By increasing the gas velocity to the high value, the bed expands significantly, resulting in a substantial decrease in the coordination number, which drops to zero for the majority of the particles.

Figures 6.41 and 6.42 show the time derivative $\partial(\alpha_p \langle CN \rangle) / \partial t$ and the divergence $\partial(\alpha_p U_{p,i} \langle CN \rangle) / \partial x_i$ for the test cases at low and high gas velocities, respectively. In Figure 6.41, we observe that the time derivative is zero within the bed, indicating a stable solid volume fraction and mean coordination number over time. However, high values of the time derivative are observed in two cells due to slight increases in the mean coordination number between consecutive time steps (the time step is of the order of 10^{-7} s). Figure 6.41 also demonstrates relatively low divergence values, reflecting minor spatial variations in $\alpha_p U_{p,i} \langle CN \rangle$ within the static bed.

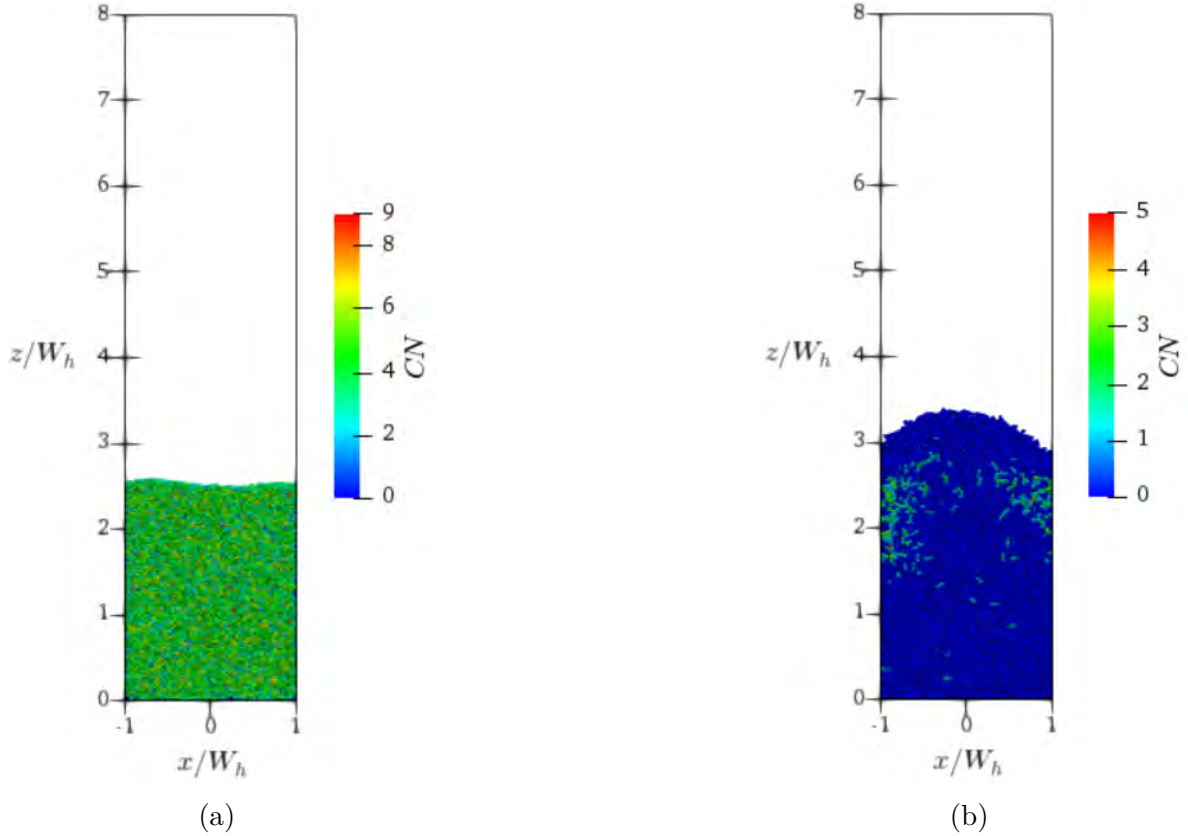


Figure 6.40 Instantaneous coordination number distribution inside a bed of Geldart A particles at (a) low and (b) high gas velocities. W_h represents half the width of the cuboid.

These variations intensify at the top of the bed, correlating with increased divergence values in this region.

Figure 6.42 illustrates the presence of both negative and positive values of the time derivative, indicating respective decreases and increases in $\alpha_p \langle CN \rangle$ between the preceding and current iterations. Additionally, negative and positive values of the divergence exist, signifying net inward and outward fluxes of $\alpha_p U_{p,i} \langle CN \rangle$, respectively. In the fluidized state (refer to Figure 6.42), the magnitudes of both the time derivative and the divergence are elevated compared to those in the static bed state (refer to Figure 6.41). This disparity stems from the dynamic nature of the fluidized state, which results in more significant variations in both time and space.

Figure 6.43 presents the distributions of the coordination number source term obtained using the direct Lagrangian and mesoscopic Eulerian methods at the low gas velocity. These results show an equivalence between the two methods. The elevated values in the two cells are

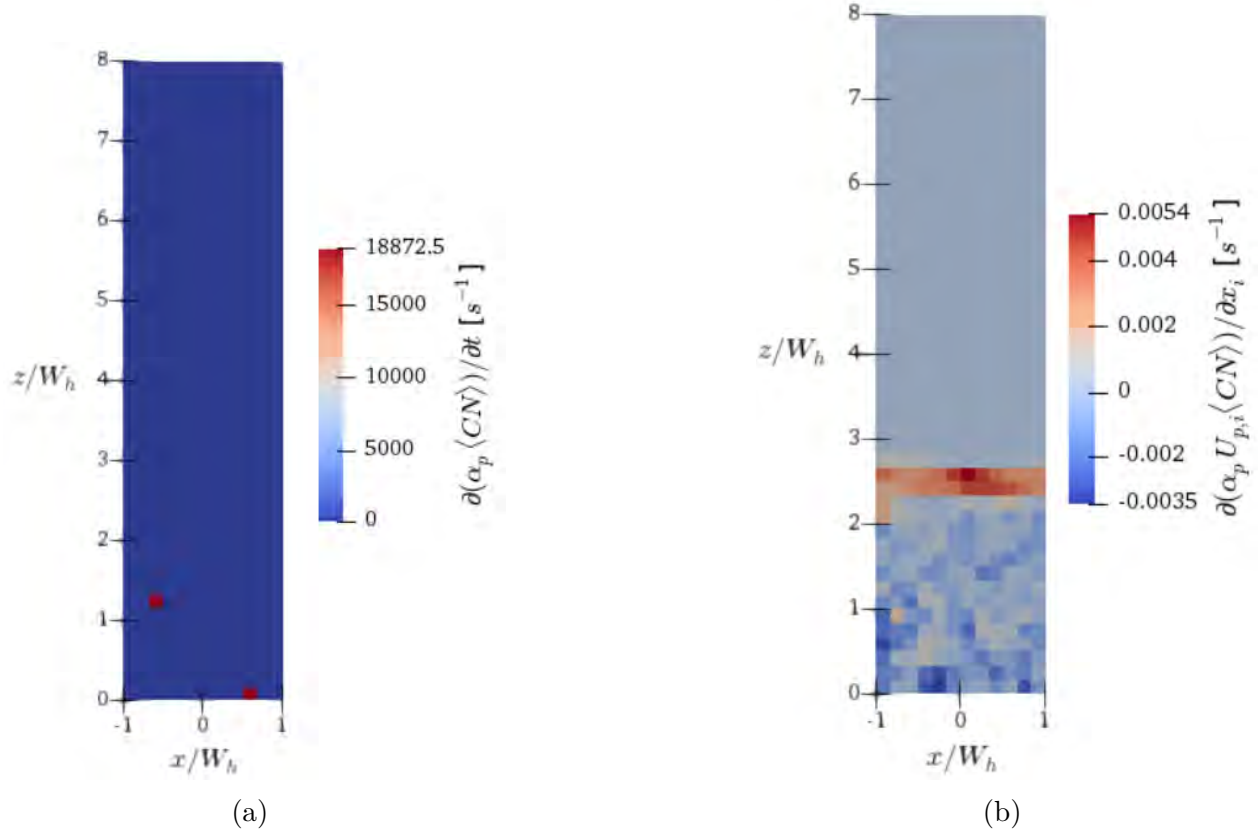


Figure 6.41 Instantaneous distribution of (a) time derivative and (b) divergence (Equation 5.45) in a bed of Geldart A particles at low gas velocity.

attributed to their high time derivative values (see Figure 6.41).

Figure 6.44 displays the distributions of the coordination number source term at the high gas velocity, obtained using the direct Lagrangian and mesoscopic Eulerian methods. The two distributions are identical, indicating consistency between the two methods. The positive source term values imply an increase in the coordination number, while the negative source term values imply a decrease in the coordination number.

We propose the following source term for the Eulerian transport equation of the coordination number, which enables the relaxation of the average coordination number within a cell, denoted as $\langle CN \rangle$, towards the equilibrium value $\langle CN \rangle_r$:

$$n_p \langle S_{CN} \rangle = C_s \frac{\alpha_p}{v_p} [\langle CN \rangle_r - \langle CN \rangle]. \quad (6.42)$$

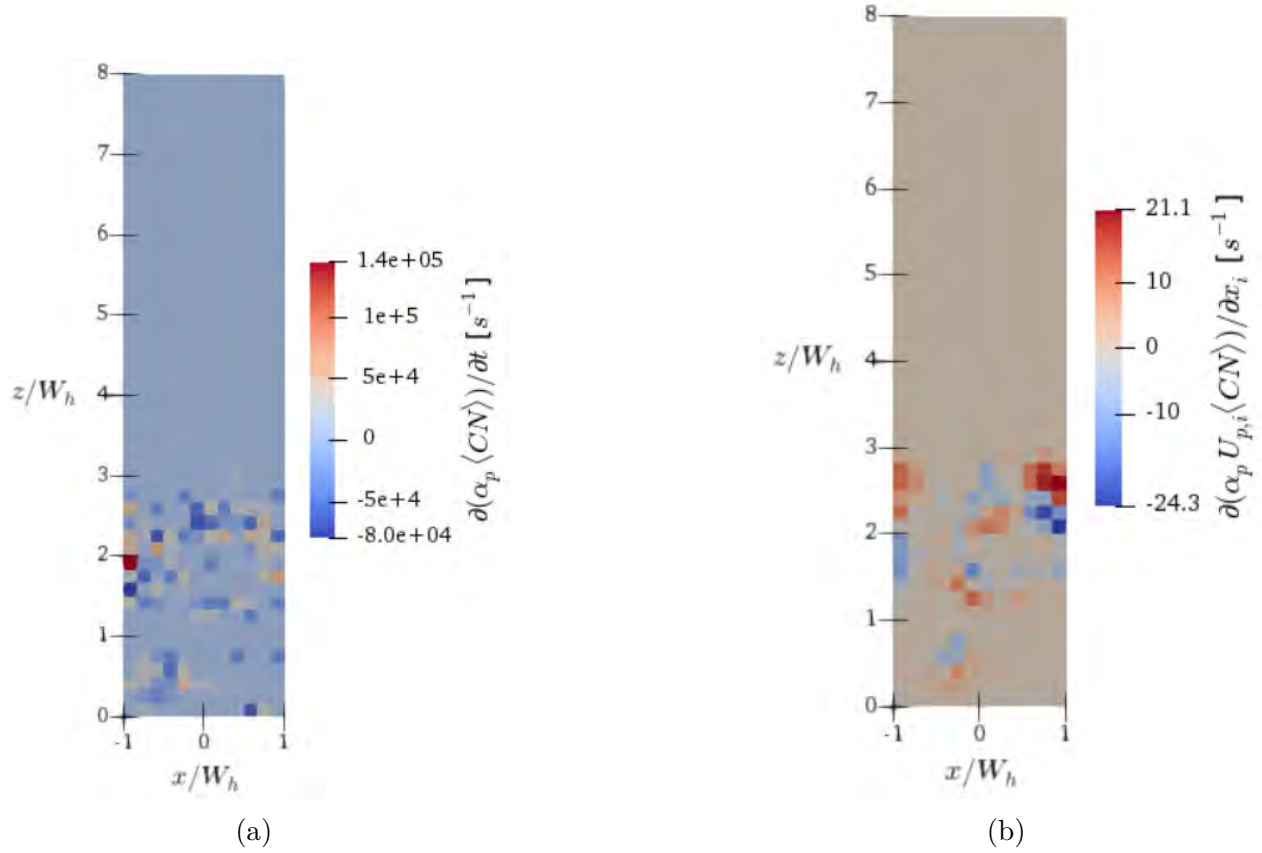


Figure 6.42 Instantaneous distribution of (a) time derivative and (b) divergence (Equation 5.45) in a bed of Geldart A particles at high gas velocity.

Then, C_s can be computed as:

$$C_s = v_p \frac{n_p \langle S_{CN} \rangle}{\alpha_p [\langle CN \rangle_r - \langle CN \rangle]}, \quad (6.43)$$

where $n_p \langle S_{CN} \rangle$ can be calculated using the direct Lagrangian or mesoscopic Eulerian method. $\langle CN \rangle_r$ represents the coordination number associated with a particular flow regime. The value of $\langle CN \rangle_r$ was determined as the spatial average of $\langle CN \rangle$ below the height $H = 3.3$ mm, which is slightly lower than the bed height at the low gas velocity. We found $\langle CN \rangle_r = 4.754$ at the low gas velocity and $\langle CN \rangle_r = 0.086$ at the high gas velocity. We calculated $n_p \langle S_{CN} \rangle$, $\langle CN \rangle$, and α_p using Equations 5.45, 5.46, and 5.48, respectively. Then, by substituting the obtained values into Equation 6.43, we determined the distribution of C_s . Figures 6.45 and 6.46 illustrate the distributions of C_s at the low and high gas velocities, respectively. The data indicate that the magnitudes of C_s are greater in the fluidized state compared to the static state. This observation implies that the relaxation time is shorter in the fluidized state,

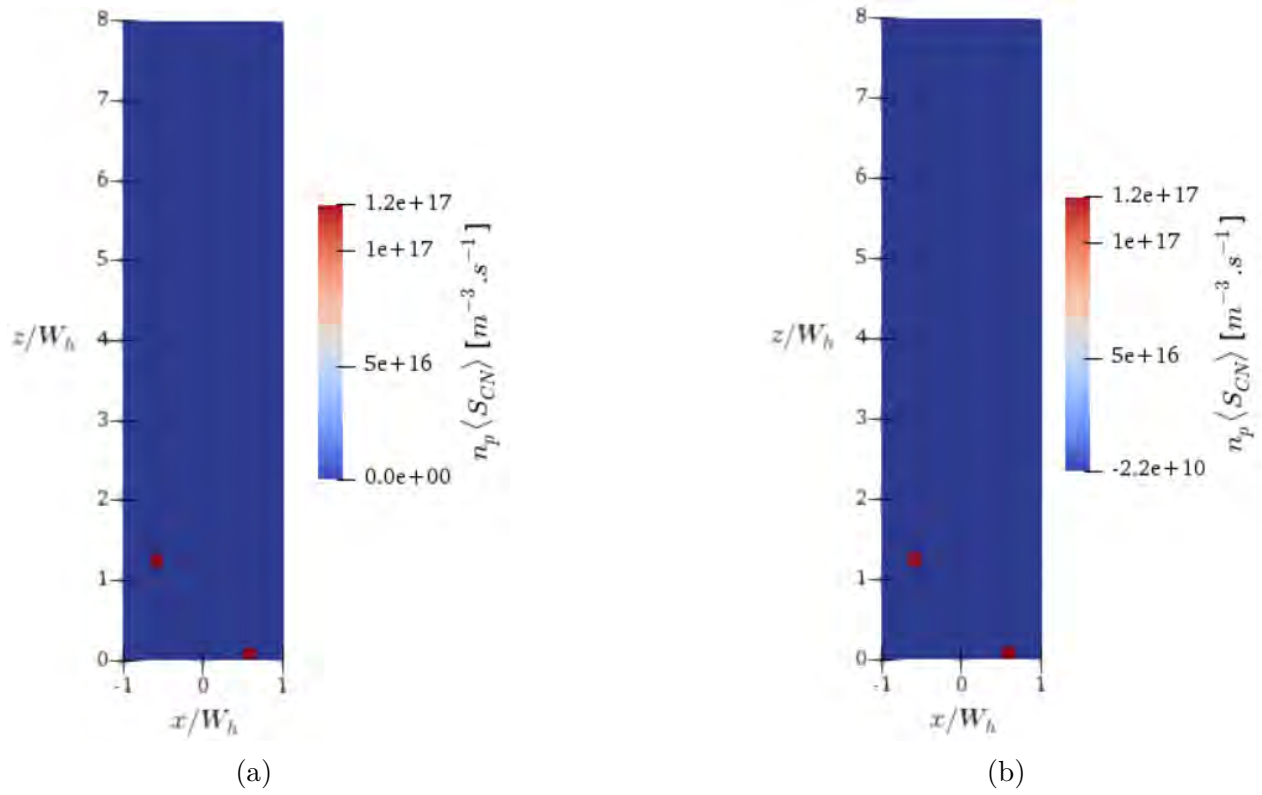


Figure 6.43 Comparison of coordination number source term distributions at low gas velocity: (a) Direct Lagrangian method vs. (b) Mesoscopic Eulerian method.

which means that the relaxation of $\langle CN \rangle$ towards $\langle CN \rangle_r$ occurs faster.

6.4 Numerical stability related to gas-solid coupling

In our CFD-DEM simulations using YALES2, we observed instability in the gas velocity and pressure contours, particularly in the fixed bed state. This instability necessitated the use of a very small CFL number in our previous simulations. In this section, we address this issue and propose potential solutions.

6.4.1 Explicit coupling

The coupling between the gas and solid phases in YALES2 is explicit [78, 194]. To solve the observed stability problem, we implemented the following stability condition [80], which is

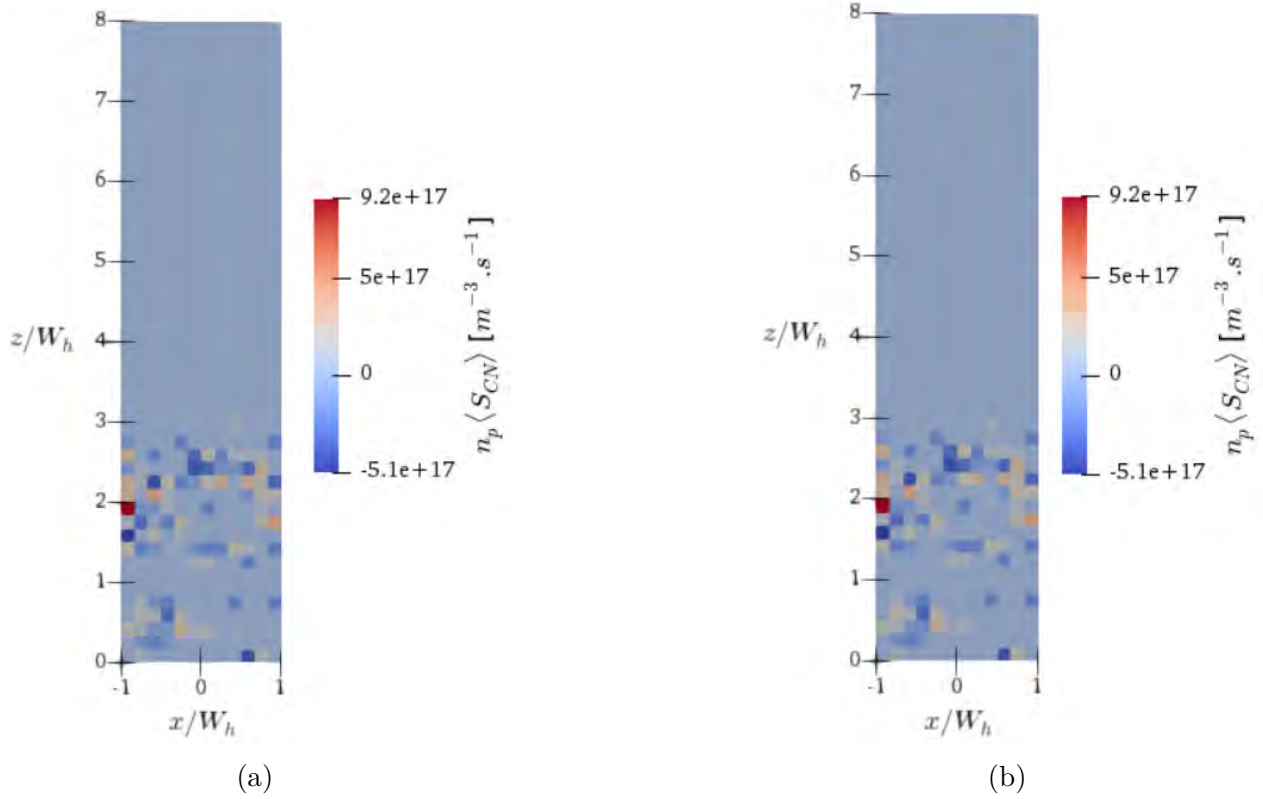


Figure 6.44 Comparison of coordination number source term distributions at high gas velocity: (a) Direct Lagrangian method vs. (b) Mesoscopic Eulerian method.

related to the gas-particle coupling, in the YALES2 code:

$$\Delta t_g \leq \min \left(\tau_r^d, \frac{\alpha_g}{1 - \alpha_g} \frac{\rho_g}{\rho_p} \tau_r^d \right), \quad (6.44)$$

where τ_r^d denotes the drag relaxation time. When $\alpha_g / (1 - \alpha_g)$ is very small compared to 1, which occurs in the dense state, the term $\alpha_g \rho_g \tau_r^d / [\rho_p (1 - \alpha_g)]$ determines the gas time step. Implementing the stability condition given in Equation 6.44 requires projecting the drag relaxation time from the particles to the grid nodes. The drag relaxation time at a node k was determined by averaging over the particles surrounding it:

$$\tau_r^d(\mathbf{x}_k) = \frac{\sum_{p \in C_k} \omega_k^p \tau_r^d(p)}{\sum_{p \in C_k} \omega_k^p}, \quad (6.45)$$

where ω_k^p denotes the projection weight of particle p on node k , and $p \in C_k$ signifies that the center of particle p is positioned within one of the adjacent cells of node k .

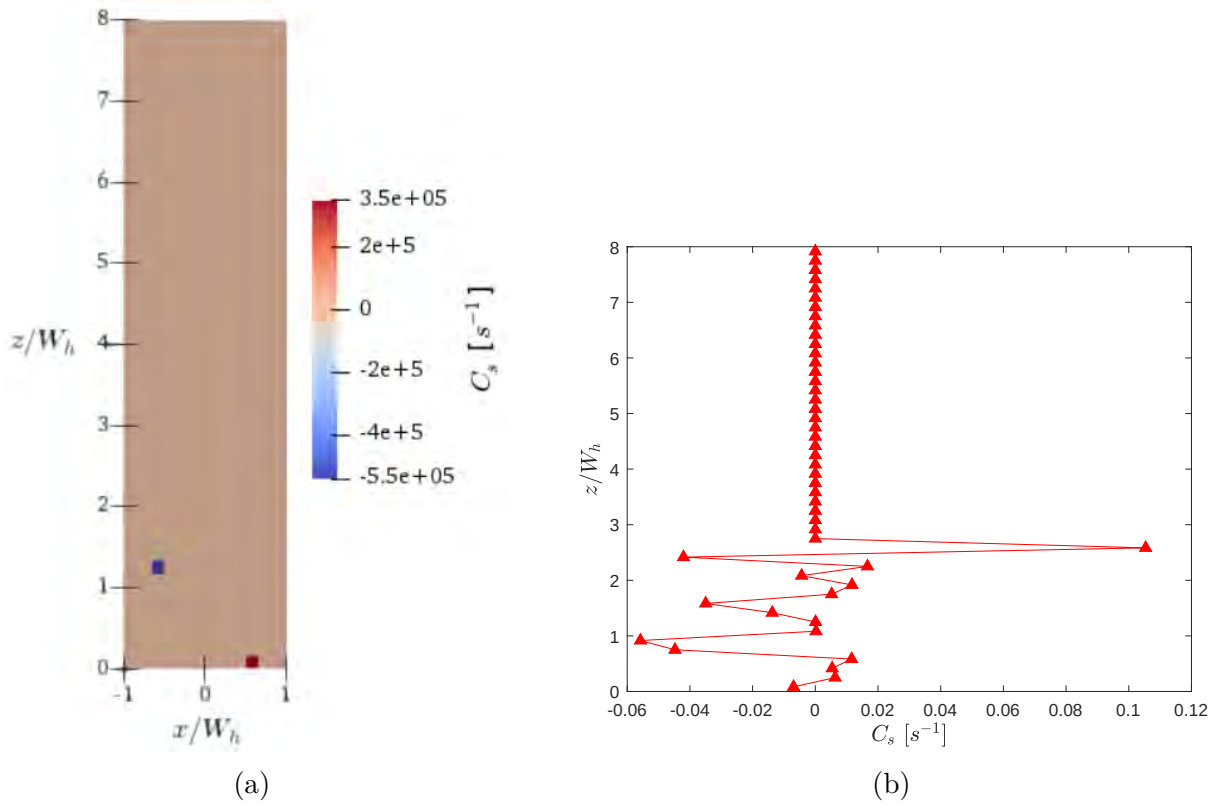


Figure 6.45 Instantaneous distribution of C_s in the bed at low gas velocity: (a) 2D visualization and (b) variation of C_s with height in the middle of the cuboid.

We tested the additional stability condition using particles of diameter $d_p = 75$ microns and density $\rho_p = 1495$ kg/m³, and a gas with density $\rho_g = 1.1979$ kg/m³ and viscosity $\mu_g = 1.8 \times 10^{-5}$ Pa.s. We seeded the particles in batches and allowed them to settle under gravity onto a distributor plate positioned in the middle of a cuboid geometry using DEM only (no gas). The obtained fluid fraction profile is shown in Figure 6.47. Then, we imposed a gas mass flow rate at the bottom boundary of the cuboid, corresponding to a superficial gas velocity $U_g \approx 0.2U_{mf}$.

Figure 6.48 illustrates the gas velocity contours within the particle bed before and after implementing the additional stability condition, highlighting the improvement in stability. As observed, before implementing the stability condition, there was an unstable loop in the gas velocity within the fixed bed, which is not physically realistic. After implementing the stability condition, the gas flows across the bed with its velocity oriented along the z -direction, achieving a stable and physically realistic state. It is worth mentioning that this simulation was performed without filtering.

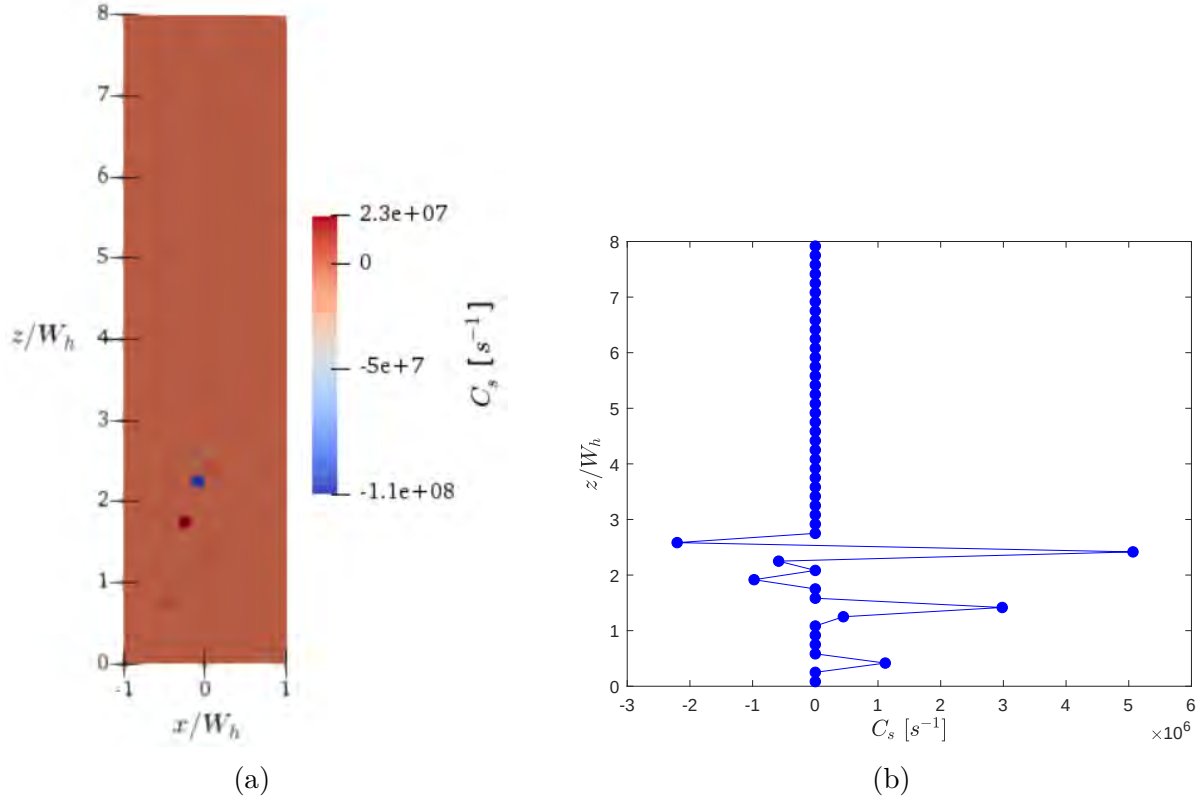


Figure 6.46 Instantaneous distribution of C_s in the bed at high gas velocity: (a) 2D visualization and (b) variation of C_s with height in the middle of the cuboid.

Before implementing the stability condition, the ratio between the gas and particle time steps was high, specifically during the first iteration. This appears to be the cause of the stability issues we observed. Adding the stability condition resulted in a reduced ratio between the gas and particle time steps and significantly smaller gas time steps (of the order of 10^{-7} seconds).

We tested the stability condition at low and high gas velocities, corresponding to static and fluidized bed regimes, and it performed satisfactorily. However, a defluidization test using a step-wise approach failed around the minimum fluidization velocity. It seems that the explicit coupling method, even with the implementation of the additional stability condition, suffers from a snowball effect in terms of instability. This means that the instability grows over time during the defluidization test. Therefore, in the following section, we propose a semi-implicitation of the gas-solid interaction forces (drag and Archimedes forces) through a penalization approach.

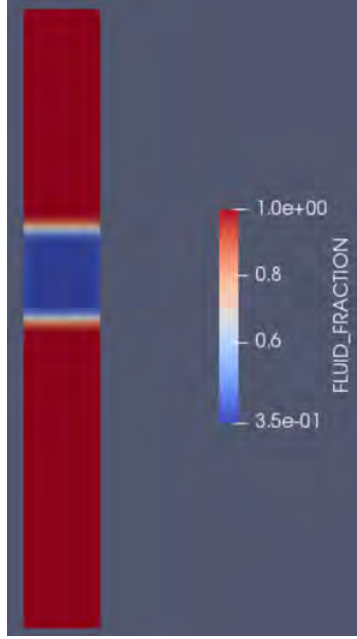
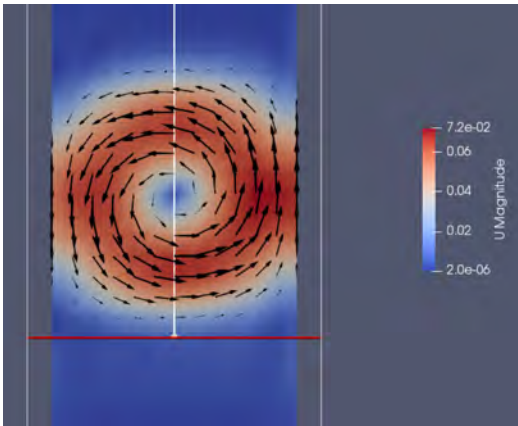
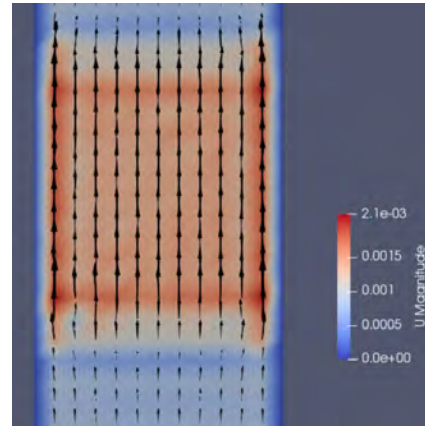


Figure 6.47 Fluid fraction profile within a cuboid. Numerical stability test.



(a)



(b)

Figure 6.48 Gas velocity contour in a fixed bed at a superficial gas velocity of $0.2U_{mf}$: (a) before and (b) after implementing the additional stability condition. The horizontal red line indicates a distributor plate, above which the particles are settled.

6.4.2 Semi-implicit coupling

In YALES2, the momentum transfer term at a given node k is determined by projecting the particle data $\mathbf{F}_{p \rightarrow g}^r$ to this node as follows:

$$\mathbf{I}_{p \rightarrow g}^n(\mathbf{x}_k) = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p \mathbf{F}_{p \rightarrow g}^r \Big|_n, \quad (6.46)$$

where the sum at time n is calculated by averaging over the particle time steps as follows:

$$\sum_{p \in C_k} \omega_k^p \mathbf{F}_{p \rightarrow g}^r \Big|_n = \frac{\sum_{m=1}^{N_{st}} \left(\sum_{p \in C_k} \omega_k^p \mathbf{F}_{p \rightarrow g}^r \right)_m \Delta t_{p,m}}{\sum_{m=1}^{N_{st}} \Delta t_{p,m}}, \quad (6.47)$$

where N_{st} is the number of sub-steps in a given gas time step, and $\mathbf{F}_{p \rightarrow g}^r$ represents a relaxed particle-gas interaction force:

$$\mathbf{F}_{p \rightarrow g}^r|_m = -\frac{1}{2} \left(\mathbf{F}_{g \rightarrow p}|_m + \mathbf{F}_{g \rightarrow p}|_{m-1} \right), \quad (6.48)$$

with

$$\mathbf{F}_{g \rightarrow p} = \frac{m_p}{\tau_r^d} (\mathbf{u}_{g@p} - \mathbf{u}_p) - V_p \nabla P_{g@p}, \quad (6.49)$$

where $\mathbf{u}_{g@p}|_m$ is the velocity of the gas at the current Δt_g interpolated at the position of the particle at $\Delta t_{p,m}$.

To achieve semi-implicit coupling, we added the time increment of $\mathbf{I}_{p \rightarrow g}$ to $\mathbf{I}_{p \rightarrow g}^n$ as follows:

$$\mathbf{I}_{p \rightarrow g}^n(\mathbf{x}_k) = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p \mathbf{F}_{p \rightarrow g}^r \Big|_n + \Delta \mathbf{I}_{p \rightarrow g}(\mathbf{x}_k), \quad (6.50)$$

where the time increment of $\mathbf{I}_{p \rightarrow g}$ is expressed as:

$$\Delta \mathbf{I}_{p \rightarrow g}(\mathbf{x}_k) = -\frac{1}{V_k} \sum_{p \in C_k} \omega_k^p \frac{m_p}{\tau_r^d} \Big|_n (\Delta \mathbf{u}_{g@p} - \Delta \mathbf{u}_p) + \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p V_p \Big|_n \nabla (\Delta P_{g@p}). \quad (6.51)$$

By assuming $\Delta \mathbf{u}_p = 0$ (valid for a fixed bed), $\Delta \mathbf{u}_{g@p} = \Delta \mathbf{U}_g$, and $\Delta P_{g@p} = \Delta P_g$, the time increment of $\mathbf{I}_{p \rightarrow g}$ can be written as:

$$\Delta \mathbf{I}_{p \rightarrow g}(\mathbf{x}_k) = -\lambda_{p,k} (\mathbf{U}_{g,k}^{n+1} - \mathbf{U}_{g,k}^n) + \eta_{p,k} \nabla (P_{g,k}^{n+1/2} - P_{g,k}^{n-1/2}), \quad (6.52)$$

with

$$\lambda_{p,k} = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p \frac{m_p}{\tau_r^d} \Big|_n, \quad (6.53)$$

and

$$\eta_{p,k} = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p V_p \Big|_n. \quad (6.54)$$

$\lambda_{p,k}$ and $\eta_{p,k}$ can be computed in a manner similar to that in Equation 6.47. $\lambda_{p,k}$ was calculated as:

$$\lambda_{p,k} = \frac{1}{V_k} \frac{\sum_{m=1}^{N_{st}} \left(\sum_{p \in C_k} \omega_k^p \Lambda_p^r \right)_m \Delta t_{p,m}}{\sum_{m=1}^{N_{st}} \Delta t_{p,m}}, \quad (6.55)$$

where

$$\Lambda_p^r|_m = \frac{1}{2} \left(\Lambda_p|_m + \Lambda_p|_{m-1} \right), \quad (6.56)$$

with

$$\Lambda_p = \frac{m_p}{\tau_r^d}. \quad (6.57)$$

Similarly, $\eta_{p,k}$ was computed as:

$$\eta_{p,k} = \frac{1}{V_k} \frac{\sum_{m=1}^{N_{st}} \left(\sum_{p \in C_k} \omega_k^p H_p^r \right)_m \Delta t_{p,m}}{\sum_{m=1}^{N_{st}} \Delta t_{p,m}}, \quad (6.58)$$

where

$$H_p^r|_m = \frac{1}{2} \left(H_p|_m + H_p|_{m-1} \right), \quad (6.59)$$

with

$$H_p = V_p. \quad (6.60)$$

In our tests, $H_p|_m = H_p|_{m-1} = V_p$.

The momentum equation of the gas can be discretized in the following way:

$$\frac{\mathbf{U}_{g,k}^{n+1} - \mathbf{U}_{g,k}^n}{\Delta t_g} = \mathbf{A}^n - \frac{1}{\alpha_g \rho_g} \nabla (\Delta P_g) - \frac{\lambda_{p,k}}{\alpha_g \rho_g} (\mathbf{U}_{g,k}^{n+1} - \mathbf{U}_{g,k}^n) + \frac{\eta_{p,k}}{\alpha_g \rho_g} \nabla \left(P_{g,k}^{n+1/2} - P_{g,k}^{n-1/2} \right), \quad (6.61)$$

with

$$\mathbf{A}^n = -\nabla \cdot (\mathbf{U}_g^n \otimes \mathbf{U}_g^n) + \frac{1}{\rho_g} \nabla \cdot \boldsymbol{\varepsilon}_g^n - \frac{1}{\alpha_g \rho_g} \nabla P_{g,k}^{n-1/2} + \frac{1}{\alpha_g \rho_g V_k} \sum_{p \in C_k} \omega_k^p \mathbf{F}_{p \rightarrow g}^r \Big|_n. \quad (6.62)$$

Equation 6.61 can be written as:

$$\begin{aligned} \mathbf{U}_{g,k}^{n+1} \left(1 + \frac{\lambda_{p,k}}{\alpha_g \rho_g} \Delta t_g \right) &= \mathbf{U}_{g,k}^n \left(1 + \frac{\lambda_{p,k}}{\alpha_g \rho_g} \Delta t_g \right) + \mathbf{A}^n \Delta t_g + \frac{\Delta t_g}{\alpha_g \rho_g} \nabla P_{g,k}^{n-1/2} \\ &\quad - \frac{\Delta t_g}{\alpha_g \rho_g} \nabla P_{g,k}^{n+1/2} + \frac{\Delta t_g}{\alpha_g \rho_g} \eta_{p,k} \nabla P_{g,k}^{n+1/2} - \frac{\Delta t_g}{\alpha_g \rho_g} \eta_{p,k} \nabla P_{g,k}^{n-1/2}. \end{aligned} \quad (6.63)$$

Then, Equation 6.63 can be expressed as:

$$\mathbf{U}_{g,k}^{n+1} = \mathbf{U}_{g,k}^{**} - \frac{\Delta t_g}{\gamma \alpha_g \rho_g} (1 - \eta_{p,k}) \nabla P_{g,k}^{n+1/2}, \quad (6.64)$$

with

$$\mathbf{U}_{g,k}^{**} = \mathbf{U}_{g,k}^n + \frac{\Delta t_g}{\gamma} \mathbf{A}^n + \frac{\Delta t_g}{\gamma \alpha_g \rho_g} (1 - \eta_{p,k}) \nabla P_{g,k}^{n-1/2}, \quad (6.65)$$

and

$$\gamma = 1 + \frac{\lambda_{p,k}}{\alpha_g \rho_g} \Delta t_g. \quad (6.66)$$

Equations 6.65 and 6.64 represent the prediction and correction steps, respectively. This method ensures a strong coupling between the pressure gradient and drag.

By applying the divergence operator to Equation 6.64, we obtained the following equation:

$$\nabla \cdot \left(\frac{1 - \eta_{p,k}}{\gamma} \nabla P_{g,k}^{n+1/2} \right) = \frac{1}{\Delta t_g} \left(\nabla \cdot (\alpha_g \rho_g \mathbf{U}_{g,k})^{**} - \nabla \cdot (\alpha_g \rho_g \mathbf{U}_{g,k})^{n+1} \right). \quad (6.67)$$

Then, using the following mass conservation equation:

$$\nabla \cdot (\alpha_g \rho_g \mathbf{U}_{g,k})^{n+1} = - \frac{(\alpha_g \rho_g)^{n+3/2} - (\alpha_g \rho_g)^{n+1/2}}{\Delta t_g}, \quad (6.68)$$

the modified Poisson equation below can be obtained:

$$\nabla \cdot \left(\frac{1 - \eta_{p,k}}{\gamma} \nabla P_{g,k}^{n+1/2} \right) = \frac{1}{\Delta t_g} \left(\nabla \cdot (\alpha_g \rho_g \mathbf{U}_{g,k})^{**} + \frac{(\alpha_g \rho_g)^{n+3/2} - (\alpha_g \rho_g)^{n+1/2}}{\Delta t_g} \right). \quad (6.69)$$

The gas time step was limited by the following condition to ensure that the penalization

factor γ is not too large:

$$\Delta t_g \leq C_{im} \frac{\alpha_g \rho_g}{\lambda_{p,k}}, \quad (6.70)$$

where C_{im} represents a constant selected by the user to attain stability.

We tested the semi-implication of the drag and Archimedes forces using particles of diameter $d_p = 67$ microns and density $\rho_p = 2595$ kg/m³, and a gas with density $\rho_g = 1.2$ kg/m³ and viscosity $\mu_g = 1.8 \times 10^{-5}$ Pa.s. We employed a cuboid geometry and imposed a gas velocity of $0.317U_{mf}$ at its bottom boundary (Dirichlet boundary condition). In this simulation, C_{im} in Equation 6.70 was set to 5. Figure 6.49 shows the obtained fluid fraction, gas velocity, and pressure profiles. As seen in this figure, the gas velocity and pressure profiles appear stable and physically realistic.

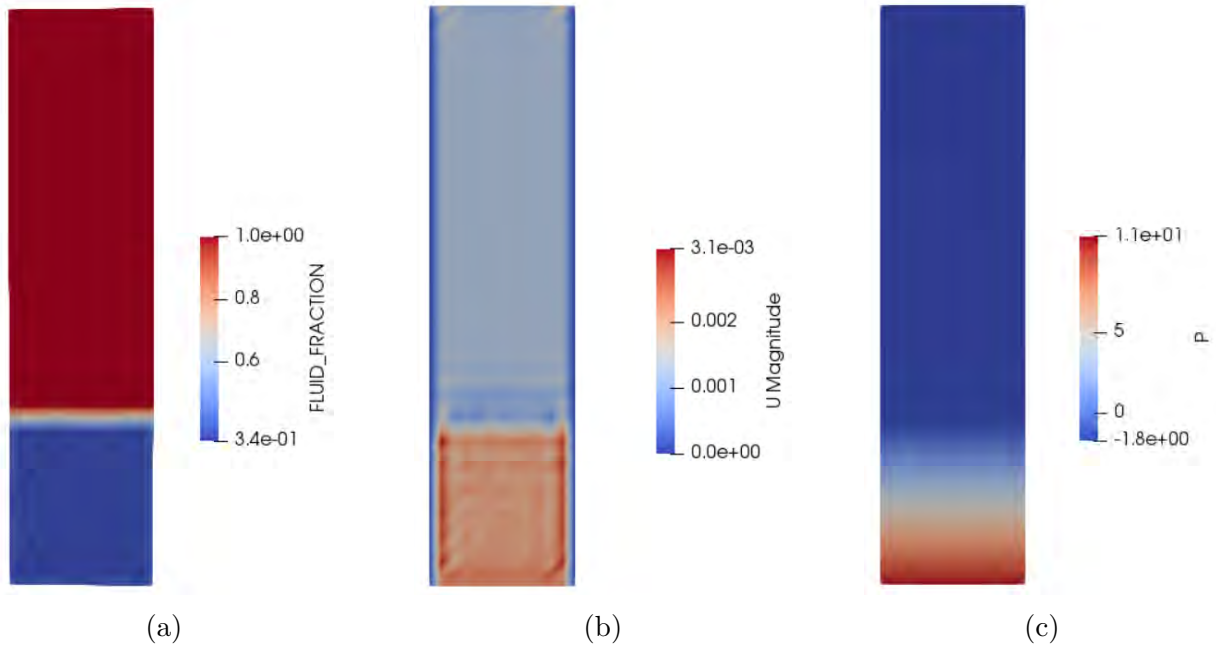


Figure 6.49 Simulation at $0.317U_{mf}$ using the penalization approach: instantaneous profiles of (a) fluid fraction, (b) gas velocity, and (c) pressure.

The stability conditions for the explicit and semi-implicit coupling methods (Equations 6.44 and 6.70, respectively) are the same except that the constant used in the explicit method is 1, while that used in the semi-implicit method is $C_{im} = 5$. This implies that larger gas time steps can be used with the semi-implicit method, thus lowering computational cost (a small improvement). It should be noted that momentum conservation was not maintained because while a term was added to the momentum equation of the gas, nothing was added to the particle momentum equation. However, our primary concern is stability rather than

accuracy.

Some researchers used an implicit scheme that does not need to satisfy any stability conditions on the gas side [195]. A fully implicit approach could be the solution to the stability problem.

6.4.3 Settling of a particle in a fluid

In this section, we perform CFD-DEM simulations of a particle settling in water under gravity. The purpose of this test is to identify the causes of the numerical stability problem. The parameters for this test, which is similar to the one conducted by El Geitani and Blais [196], are provided in Table 6.11. The inlet fluid velocity was set to zero, and no spatial filtering

Table 6.11 Simulation parameters for particle settling in fluid.

<i>Particle properties</i>	
Diameter, d_p	5 mm
Density, ρ_p	2500 kg/m ³
<i>Cuboid geometry</i>	
Width (x -direction), W	100 mm
Thickness (y -direction), T	100 mm
Height (z -direction), H	300 mm
<i>Hexahedral mesh</i>	
Number of cells in the x -direction, N_c^x	14
Number of cells in the y -direction, N_c^y	14
Number of cells in the z -direction, N_c^z	36
<i>Particle loading</i>	
Number of particles, N_{tot}	1
<i>Time advancement of the particle</i>	
Numerical scheme	Groot-Warren [82]
Particle time step, Δt_p	10^{-3} s
<i>Fluid properties</i>	
Density, ρ_f	997 kg/m ³
Viscosity, μ_f	1.002×10^{-3} Pa.s
<i>Advancement of fluid</i>	
Time integration scheme	TFV4A [85]
Spatial integration scheme	4th-order centered
Fluid time step, Δt_f	10^{-3} s
<i>Fluid-particle interaction</i>	
Drag model	Gobin et al. [81]

operations were applied. The particle centroid method was employed to calculate the fluid

fraction. The simulation duration was 0.2 seconds. Figure 6.50 shows the initial fluid fraction profile. As observed, the fluid fraction spreads significantly across adjacent cells.

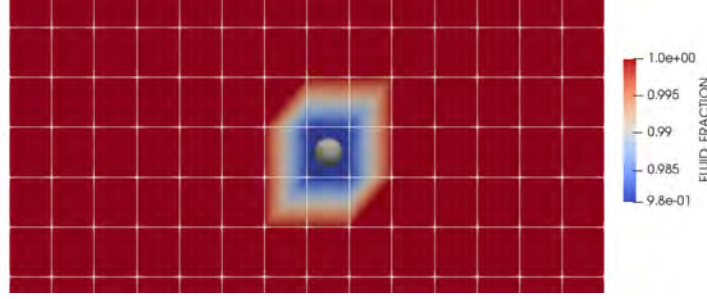


Figure 6.50 Initial distribution of fluid fraction in particle settling simulation.

When the force of gravity is balanced by the drag and Archimedes forces, the particle reaches its terminal velocity. The terminal velocity of the particle can be determined through a trial-and-error approach using the following expression [196]:

$$u_p^T = \sqrt{\frac{2v_p g (\rho_p - \rho_f)}{A_p C_d \rho_f}}. \quad (6.71)$$

Here, g denotes the acceleration due to gravity, C_d represents the drag coefficient, v_p stands for the particle volume, and A_p signifies the particle cross-sectional area. Using Equation (6.71), the terminal velocity is 0.459 m/s. Figure 6.51 shows the particle velocity profile. The particle velocity increases over time until it reaches the terminal velocity.

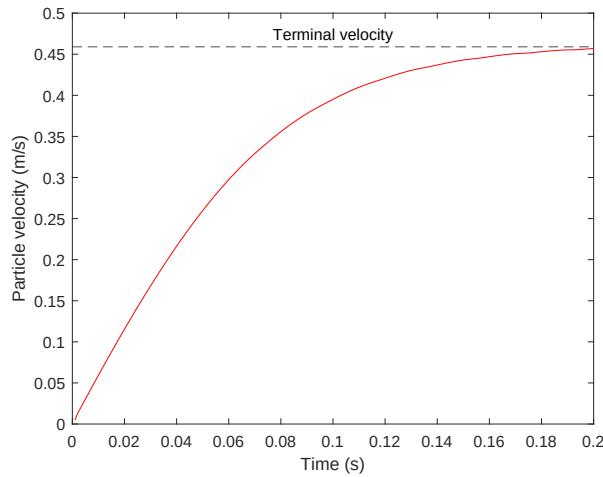


Figure 6.51 Velocity profile of a particle settling in water.

We investigated the effect of the time step (the fluid time step is equal to the particle time

step) on the particle velocity profile. As shown in Figure 6.52a, decreasing the time step to 10^{-5} s leads to instability in the velocity profile. This instability becomes severe at Δt equal to 10^{-6} s, as illustrated in Figure 6.52b. This issue may be attributed to the particle centroid method. An alternative method for calculating the fluid fraction, such as the quadrature-centered method [196], could potentially solve this stability issue.

When an additional stability condition for explicit coupling was implemented, the time step became very small, causing a defluidization simulation to fail at a superficial fluid velocity close to U_{mf} (balance between drag and gravitational forces). We hypothesize that the simulation failure is due to numerical instability resulting from the use of the particle centroid method with very small time steps.

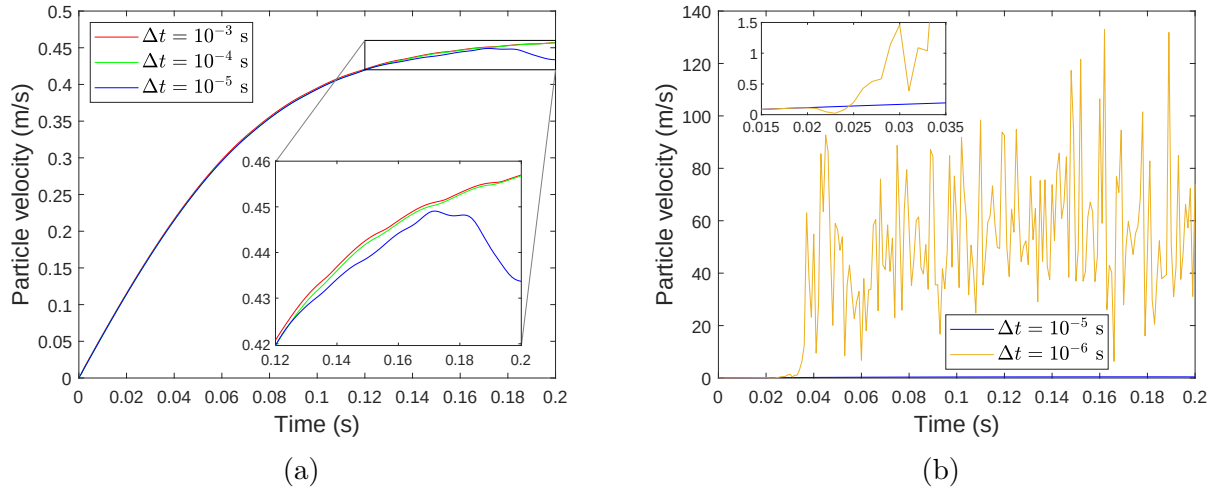


Figure 6.52 Influence of the time step on the velocity of a particle settling in water.

In addition, we examined the influence of cell size on the particle velocity profile using a particle diameter of 10 mm. For these tests, the particle time step was set equal to the fluid time step, both being 10^{-3} s. Figure 6.53 illustrates the influence of cell size on the particle velocity profile. As shown in this figure, reducing the cell size to $0.625d_p$ leads to numerical instability.

6.4.4 Fixing the gas-solid force during the sub-steps

In addition to the penalization approach, keeping the gas-solid force constant during the sub-steps may achieve stability in all flow regimes and during the transitions between them. This will be discussed in this section.

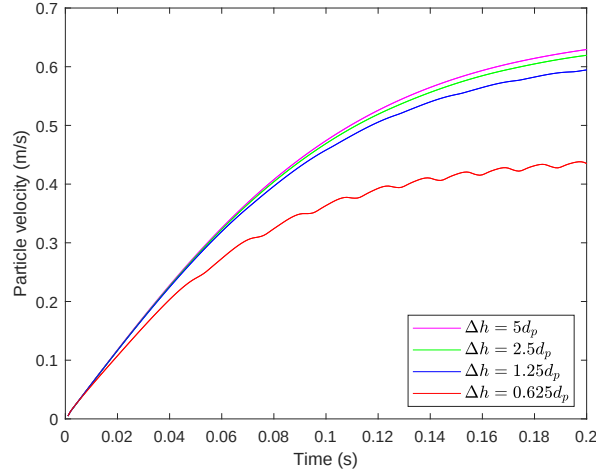


Figure 6.53 Influence of the cell size (Δh) on the velocity of a particle settling in water.

The following steps can be used to couple the gas and solid phases:

1. Advance the gas from time t_g^0 to time t_g^1 (transition from point ① to point ② in Figure 6.54). To perform this, the solid-gas momentum transfer term $\mathbf{I}_{p \rightarrow g}$ and the penalization parameters λ and η should first be computed. Additionally, an initial guess for the gas volume fraction α_g^1 (set as $\alpha_g^1 = \alpha_g^0$) is needed to compute the discretized time derivative of $\alpha_g \rho_g$ in the Poisson equation.
2. Calculate the force exerted by the gas on the particles $\mathbf{F}_{g \rightarrow p}$ using the gas velocity $\mathbf{u}_g^1$ (transition from point ② to point ③ in Figure 6.54) if the convergence condition $\|\mathbf{u}_g^1 - \mathbf{u}_g^0\| \leq \varepsilon_u$ (where ε_u is the convergence tolerance for the gas velocity) is satisfied. Otherwise, restart from point ①.
3. Advance the particles from time t_p^0 to t_p^w (transition from point ③ to point ④).
4. Compute the gas volume fraction α_g^1 and check for convergence ($\|\alpha_g^1 - \alpha_g^0\| \leq \varepsilon_\alpha$, where ε_α is the convergence tolerance for the gas volume fraction). If convergence is achieved, compute the solid-gas momentum transfer term and the penalization parameters (transition from point ④ to point ⑤). If not, restart (transition from point ④ back to point ①) and advance the gas from t_g^0 to t_g^1 using the computed α_g^1 in the Poisson equation.

To simplify the process, the discretized time derivative of $\alpha_g \rho_g$ in the Poisson equation may be estimated rather than performing additional iterations until convergence. This estimation

may be done using the following expression:

$$(\alpha_g \rho_g)^{n+3/2} - (\alpha_g \rho_g)^{n+1/2} = (\alpha_g \rho_g)^{n+1/2} - (\alpha_g \rho_g)^{n-1/2}. \quad (6.72)$$

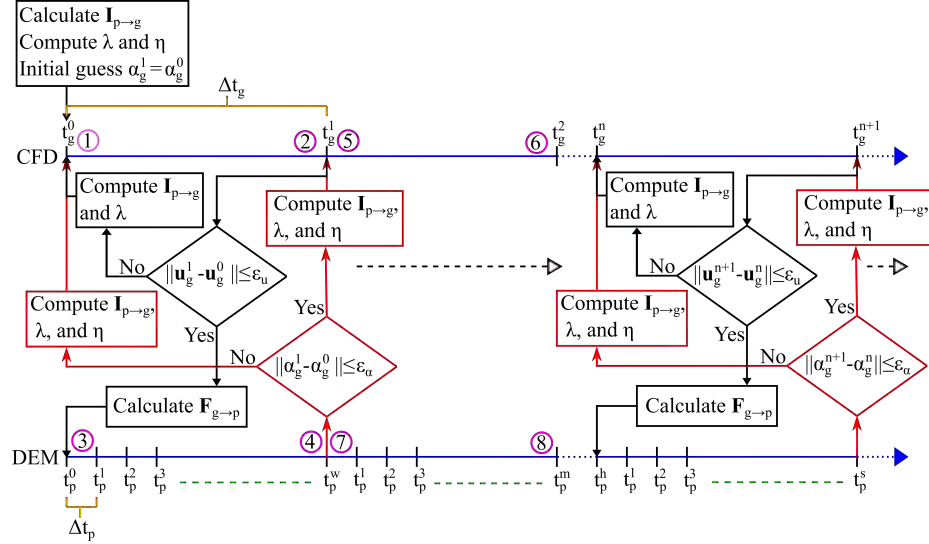


Figure 6.54 Gas-particle coupling process.

Let j be an index referring to discrete times for particle advancement ($j \in [0, N_{st}]$, where N_{st} is the number of particle time steps within a given gas time step). The momentum transfer term should be computed at $j = 0$ as follows:

$$\mathbf{I}_{p \rightarrow g}^n(\mathbf{x}_k) = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p \mathbf{F}_{p \rightarrow g} \Big|_n = -\frac{1}{V_k} \left(\sum_{p \in C_k} \omega_k^p \mathbf{F}_{g \rightarrow p}^n \right)_{j=0}, \quad (6.73)$$

with

$$\mathbf{F}_{g \rightarrow p}^n|_{j=0} = \frac{m_p}{\tau_r^d} \left(\mathbf{u}_{g@p}^n|_{j=0} - \mathbf{u}_p|_{j=0} \right) - V_p \nabla P_{g@p}^n|_{j=0}, \quad (6.74)$$

where $\mathbf{u}_{g@p}^n|_{j=0}$ is the velocity of the gas at time t_g^n , interpolated at the particle position $\mathbf{x}_p|_{j=0}$. The penalization parameters should also be calculated at $j = 0$ as follows:

$$\lambda_{p,k} = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p \frac{m_p}{\tau_r^d} \Big|_n = \frac{1}{V_k} \left(\sum_{p \in C_k} \omega_k^p \frac{m_p}{\tau_r^d} \right)_{j=0}, \quad (6.75)$$

$$\eta_{p,k} = \frac{1}{V_k} \sum_{p \in C_k} \omega_k^p V_p \Big|_n = \frac{1}{V_k} \left(\sum_{p \in C_k} \omega_k^p V_p \right)_{j=0}. \quad (6.76)$$

Equations (6.73), (6.75), and (6.76) are employed for gas advancement.

For particle advancement using the Groot-Warren scheme [82], the gas-particle force $\mathbf{F}_{g \rightarrow p}$ (including drag and Archimedes forces) should be computed at $j = 0$. Since the gas is updated before the particles, this force is a function of the gas velocity and pressure at time t_g^{n+1} . This constant gas-solid force should be applied to advance the particles during each sub-step within a given gas time step.

In summary, the modifications to be implemented in the YALES2 code are as follows: advance the gas before advancing the particles (initially compute the momentum transfer term and penalization parameters and provide an initial guess for α_g^1); do not accumulate the gas-solid force and penalization parameters during the sub-steps (calculate them at $j = 0$ instead); and solve iteratively until the fluid converges, or alternatively, use the estimation given by Equation (6.72).

6.5 Conclusion

In this chapter, we validated the static-dynamic friction and Van der Waals adhesion models implemented in DEM. The rebound angles obtained for particle-wall and particle-particle collisions using the static-dynamic friction model were in strong agreement with Walton's theory. The vertical interparticle contact stress profile in a static bed of soft spheres, determined from DEM simulation using the static-dynamic friction model, matched Janssen's theory. The mass flow rate of powder exiting a hopper, obtained from our DEM simulation, closely matched the value from the Beverloo correlation. The angle of repose increased with an increasing dynamic friction coefficient. Particle-wall and particle-particle collision tests with Van der Waals adhesion showed that increasing the Hamaker constant decreases the rebound translational velocity, increases the rebound rotational velocity, extends the contact time, and increases the maximum normal overlap.

Additionally, we conducted preliminary two-fluid simulations using a coordination number transport equation, which showed pressure-drop hysteresis between decreasing and increasing velocity paths. The results of these simulations indicated that the proposed expression for the source term in the coordination number transport equation needs further refinement. To address this, we computed the source term via CFD-DEM simulations, which allowed us to determine the relaxation time of the coordination number. The time of relaxation towards the equilibrium coordination number was smaller in the fluidized bed state compared to the fixed bed state. Evaluating potential correlations between the relaxation time of the coordination number and local Eulerian variables, such as collisional pressure, through statistical analysis could assist in developing a model for the coordination number source term.

Finally, we tackled a stability issue arising from the coupling between the fluid and particle phases using two approaches. The first approach involves adding a stability condition for explicit coupling, while the second approach uses penalization to achieve semi-implicit coupling. Both approaches enhanced numerical stability in our CFD-DEM simulations, particularly in the fixed-bed regime, ensuring physically realistic gas velocity and pressure contours.

CHAPTER 7 GENERAL DISCUSSION

The aim of this thesis was to quantify the macroscopic impact of the Van der Waals adhesion force on gas-solid fluidized bed hydrodynamics. To meet this objective, we opted for multi-scale numerical simulations. This approach allows us to extract meso-scale information from CFD-DEM simulations and employ it to develop closures required for the two-fluid model at the macroscopic scale. The two-fluid approach is commonly used to simulate large fluidized beds, including those at pilot and industrial scales. Macro-scale models representing the Van der Waals force are rare, and their applicability in all flow regimes, including the fixed-bed regime, is questionable. To achieve our overall goal, we encountered a number of surprises and challenges. In the following paragraphs, we provide an overview of the three main chapters in this thesis, discussing the challenges they represent and highlighting the links between them.

Chapter 4 provides a review of macro-scale Van der Waals adhesion models found in the literature. At the beginning of this project, our approach was to consider Van der Waals adhesion using a macro-scale model based on kinetic theory. However, upon integrating this model into our two-fluid simulations, it became evident that it failed to predict the pressure-drop overshoot observed during the transition from static to fluidized bed states. This deficiency was attributed to the neglect of long-duration and multiple contacts in the kinetic theory approach. The identification of this limitation prompted us to seek a more appropriate model. Consequently, we developed a novel coordination number-based model, offering broader applicability in modeling adhesion across various flow regimes, contingent upon knowledge of the coordination number of the particles. To determine the coordination number, we utilized CFD-DEM correlations from the literature, which relate the coordination number to the particle volume fraction. Using this new model enabled the generation of the pressure-drop overshoot. Nevertheless, we realized the need for further development, specifically aimed at modeling the coordination number evolution to predict hysteresis in pressure drop. Therefore, we proposed an expression for the source term in a coordination number transport equation and integrated it into our two-fluid simulations (in chapter 6). Our proposition successfully predicted the pressure-drop hysteresis. However, an analysis of various profiles, including bed voidage and coordination number profiles, revealed the need for further refinement in the source term expression. This refinement process necessitates guidance provided by CFD-DEM measurements of the coordination number source term. The Eulerian transport equation for the coordination number can then be validated by comparing its predictions with results from CFD-DEM simulations.

In chapter 5, we used the YALES2 code to conduct CFD-DEM simulations of fluidized beds. The primary objective of these simulations was to gather mesoscopic data necessary to guide the development of our macroscopic adhesion model to predict the hysteresis phenomenon. Our findings indicated that both Van der Waals force and static wall friction contribute to the pressure-drop overshoot. We implemented the Van der Waals adhesion and static-dynamic friction models for both interparticle and particle-wall interactions in the YALES2 code, which is massively parallel. This implementation was verified through micro-scale and macro-scale tests (in chapter 6). We opted to consider solely the Van der Waals interactions among particles in contact, neglecting those between particles not in contact. This decision was motivated by the quick decrease in Van der Waals force with increasing separation between the surfaces of the two interacting particles, as well as for the sake of simplification. Moreover, we computed the adhesive and repulsive particle pressures. We observed that Van der Waals adhesion has a marked effect on pressure drop (overshoot), voidage, coordination number, fabric, and effective solid pressure profiles. From our CFD-DEM tests, we concluded that adhesion is essential for predicting the homogeneous fluidization regime. Considering the small bed width in our simulations, Van der Waals adhesion and static friction each contribute to around 50% of the overshoot. It is worth noting that increasing the bed width decreases the effect of static wall friction. This could be investigated through additional CFD-DEM tests. Additionally, studying the impact of the Hamaker constant, particle-wall dynamic friction coefficient, and spring stiffness on the pressure-drop overshoot would be insightful. However, our progress was impeded by an instability in the gas velocity field, which was particularly evident in the fixed-bed regime. We attempted to solve this stability problem first by implementing a stability condition for the explicit gas-particle coupling and then by semi-implicitation of the drag and Archimedes forces (in chapter 6). The latter method showed a small improvement in terms of computational cost compared to the former. These implementations enabled us to simulate static or fluidized beds without stability problems. Nevertheless, the gas time step was very small, and neither of these two approaches enabled us to successfully simulate the entire defluidization cycle. It appears that instability was growing over time during the defluidization cycle. Implementing a fully implicit scheme may solve the problem, but it would be rather complicated to do that in the granular flow solver in YALES2, which relies on a variable-density formulation. While we acknowledge the potential impact of the stability issue on the results obtained for each configuration studied, we remain confident in the validity of our conclusions drawn from comparing the results of these configurations.

Chapter 6 is intended to open the door to a better understanding of coordination number evolution at the macroscale and to develop an Eulerian adhesion closure capable of predicting

pressure-drop hysteresis. This chapter covers the computation of the source term in the Eulerian transport equation of the coordination number using CFD-DEM simulations. Two methods were employed for this measurement, both yielding identical results. The source term was calculated in the static and fluidized bed states. Moreover, we introduced an Eulerian relaxation expression for this source term and determined the coordination number relaxation time using our CFD-DEM measurements. The combination of chapters 5 and 6 involves the computation of various parameters that can contribute to the development of an Eulerian adhesion model capable of producing pressure hysteresis.

Finally, a significant aspect of numerical modeling involves learning software, creating meshes, writing input scripts (pre-processing), and analyzing results (post-processing). The scripts and test case files developed and utilized during this thesis have been uploaded to the GitLab repository at: https://gitlab.imft.fr/LGCRestreint/dem-cfd_yales2. Additionally, the main developments made in YALES2 during this research can be accessed on the YALES2 remote Git repository at: <https://gitlab.coria-cfd.fr>.

Thus, through the writing of this thesis, we believe we have successfully achieved the main objective.

CHAPTER 8 CONCLUSION

8.1 Summary of the work

The aim of this section is to summarize the main results of this thesis and outline its scientific contributions to the field.

Chapter 4: Macro-scale numerical investigation of the contribution of Van der Waals force to the pressure-drop overshoot in fine-particle fluidized beds

The main findings and scientific contributions in this chapter are described below.

- **Development of adhesion pressure closures:** Two adhesion pressure closures were proposed to account for the Van der Waals force effect in a two-fluid model. The first closure was developed within the context of the kinetic theory of rapid granular flows, while the second was based on the coordination number.
- **Limitations of the kinetic theory:** The kinetic theory adhesion model proved inadequate in predicting a pressure overshoot observed in fluidized beds due to its underestimation of the adhesion effect. This was attributed to its inability to consider long-term and multiple particle-particle contacts, highlighting the need for a more comprehensive adhesion model.
- **Success of the coordination-number-based adhesion model:** The adhesion model based on the coordination number, which represents long-lasting interparticle contacts, was able to create the pressure drop overshoot. This model makes use of CFD-DEM correlations that relate the coordination number to the solid volume fraction for various flow conditions.
- **Role of the interparticle Van der Waals force:** The contribution of the interparticle Van der Waals force to the pressure overshoot phenomenon was demonstrated. Taking this adhesive interaction into account is critical for comprehensively understanding and accurately modeling the fluidization behavior of particles belonging to Geldart group A.

Chapter 5: Meso-scale numerical analysis of the role of Van der Waals adhesion and static friction in fluidized beds of fine solids

The main scientific contributions and findings in Chapter 5 are outlined below.

- **Implementation and verification of static-dynamic friction in DEM:** The Coulomb dynamic friction model available in YALES2 is valid for rapid granular flows but is not suitable for fixed beds. We have implemented a static-dynamic friction model in the massively parallel YALES2 code, appropriate for any flow regime. This model was implemented for both interparticle and particle-wall interactions and was validated at both micro and macro scales by comparing its results to those obtained from theoretical models (Walton and Janssen) and an empirical correlation (Beverloo). The results of these tests are presented in Chapter 6.
- **Implementation and verification of Van der Waals force in DEM:** We have implemented the Van der Waals adhesion force for particle-particle and particle-wall interactions in the YALES2 code. This implementation was qualitatively validated at the microscale by predicting the effect of adhesion on rebound translational and rotational velocities, contact time, and maximum normal overlap, and at the macroscale by producing a pressure overshoot. The outcomes of the microscale tests are provided in Chapter 6.
- **Predicting pressure-drop hysteresis using CFD-DEM:** We have predicted hysteresis in the pressure drop across a fine particle bed and quantified the contributions of Van der Waals adhesion and static friction to this phenomenon.
- **Building a CFD-DEM database:** We have extracted new numerical data from fluidization and defluidization CFD-DEM simulations. This dataset encompasses various parameters, including adhesion pressure, wall shear stress, repulsive pressure, coordination number, fabric tensor, pressure drop, and voidage. These data may be utilized to guide the development of and validate Eulerian models for adhesion and friction, enabling the prediction of hysteresis in the bed pressure drop at the macroscopic scale.
- **Van der Waals adhesion causing homogeneous fluidization:** We have shown that predicting the homogeneous bed expansion between the minimum fluidization and minimum bubbling velocities requires accounting for Van der Waals adhesion.
- **Computation of the coordination number source term:** We have computed the source term of the coordination number transport equation from CFD-DEM simulations using two methods. The coordination number source term was shown to be influenced by the Van der Waals forces and superficial gas velocity.

Chapter 6: CFD-DEM validation and coordination number source term formulation

The key results and scientific contributions in Chapter 6 are summarized below.

- **Proposing an Eulerian expression for the coordination number source term:** We have calculated the coordination number source term from CFD-DEM simulations at both low and high gas velocities, corresponding respectively to static and fluidized beds. We have then proposed an Eulerian relaxation expression for the coordination number source term and computed the relaxation time of the coordination number using our CFD-DEM measurements. The time of relaxation towards the equilibrium coordination number was smaller in the fluidized bed state compared to the fixed bed state. The postulated source term expression may be used in two-fluid simulations to predict the hysteresis in pressure drop.
- **Improving stability:** To solve a stability problem related to gas-solid coupling, we have implemented in YALES2 a stability condition for explicit coupling and a semi-implicit treatment of drag and Archimedes forces using a penalization approach. These two methods were tested at both low and high gas velocities, corresponding respectively to static and fluidized beds, and resulted in stable gas velocity and pressure fields.

8.2 Limitations of the proposed solution

The main limitations of the work carried out in this thesis are discussed here.

Our Eulerian model accounts only for the contribution of the interparticle Van der Waals force to the bed pressure drop overshoot. Static wall friction, which depends on the non-sphericity of the particles and roughness parameters, can also contribute to the pressure overshoot. This wall impact is significant for small bed diameters.

Our study is limited to ambient pressure and temperature. At elevated conditions, we may change the Hamaker constant value, but other inter-particle forces, such as solid and liquid bridge forces, could significantly contribute to the pressure overshoot.

Regarding static-dynamic friction between particles and walls, our implementation is limited to planar walls. For non-planar walls, different scenarios (contact with face, edge, and/or vertex) should be considered while accumulating the tangential overlap.

An often-mentioned limitation in CFD-DEM simulations is the high computation time, which depends heavily on the number of particles. For instance, our simulation with 36,000 fine particles in the presence of adhesion required about 15 days using 36 processors to complete the fluidization branch (equivalent to 36 seconds of physical time). To improve this aspect, some CFD-DEM codes enable adaptive and simultaneous parallelization of the simulation domain, meaning that the distribution of processors adapts to particle movement, ensuring optimal resource utilization. This improvement is available in a CFD-DEM code developed at

Polytechnique Montréal called Lethe (<https://github.com/chaos-polymtl/lethe/wiki>).

8.3 Future improvements

This research project opens the door to numerous future avenues.

The next logical step would be to extend our Eulerian adhesion model to accurately predict the hysteresis in the pressure drop and to obtain precise coordination number evolution at the macroscale compared to CFD-DEM results. Future work could also include accounting for the effect of adhesion on solid viscosity. Additionally, developing and implementing an Eulerian boundary condition for adhesion in the `neptune_cfd` code would enhance the model's accuracy and applicability.

In the CFD-DEM model, an improvement would be to account for Van der Waals forces between particles not in contact. Additionally, it is important to study the influence of spring stiffness on the pressure overshoot, as it impacts the contact duration. Further studies could investigate the effect of adhesion on the flow behavior in the fluidized bed regime, for example, by examining its influence on variables such as cluster size.

Moreover, there is potential to develop an Eulerian model for static friction, which would enhance the applicability of the two-fluid model. The wall shear stress measured from the CFD-DEM simulations, along with other measured parameters, could guide the development of a static-dynamic friction boundary condition, extending the dynamic boundary condition developed by Dupuy et al. [76]. Furthermore, the measured repulsive particle pressure and other valuable data and statistics obtained from CFD-DEM simulations could be utilized to develop a more sophisticated frictional pressure model, potentially through the use of machine learning techniques.

Extending the implementation of static-dynamic friction in the CFD-DEM model to handle cases with periodic boundaries and/or non-planar walls could be a subject of future work. Optimizing the implementation of the static-dynamic friction model to decrease computational and memory costs is also an avenue for improvement. Implementing non-linear contact models, which accurately predict the experimental evolution of parameters such as the restitution coefficient, is a potential improvement. Additionally, rolling friction represented using a spring-dashpot system could enhance the predictions of the DEM model in the static state where the relative angular velocity is zero. Furthermore, investigating the effects of roughness and non-sphericity on friction and pressure overshoot and extending the implementation in the YALES2 code from monodisperse to polydisperse particles to analyze the impact of polydispersity on the fluidization quality index are important areas for future work.

Implementing a fully implicit scheme in YALES2 to improve stability without limiting the fluid time step by a stability condition could be a direction for future study. In addition, investigating spatial filtering is necessary because we observed an issue in the gas velocity field in the fixed-bed regime when using this technique. Implementing a more accurate method than the particle centroid method, such as the divided approach [80], could be a future enhancement.

After validating the ability of our Eulerian adhesion model to predict pressure-drop hysteresis accurately compared to CFD-DEM results, it should be validated by comparison with experimental data. Further validation may include checking the model's ability to predict experimental results upon changing parameters such as particle properties, gas properties, and bed diameter. Then, with simulations, we can realize specific operating conditions and bed geometries that are not available in the lab.

Finally, the implementation of interparticle force models in the YALES2 CFD-DEM code during this thesis opens avenues for the integration of additional interparticle forces, such as electrostatic forces. Subsequently, the data obtained from CFD-DEM simulations could guide the development of Eulerian models for these interparticle forces.

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APPENDIX A IMPLEMENTATION OF THE ADHESION PRESSURE IN THE TWO-FLUID MODEL

Implementation of the kinetic-theory-based adhesion model

The kinetic-theory-based adhesive pressure was incorporated into the subroutine that computes the frictional pressure as follows:

□ If $\alpha_p \leq \alpha_{p,min}$:

The frictional pressure model was activated for α_p values greater than $\alpha_{p,min}$. The effective pressure and its derivative with respect to α_p were written as:

$$P_p^e = P_p^a, \quad (\text{A.1})$$

$$\frac{\partial P_p^e}{\partial \alpha_p} = \frac{\partial P_p^a}{\partial \alpha_p}, \quad (\text{A.2})$$

where the adhesive particle pressure, P_p^a , and its derivative with respect to α_p were expressed as:

$$P_p^a = -\frac{B}{d_p^3} 2\alpha_{p,max}^2 \left[\frac{25}{6} + \left(-\frac{3}{2} \frac{\alpha_p^2}{\alpha_{p,max}^2} + \frac{20}{3} \frac{\alpha_p}{\alpha_{p,max}} - \frac{25}{6} \right) g_0 \right], \quad (\text{A.3})$$

$$\begin{aligned} \frac{\partial P_p^a}{\partial \alpha_p} = -\frac{B}{d_p^3} 2\alpha_{p,max}^2 & \left[\left(-3 \frac{\alpha_p}{\alpha_{p,max}^2} + \frac{20}{3} \frac{1}{\alpha_{p,max}} \right) g_0 \right. \\ & \left. + \left(-\frac{3}{2} \frac{\alpha_p^2}{\alpha_{p,max}^2} + \frac{20}{3} \frac{\alpha_p}{\alpha_{p,max}} - \frac{25}{6} \right) \frac{\partial g_0}{\partial \alpha_p} \right], \end{aligned} \quad (\text{A.4})$$

with

$$B = A \frac{3}{\pi} \ln \left(\frac{d_p}{S_0} \right). \quad (\text{A.5})$$

The radial distribution function, g_0 , and its derivative with respect to α_p were given by:

$$g_0 = \left(1 - \frac{\alpha_p}{\alpha_{p,max}} \right)^{-2.5\alpha_{p,max}}, \quad (\text{A.6})$$

$$\frac{\partial g_0}{\partial \alpha_p} = \frac{2.5g_0}{1 - \frac{\alpha_p}{\alpha_{p,max}}}. \quad (\text{A.7})$$

□ If $\alpha_p > \alpha_{p,min}$:

As α_p tends to $\alpha_{p,max}$, both the radial distribution function (g_0) and the frictional particle pressure (P_p^f) tend to infinity (division by zero), leading to the termination of the simulation. To avoid this division by zero, we employed the parameter $\alpha_{p,s}$, defined as:

$$\alpha_{p,s} = \alpha_{p,max} - \varepsilon \alpha_{p,max}, \quad \text{with } \varepsilon = 0.001. \quad (\text{A.8})$$

• If $\alpha_{p,min} < \alpha_p \leq \alpha_{p,s}$:

The effective pressure and its derivative with respect to α_p were written as:

$$P_p^e = P_p^f + P_p^a, \quad (\text{A.9})$$

$$\frac{\partial P_p^e}{\partial \alpha_p} = \frac{\partial P_p^f}{\partial \alpha_p} + \frac{\partial P_p^a}{\partial \alpha_p}, \quad (\text{A.10})$$

where the expressions for the frictional pressure, P_p^f , and its derivative with respect to α_p were given by:

$$P_p^f = Fr \frac{(\alpha_p - \alpha_{p,min})^n}{(\alpha_{p,max} - \alpha_p)^m}, \quad (\text{A.11})$$

$$\frac{\partial P_p^f}{\partial \alpha_p} = Fr \left[n \frac{(\alpha_p - \alpha_{p,min})^{n-1}}{(\alpha_{p,max} - \alpha_p)^m} + m \frac{(\alpha_p - \alpha_{p,min})^n}{(\alpha_{p,max} - \alpha_p)^{m+1}} \right]. \quad (\text{A.12})$$

The adhesion pressure, P_p^a , and its derivative with respect to α_p were given by Equations (A.3) and (A.4), respectively.

• If $\alpha_p > \alpha_{p,s}$:

The effective pressure and its derivative with respect to α_p were given by Equations (A.9) and (A.10), respectively. A Taylor series expansion of P_p^f about $\alpha_{p,s}$ was used:

$$\begin{aligned} P_p^f(\alpha_p) &= P_p^f(\alpha_{p,s} + \Delta\alpha_p) \quad \text{with } \Delta\alpha_p = \alpha_p - \alpha_{p,s} \\ &\approx P_p^f(\alpha_{p,s}) + \Delta\alpha_p \left. \frac{\partial P_p^f}{\partial \alpha_p} \right|_{\alpha_p=\alpha_{p,s}} + \frac{(\Delta\alpha_p)^2}{2} \left. \frac{\partial^2 P_p^f}{\partial \alpha_p^2} \right|_{\alpha_p=\alpha_{p,s}} \\ &= Fr \frac{(\alpha_{p,s} - \alpha_{p,min})^n}{(\varepsilon \alpha_{p,max})^m} + (\alpha_p - \alpha_{p,s}) Fr \left[n \frac{(\alpha_{p,s} - \alpha_{p,min})^{n-1}}{(\varepsilon \alpha_{p,max})^m} + m \frac{(\alpha_{p,s} - \alpha_{p,min})^n}{(\varepsilon \alpha_{p,max})^{m+1}} \right] \\ &\quad + \frac{(\alpha_p - \alpha_{p,s})^2}{2} Fr \left[n(n-1) \frac{(\alpha_{p,s} - \alpha_{p,min})^{n-2}}{(\varepsilon \alpha_{p,max})^m} \right. \\ &\quad \left. + 2mn \frac{(\alpha_{p,s} - \alpha_{p,min})^{n-1}}{(\varepsilon \alpha_{p,max})^{m+1}} + m(m+1) \frac{(\alpha_{p,s} - \alpha_{p,min})^n}{(\varepsilon \alpha_{p,max})^{m+2}} \right]. \end{aligned} \quad (\text{A.13})$$

Then, the derivative of P_p^f with respect to α_p can be formulated as follows:

$$\begin{aligned} \frac{\partial P_p^f}{\partial \alpha_p} = Fr \left[n \frac{(\alpha_{p,s} - \alpha_{p,min})^{n-1}}{(\varepsilon \alpha_{p,max})^m} + m \frac{(\alpha_{p,s} - \alpha_{p,min})^n}{(\varepsilon \alpha_{p,max})^{m+1}} \right] \\ + (\alpha_p - \alpha_{p,s}) Fr \left[n(n-1) \frac{(\alpha_{p,s} - \alpha_{p,min})^{n-2}}{(\varepsilon \alpha_{p,max})^m} \right. \\ \left. + 2mn \frac{(\alpha_{p,s} - \alpha_{p,min})^{n-1}}{(\varepsilon \alpha_{p,max})^{m+1}} + m(m+1) \frac{(\alpha_{p,s} - \alpha_{p,min})^n}{(\varepsilon \alpha_{p,max})^{m+2}} \right]. \quad (A.14) \end{aligned}$$

A Taylor series expansion of g_0 about $\alpha_{p,s}$ was employed:

$$\begin{aligned} g_0(\alpha_p) &= g_0(\alpha_{p,s} + \Delta\alpha_p) \quad \text{with } \Delta\alpha_p = \alpha_p - \alpha_{p,s} \\ &\approx g_0(\alpha_{p,s}) + \Delta\alpha_p \left. \frac{\partial g_0}{\partial \alpha_p} \right|_{\alpha_p=\alpha_{p,s}} + \frac{(\Delta\alpha_p)^2}{2} \left. \frac{\partial^2 g_0}{\partial \alpha_p^2} \right|_{\alpha_p=\alpha_{p,s}} \\ &= \varepsilon^{-2.5\alpha_{p,max}} + 2.5(\alpha_p - \alpha_{p,s}) \varepsilon^{-2.5\alpha_{p,max}-1} \\ &\quad + 2.5 \frac{(\alpha_p - \alpha_{p,s})^2}{2} \varepsilon^{-2.5\alpha_{p,max}-2} \left(2.5 + \frac{1}{\alpha_{p,max}} \right). \quad (A.15) \end{aligned}$$

Then, the derivative of g_0 with respect to α_p can be expressed as follows:

$$\frac{\partial g_0}{\partial \alpha_p} = 2.5 \varepsilon^{-2.5\alpha_{p,max}-1} + 2.5(\alpha_p - \alpha_{p,s}) \varepsilon^{-2.5\alpha_{p,max}-2} \left(2.5 + \frac{1}{\alpha_{p,max}} \right). \quad (A.16)$$

The equations for the adhesive pressure (P_p^a) and its derivative with respect to α_p are identical to Equations (A.3) and (A.4), but with the expressions for g_0 and its derivative given by Equations (A.15) and (A.16).

Implementation of the coordination-number-based adhesion model

► Constant coordination number

The coordination-number-based adhesive pressure with constant coordination number was incorporated into the subroutine that computes the frictional pressure as follows:

□ If $\alpha_p \leq \alpha_{p,min}$:

The effective pressure and its derivative with respect to α_p were written as:

$$P_p^e = P_p^a, \quad (A.17)$$

$$\frac{\partial P_p^e}{\partial \alpha_p} = \frac{\partial P_p^a}{\partial \alpha_p}, \quad (\text{A.18})$$

where the adhesive pressure (P_p^a) and its derivative with respect to α_p were expressed as:

$$P_p^a = -\frac{\alpha_p}{\pi d_p^2} CN \frac{Ad_p}{24S_0^2}, \quad (\text{A.19})$$

$$\frac{\partial P_p^a}{\partial \alpha_p} = -\frac{1}{\pi d_p^2} CN \frac{Ad_p}{24S_0^2}. \quad (\text{A.20})$$

□ If $\alpha_p > \alpha_{p,min}$:

- If $\alpha_{p,min} < \alpha_p \leq \alpha_{p,s}$, with $\alpha_{p,s} = \alpha_{p,max} - 0.001\alpha_{p,max}$:

The expressions for the effective pressure and its derivative with respect to α_p were given by:

$$P_p^e = P_p^f + P_p^a, \quad (\text{A.21})$$

$$\frac{\partial P_p^e}{\partial \alpha_p} = \frac{\partial P_p^f}{\partial \alpha_p} + \frac{\partial P_p^a}{\partial \alpha_p}. \quad (\text{A.22})$$

The frictional pressure and its derivative with respect to α_p are given by Equations (A.11) and (A.12), respectively. The adhesive pressure and its derivative with respect to α_p are given by Equations (A.19) and (A.20), respectively.

- If $\alpha_p > \alpha_{p,s}$:

A Taylor series expansion of P_p^f about $\alpha_{p,s}$ was used. The frictional pressure and its derivative with respect to α_p are given by Equations (A.13) and (A.14), respectively. The adhesive pressure and its derivative with respect to α_p are given by Equations (A.19) and (A.20), respectively.

► Coordination number determined using an expanded-bed correlation

The adhesive pressure was expressed as:

$$P_p^a = -\frac{\alpha_p}{\pi d_p^2} CN \frac{Ad_p}{24S_0^2}, \quad (\text{A.23})$$

with

$$CN = 2 + 3.25\alpha_p^{0.4}.$$

Then,

$$P_p^a = -\frac{\alpha_p}{\pi d_p^2} \frac{Ad_p}{24S_0^2} (2 + 3.25\alpha_p^{0.4}), \quad (\text{A.24})$$

$$\frac{\partial P_p^a}{\partial \alpha_p} = -\frac{1}{\pi d_p^2} \frac{Ad_p}{24S_0^2} (2 + 4.55\alpha_p^{0.4}). \quad (\text{A.25})$$

Using Equations (A.24) and (A.25), the adhesive pressure can be incorporated into the subroutine that calculates the frictional pressure, employing a method analogous to that used for a constant coordination number. The expressions for the adhesive pressure and its derivative involve $\alpha_p^{0.4}$. A test revealed that α_p can be negative zero (approximately), which caused an error in the simulation because a negative α_p raised to the power of 0.4 is not a number. To resolve this problem, we used an α_p of zero in Equations (A.24) and (A.25) if α_p was less than zero.

► Coordination number determined using a fluidized-bed correlation

The adhesive pressure was written as:

$$P_p^a = -\frac{\alpha_p}{\pi d_p^2} CN \frac{Ad_p}{24S_0^2}, \quad (\text{A.26})$$

with

$$CN = 4.87 \times 10^{-5} \frac{1 - (1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{11.6}}. \quad (\text{A.27})$$

Then,

$$P_p^a = -4.87 \times 10^{-5} \frac{\alpha_p}{\pi d_p^2} \frac{Ad_p}{24S_0^2} \frac{1 - (1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{11.6}}, \quad (\text{A.28})$$

$$\frac{\partial P_p^a}{\partial \alpha_p} = -\frac{4.87 \times 10^{-5}}{\pi d_p^2} \frac{Ad_p}{24S_0^2} \frac{1 + 10.6\alpha_p - (1 - \alpha_p)^{3.8} - 8.8\alpha_p(1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{12.6}}. \quad (\text{A.29})$$

Using Equations (A.28) and (A.29), the adhesive pressure can be incorporated into the subroutine that calculates the frictional pressure, employing a method analogous to that used for a constant coordination number.

APPENDIX B PARTICLE PRESSURES AS A FUNCTION OF SOLID VOLUME FRACTION

Kinetic-theory-based adhesive pressure model

The adhesive pressure was computed as follows:

$$P_p^a = -\frac{B}{d_p^3} 2\alpha_{p,max}^2 \left[\frac{25}{6} + \left(-\frac{3}{2} \frac{\alpha_p^2}{\alpha_{p,max}^2} + \frac{20}{3} \frac{\alpha_p}{\alpha_{p,max}} - \frac{25}{6} \right) g_0 \right], \quad (\text{B.1})$$

with

$$g_0 = \left(1 - \frac{\alpha_p}{\alpha_{p,max}} \right)^{-2.5\alpha_{p,max}}, \quad (\text{B.2})$$

and

$$B = A \frac{3}{\pi} \ln \left(\frac{d_p}{S_0} \right). \quad (\text{B.3})$$

Using $d_p = 67 \mu\text{m}$, $A = 7.21 \times 10^{-20} \text{ J}$ (for glass beads fluidized by air at 20°C [197]), and $S_0 = 4 \times 10^{-10} \text{ m}$, the value of B is $8.3 \times 10^{-19} \text{ J}$. For Figure B.1, we used a value of B multiplied by 10^6 ($B = 8.3 \times 10^{-13} \text{ J}$). The frictional pressure was calculated as:

$$P_p^f = Fr \frac{(\alpha_p - \alpha_{p,min})^n}{(\alpha_{p,max} - \alpha_p)^m}, \quad \text{for } \alpha_p > \alpha_{p,min}, \quad (\text{B.4})$$

with $\alpha_{p,min} = 0.5$, $\alpha_{p,max} = 0.64$, $Fr = 0.05$, $n = 2$, and $m = 5$. The effective pressure was determined as:

$$P_p^e = P_p^f + P_p^a. \quad (\text{B.5})$$

Figure B.1 shows plots of the frictional, adhesion, and effective pressures as a function of the solid volume fraction (α_p) using $B = 8.3 \times 10^{-13} \text{ J}$. This figure demonstrates that at high α_p values (Figure B.1b), the frictional effect dominates, whereas at lower α_p values (Figure B.1a), there is a pressure well due to the dominance of adhesion. As α_p decreases further, the effect of adhesion diminishes. This behavior is similar to the Lennard-Jones potential.

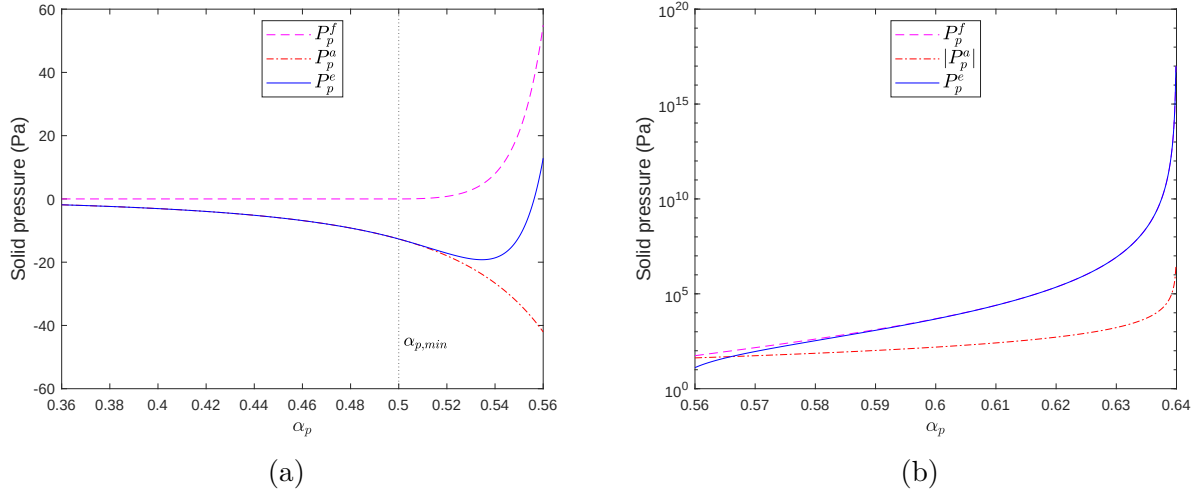


Figure B.1 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.36 \leq \alpha_p \leq 0.56$ and (b) $0.56 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the kinetic theory.

Coordination-number-based adhesive pressure model

The adhesive pressure was calculated as follows:

$$P_p^a = -\frac{\alpha_p}{\pi d_p^2} CN \frac{A d_p}{24 S_0^2}, \quad (\text{B.6})$$

with $d_p = 67 \mu\text{m}$, $A = 7.21 \times 10^{-20} \text{ J}$, and $S_0 = 4 \times 10^{-10} \text{ m}$. The coordination number was determined as [148]:

$$CN = \begin{cases} 4.77, & \text{for fixed beds,} \\ 2 + 3.25\alpha_p^{0.4}, & \text{for expanded beds,} \\ 4.87 \times 10^{-5} \frac{1 - (1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{11.6}}, & \text{for fluidized beds.} \end{cases} \quad (\text{B.7})$$

The frictional pressure was computed using Equation B.4, and the effective pressure was calculated using Equation B.5. Figures B.2, B.3, and B.4 are plots of the solid pressures as a function of the solid volume fraction using fixed-bed, expanded-bed, and fluidized-bed coordination numbers, respectively.

The coordination number may be expressed as a function of the frictional pressure in the

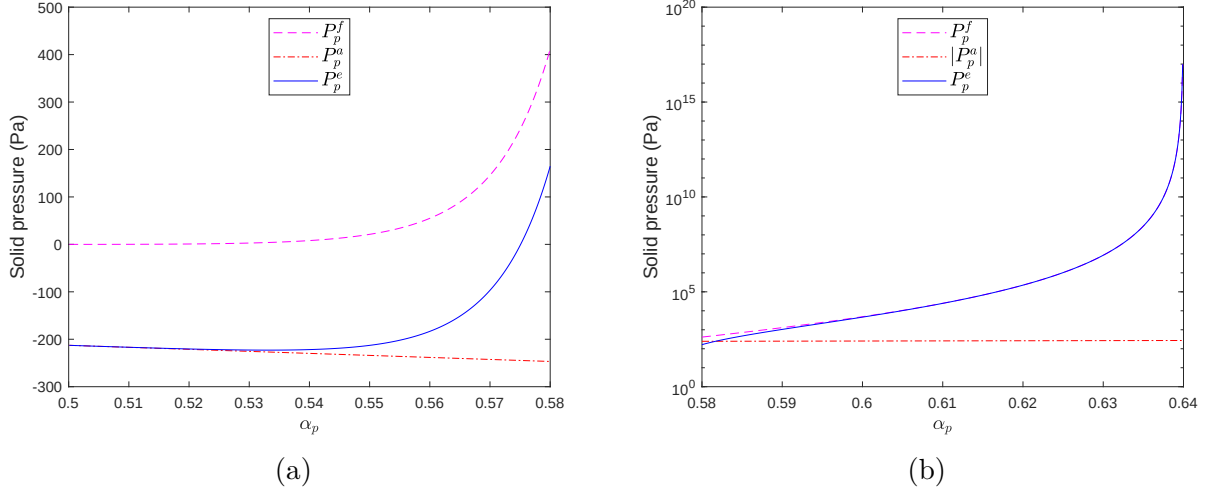


Figure B.2 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. A constant fixed-bed coordination number ($CN = 4.77$) is used.

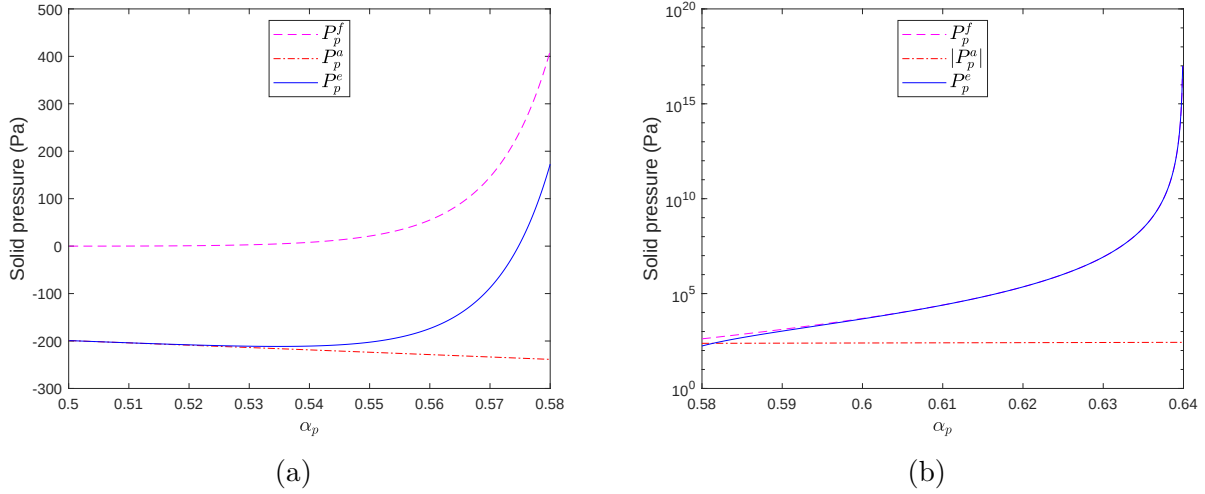


Figure B.3 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. An expanded-bed coordination number ($CN = 2 + 3.25\alpha_p^{0.4}$) is used.

following manner:

$$CN = CN_{max} \frac{P_p^f}{Fr_1 + P_p^f}. \quad (B.8)$$

This formula represents the fact that the coordination number tends towards the maximum

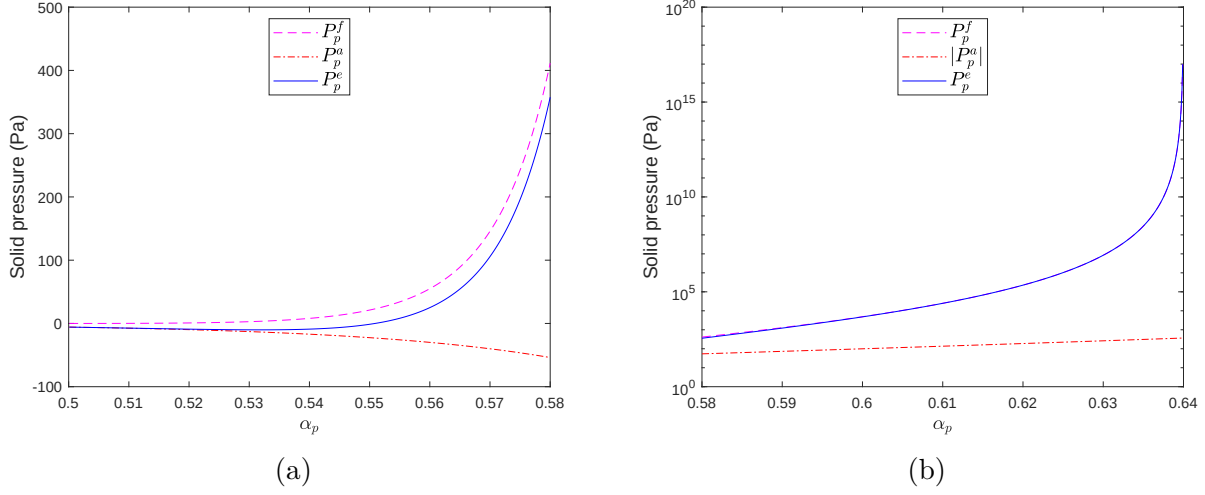


Figure B.4 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. A fluidized-bed coordination number (see Equation B.7) is used.

value (CN_{max}) for large values of P_p^f and tends towards zero for small values of P_p^f . Figure B.5 shows plots of the coordination number as a function of the solid volume fraction. $CN_{max} = 6$ (in 2D [198]) and $Fr_1 = Fr = 0.05$ were used for this figure.

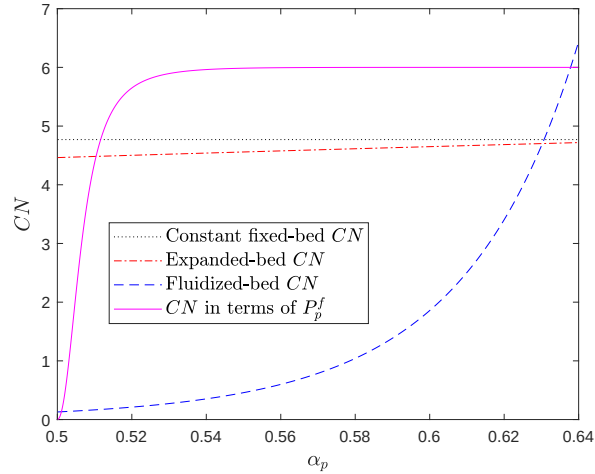


Figure B.5 Coordination number vs. solid volume fraction for different coordination number expressions.

Figures B.6, B.7, and B.8 show the solid pressures as a function of the solid volume fraction using the coordination number expressed as a function of the frictional pressure (Equation

B.8), with Fr_1 equal to 0.05, 5, and 50, respectively. The value of CN_{max} used is 6.

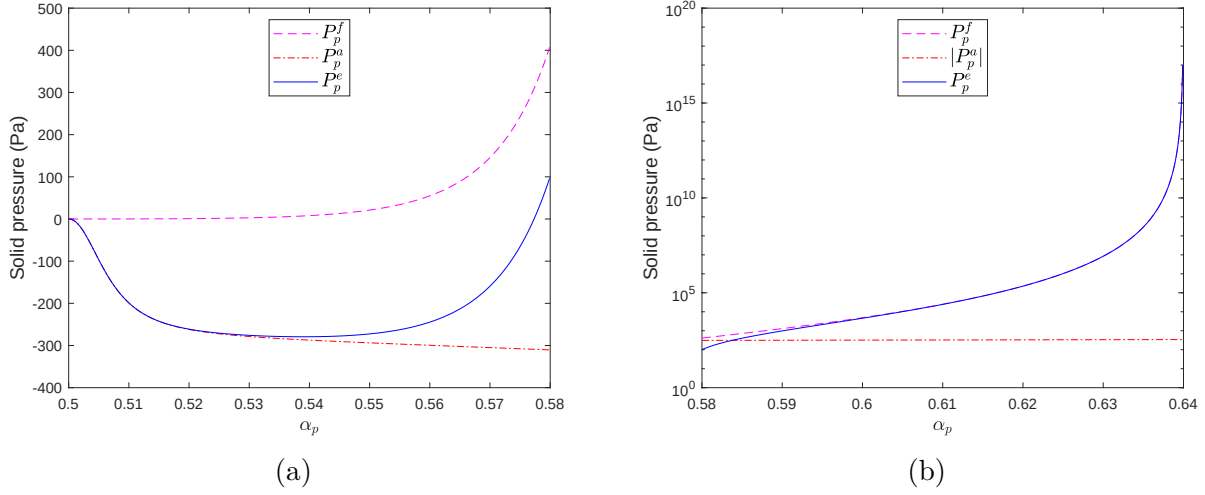


Figure B.6 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. The coordination number is expressed as a function of the frictional pressure P_p^f , with $Fr_1 = Fr = 0.05$.

The coordination number may be expressed as a combination of fixed-bed and fluidized-bed

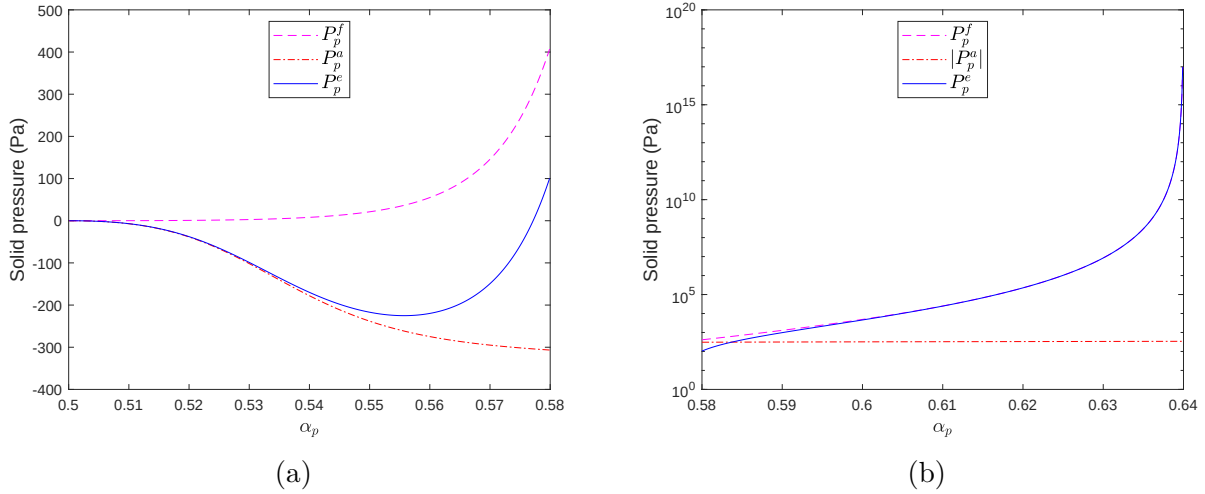


Figure B.7 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. The coordination number is expressed as a function of P_p^f , with $Fr_1 = 5$.

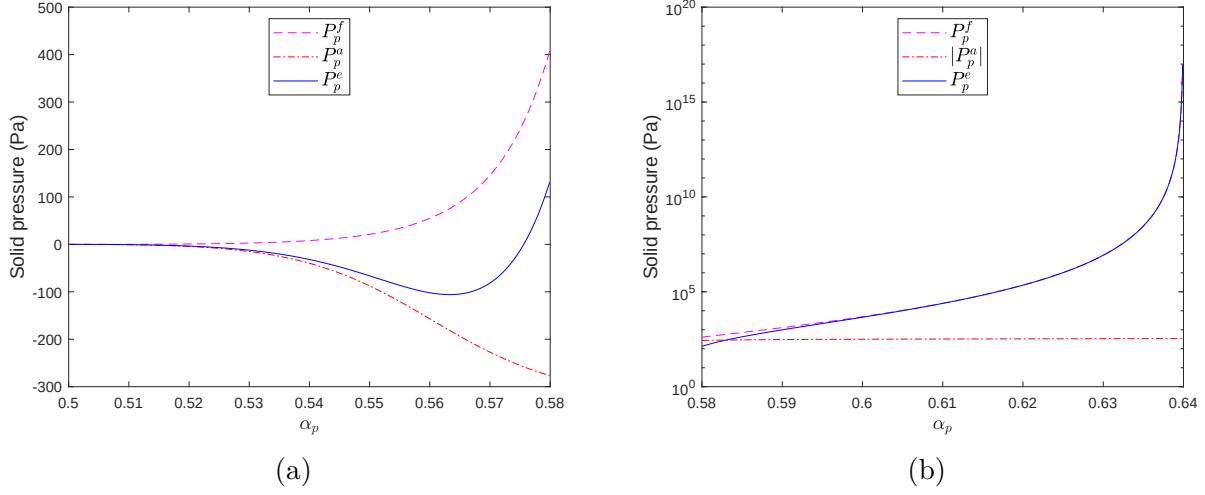


Figure B.8 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. The coordination number is expressed as a function of P_p^f , with $Fr_1 = 50$.

coordination numbers using an α_p value of 0.55 corresponding to a minimum fluidization condition as follows:

$$CN = \begin{cases} 4.77, & \text{for } \alpha_p > 0.55, \\ 4.87 \times 10^{-5} \frac{1 - (1 - \alpha_p)^{2.8}}{(1 - \alpha_p)^{11.6}}, & \text{otherwise.} \end{cases} \quad (\text{B.9})$$

In Equation B.9, the constant fixed-bed coordination number is used for $\alpha_p > 0.55$, while the fluidized-bed correlation is used for $\alpha_p \leq 0.55$. Figure B.9 shows the variation of the solid pressures as a function of the solid volume fraction using Equation B.9.

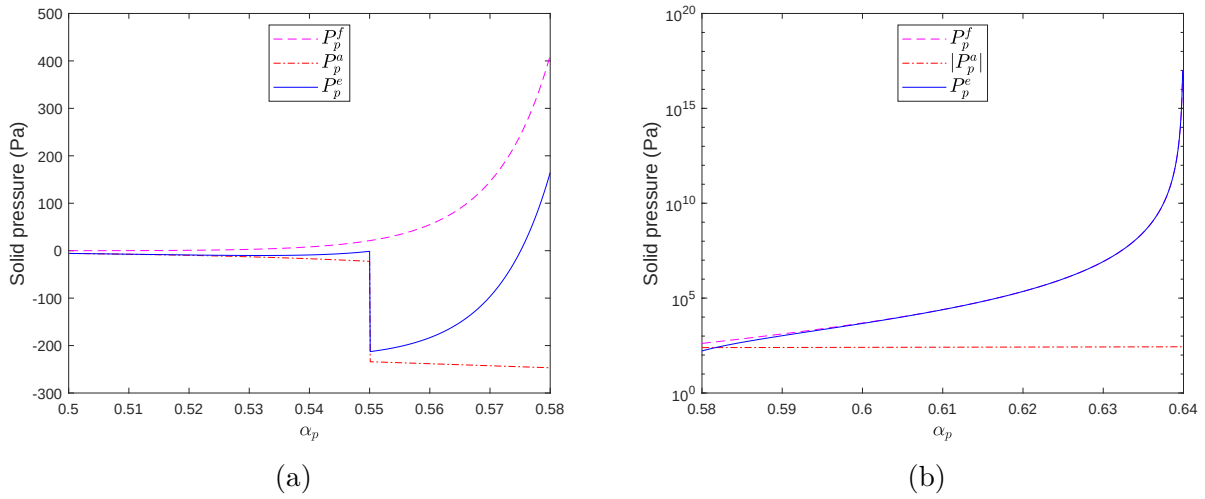


Figure B.9 Frictional, adhesive, and effective solid pressures vs. solid volume fraction (α_p) for (a) $0.5 < \alpha_p \leq 0.58$ and (b) $0.58 \leq \alpha_p < 0.64$, where the adhesive pressure is based on the coordination number. A combination of fixed-bed and fluidized-bed coordination numbers is used.

APPENDIX C FLUIDIZATION AND DEFLUIDIZATION CFD-DEM SIMULATIONS

Here we present results supplementary to those in Chapter 5.

The strain rate tensor of particles is defined as:

$$D_{p,ij} = \frac{1}{2} \left(\frac{\partial U_{p,j}}{\partial x_i} + \frac{\partial U_{p,i}}{\partial x_j} \right). \quad (\text{C.1})$$

The diagonal component $\partial U_{p,z}/\partial z$ of this tensor indicates the strain rate of a line element oriented along the z -axis in the particle phase and is represented by:

$$\frac{\partial U_{p,z}}{\partial z} = \frac{L_z^d - L_z^i}{L_z^i}, \quad (\text{C.2})$$

where L_z^i is the initial length and L_z^d is the deformed length of the line element along the z -axis. The trace of $D_{p,ij}$ signifies the dilatation rate of a particle phase element, given by:

$$\text{tr}(D_{p,ij}) = \frac{V_p^d - V_p^i}{V_p^i}, \quad (\text{C.3})$$

where V_p^i and V_p^d are the initial and deformed volumes of the particle phase element, respectively. A positive $\text{tr}(D_{p,ij})$ indicates that the particle phase is expanding, leading to a decrease in the coordination number, while a negative value suggests contraction and an increasing coordination number. The off-diagonal components of $D_{p,ij}$ reflect the shear deformation of the particle phase.

The average particle velocity in the z -direction within a particular slice is calculated as:

$$U_{p,z} = \frac{1}{n_s} \sum_{i=1}^{n_s} u_{p,z}|_i, \quad (\text{C.4})$$

where n_s represents the number of particles in the slice, and $u_{p,z}|_i$ is the z -direction velocity of particle i . The Favre-averaged particle velocity is determined using the equation:

$$\overline{U_{p,z}} = \frac{\sum_{k=1}^{N_r} (\Delta t_g \alpha_p U_{p,z})_k}{\sum_{k=1}^{N_r} (\Delta t_g \alpha_p)_k} = \frac{\sum_{k=1}^{N_r} (\Delta t_g n_s U_{p,z})_k}{\sum_{k=1}^{N_r} (\Delta t_g n_s)_k} = \frac{\sum_{k=1}^{N_r} \left(\Delta t_g \sum_{i=1}^{n_s} u_{p,z}|_i \right)_k}{\sum_{k=1}^{N_r} (\Delta t_g n_s)_k}, \quad (\text{C.5})$$

where N_r denotes the total number of gas time steps in the averaging period, Δt_g is the gas time step, and α_p is the solid volume fraction in the slice. The time-averaged gradient of the particle velocity for each slice s is computed as follows:

$$\left. \frac{\partial \overline{U_{p,z}}}{\partial z} \right|_s = \frac{\overline{U_{p,z}}|_{s+1} - \overline{U_{p,z}}|_{s-1}}{\Delta z}, \quad (\text{C.6})$$

where $s + 1$ and $s - 1$ refer to the slices above and below the slice s , and $\Delta z = 5d_p$ is the slice thickness.

Figure C.1 presents the time-averaged gradient of the particle velocity in the z -direction as a function of depth during defluidization and fluidization cycles without adhesion. The time-averaged gradient of the particle velocity remains approximately zero in the fluidization branch up to the minimum fluidization velocity, which is 3.324 mm/s. At this velocity, the gradient magnitude increases significantly. Significant increases in the gradient magnitude are also observed at velocities of 3.601 mm/s and 3.878 mm/s. This is because particle phase deformation begins when the minimum fluidization velocity is reached.

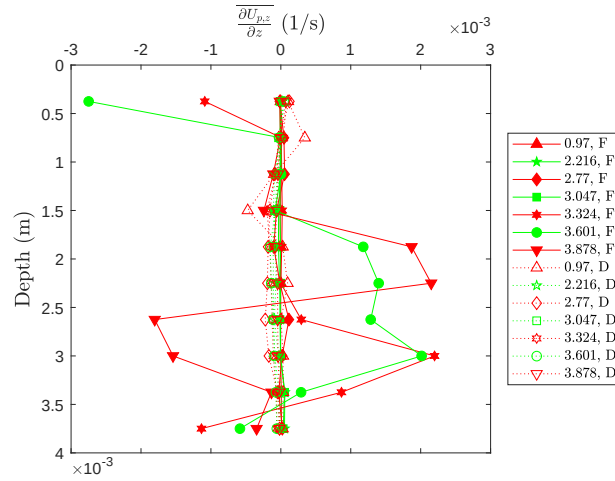


Figure C.1 Variation of the time-averaged gradient of the particle velocity in the z -direction with depth during defluidization (D) and fluidization (F) cycles without Van der Waals adhesion. The numbers in the legend of this figure and Figure C.2 are the superficial gas velocity values in mm/s.

Figure C.2 illustrates the time-averaged gradient of the particle velocity in the z -direction as a function of depth during defluidization and fluidization cycles with adhesion. It is evident that deformation in the particle phase commences at a velocity of 3.601 mm/s, which is higher than the 3.324 mm/s in the non-adhesion case (refer to Figure C.1). This increase is due to the adhesive forces impeding the deformation in the particle phase. Additionally, the

gradient magnitude reaches higher values in the presence of adhesion compared to the case without adhesion.

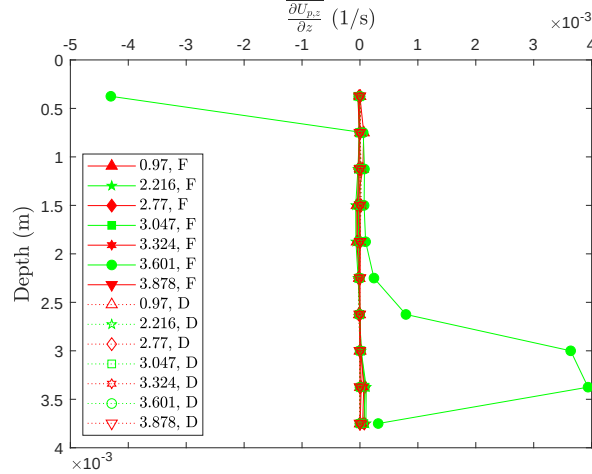


Figure C.2 Variation of the time-averaged gradient of the particle velocity in the z -direction with depth during defluidization (D) and fluidization (F) cycles with Van der Waals adhesion.

The time-averaged bed height was calculated as follows:

$$\overline{H}_b = \frac{\sum_{k=1}^{N_r} H_{b,k} \Delta t_{g,k}}{\sum_{k=1}^{N_r} \Delta t_{g,k}}. \quad (\text{C.7})$$

The variation of this average bed height throughout defluidization and fluidization cycles is illustrated in Figure C.3. This variation mirrors the observed evolution in bed voidage.

We compare our simulation results with those of Ye et al. [12]. It is worth mentioning that Ye et al. [12] employed a linear increase in superficial gas velocity over time, whereas we utilized a step-wise approach. Figure C.4 illustrates the comparison of our results for normalized bed pressure drop as a function of superficial gas velocity during a fluidization cycle without adhesion with those of Ye et al. [12]. In our simulations, the normalized bed pressure drop profile in the fixed bed state closely replicates that of Ye et al. [12]. Both simulations exhibit a normalized pressure drop reaching a value of 1 at nearly identical superficial gas velocities. Additionally, the maximum overshoot in our results is close to that in their results.

Figure C.5 presents the comparison of our results for normalized bed pressure drop as a function of superficial gas velocity for a fluidization cycle in the presence of adhesion with those of Ye et al. [12]. As shown, the overshoot intensity increases with the value of the

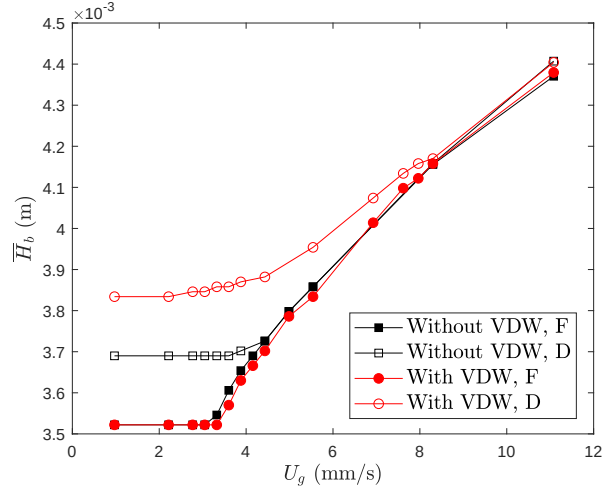


Figure C.3 Evolution of bed height during defluidization (D) and fluidization (F) cycles, without and with Van der Waals (VDW) adhesion.

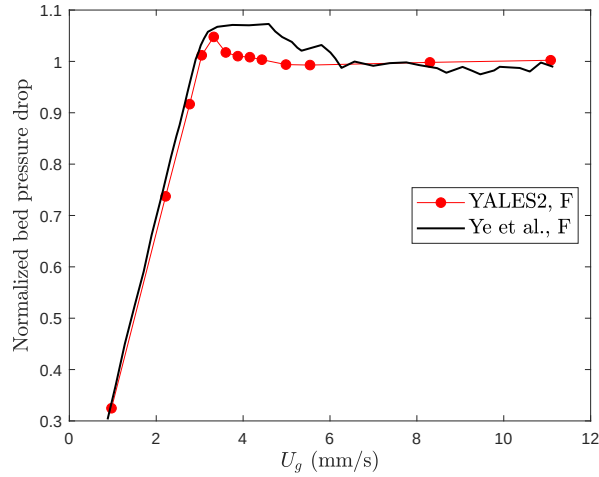


Figure C.4 Comparison between YALES2 simulation results and those obtained by Ye et al. [12] for the normalized bed pressure drop as a function of superficial gas velocity during a fluidization (F) cycle without Van der Waals adhesion.

Hamaker constant A . Our simulation results for $A = 1.96 \times 10^{-22}$ J are close to the results of Ye et al. [12] for $A = 1.0 \times 10^{-22}$ J, with a higher maximum overshoot observed in our case.

In Figure C.6, the distribution of the number of contacts per particle (CN) in the formed fixed bed is illustrated for the case without adhesion. The figure shows a homogeneous distribution of CN , with an average of approximately 5 contacts per particle.

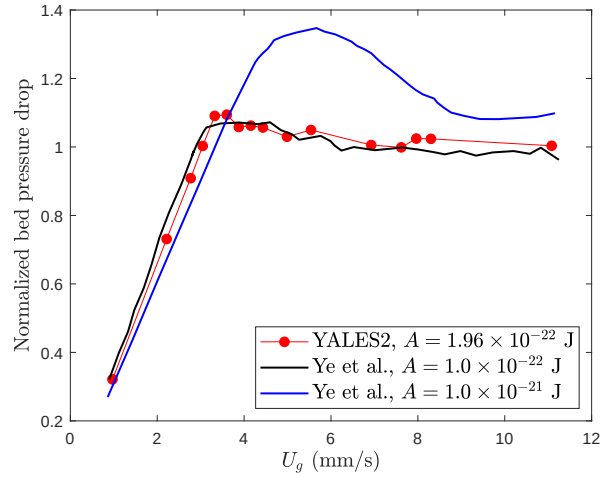


Figure C.5 Comparison between YALES2 simulation results and those obtained by Ye et al. [12] for the normalized bed pressure drop as a function of superficial gas velocity during a fluidization cycle with Van der Waals adhesion.

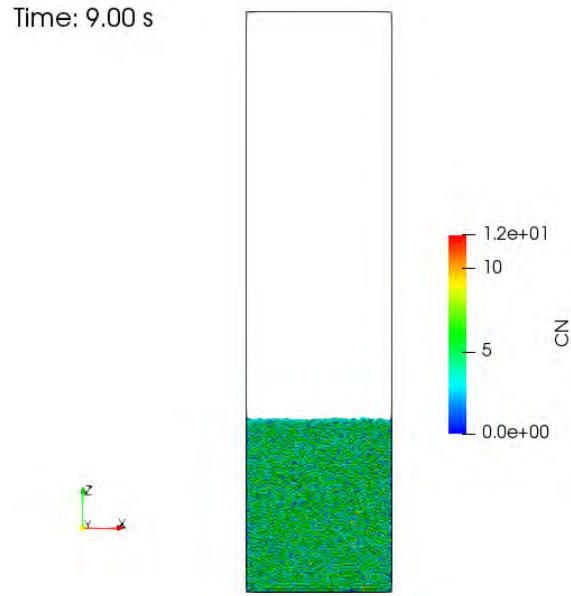


Figure C.6 Distribution of the number of contacts per particle (CN) in a gravitationally settled bed without adhesion.

Figure C.7 displays instantaneous vertical solid stress profiles at zero superficial gas velocity for test cases without and with adhesion, compared to the hydrostatic stress. In the presence of adhesion, the effective stress is the sum of repulsive and adhesive stresses. In both cases, without and with adhesion, the simulated vertical solid stress matches the hydrostatic stress in the upper bed regions but deviates from it in the lower regions. This deviation can be

attributed to particle-wall interactions.

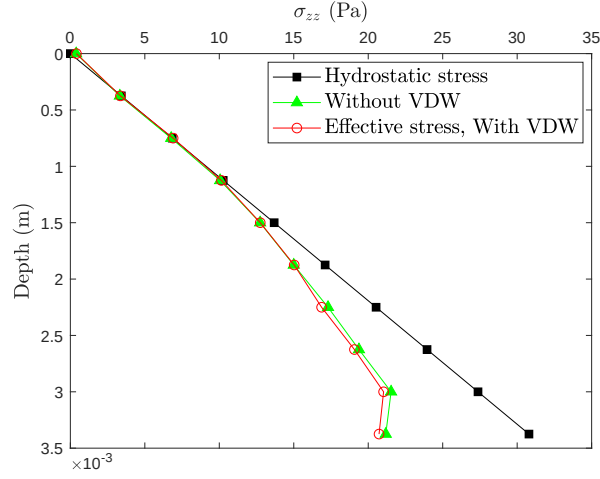


Figure C.7 Instantaneous vertical solid stress as a function of depth at zero superficial gas velocity for test cases without and with Van der Waals (VDW) adhesion, compared to the hydrostatic stress.

Figure C.8 shows the instantaneous mean interparticle contact force $F_{q \rightarrow p, z}^s / n_s$ at zero superficial gas velocity for test cases without and with adhesion, compared to the weight of a single particle. As seen, $F_{q \rightarrow p, z}^s / n_s$ coincides with the particle weight in the upper region of the bed but deviates from it in the lower region because part of the particle weight is supported by the walls.

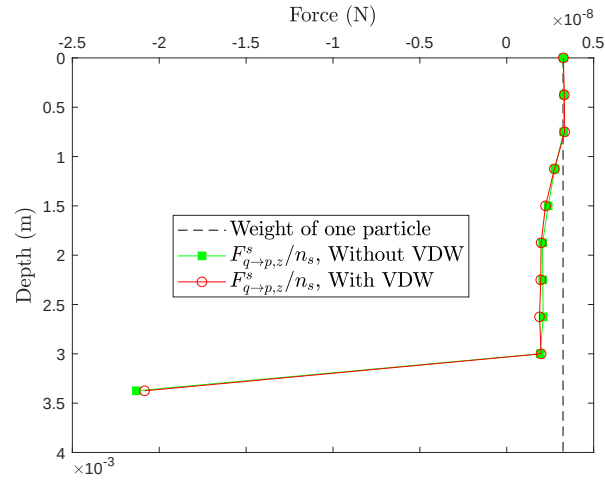


Figure C.8 Instantaneous mean interparticle contact force as a function of depth at zero superficial gas velocity for test cases without and with Van der Waals (VDW) adhesion, compared to the weight of one particle.

APPENDIX D MACRO-SCALE MODELING: EFFECTS OF PARAMETERS AND COMPARISON WITH EXPERIMENTS

Effect of particle diameter on overshoot intensity

The coordination-number-based adhesion model was used with a constant coordination number of 4.77 to study the effect of particle diameter on the intensity of the pressure-drop overshoot. Figure D.1 presents the normalized pressure drop as a function of the normalized gas velocity for particles of different diameters. The results indicate that a decrease in particle diameter significantly increases the pressure overshoot intensity, consistent with the experiments of Affleck et al. [118].

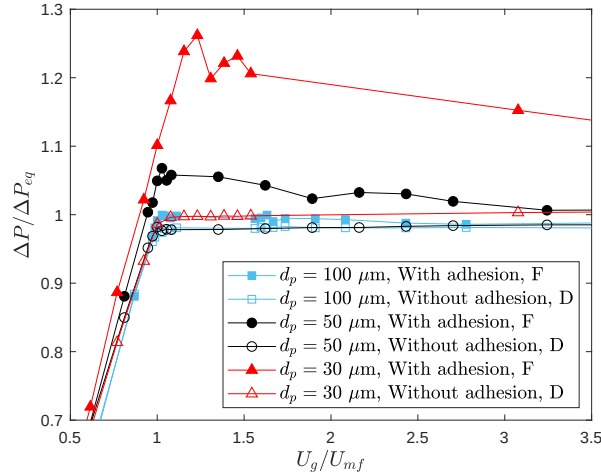


Figure D.1 Normalized pressure drop versus normalized gas velocity for particles of different diameters.

Comparison with experimental data

In this section, our two-fluid simulation results are compared with the experimental data reported by Soleimani et al. [1]. It is important to note that a smaller bed geometry was used in the simulations compared to the experimental setup. The simulation parameters are as follows: for the solid phase, the particle diameter is $d_p = 67 \mu m$, and the particle density is $\rho_p = 2595 \text{ kg/m}^3$; for the gas phase, the density is $\rho_g = 1.2 \text{ kg/m}^3$, and the dynamic viscosity is $\mu_g = 1.8 \times 10^{-5} \text{ Pa} \cdot \text{s}$. The cuboid bed dimensions are a height of $160 d_p$, a width of $40 d_p$,

and a thickness of $16 d_p$. The initial conditions include a bed height of $49 d_p$ and a solid volume fraction of 0.6.

Effect of Hamaker constant on overshoot intensity

Here, fluidization simulations with adhesion are performed to study the effect of the Hamaker constant on overshoot intensity and to compare the simulated overshoot intensity with the experimental results. The minimum cutoff distance used is $S_0 = 4 \times 10^{-10} \text{ m}$, and the coordination number in the adhesion model is defined as follows:

$$CN = \begin{cases} 4.77 & \text{if } U_g \leq U_{mf}, \\ 0 & \text{otherwise.} \end{cases} \quad (\text{D.1})$$

Figure D.2 illustrates the effect of the Hamaker constant on the pressure drop and voidage curves, and a comparison with experiments. As shown in this figure, increasing the Hamaker constant results in a higher overshoot intensity. The overshoot intensity aligns with the experimental results when a Hamaker constant of $7.21 \times 10^{-21} \text{ J}$ is used. However, a discrepancy in the bed voidage profile between the simulation and experiment is observed. This issue is addressed in the next subsection, where parameter fitting is employed to achieve agreement between simulation and experiment for both the pressure drop and the voidage.

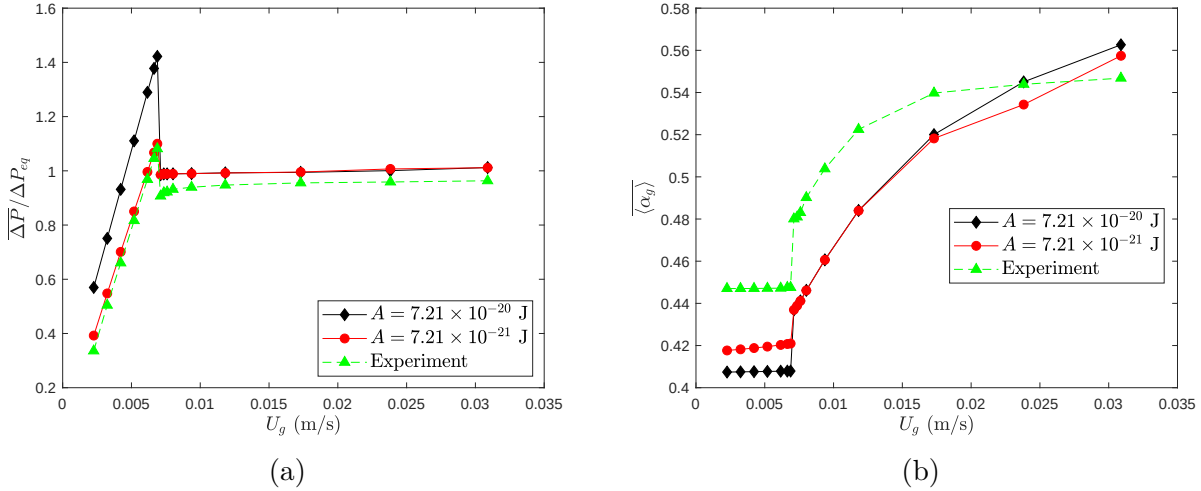


Figure D.2 Effect of the Hamaker constant on (a) pressure drop and (b) voidage profiles and comparison with experimental data.

Effect of threshold particle volume fraction for friction and sphericity coefficient on voidage and pressure drop profiles

Here, we study the influence of the threshold particle volume fraction for the activation of the frictional stress, $\alpha_{p,\min}$, and the sphericity coefficient, ϕ , on the voidage and pressure drop profiles. We use a two-step parameter fitting procedure to achieve agreement between simulations and experiments in terms of the minimum fluidization velocity, U_{mf} , and bed voidage at the lowest gas velocity. In the first step, we determine $\alpha_{p,\min}$ that gives the experimental bed voidage at the lowest gas velocity. According to Figure D.3, this value is $\alpha_{p,\min} = 0.51$. Figure D.3 shows that as $\alpha_{p,\min}$ increases, the voidage at the lowest gas velocity decreases. In the second step, using $\alpha_{p,\min} = 0.51$, we determine the value of ϕ that gives the experimental U_{mf} . According to Figure D.4, this value is $\phi = 0.85$. Figure D.4 shows that increasing ϕ causes U_{mf} to increase. It is worth noting that the method used to obtain the bed voidage in experiments is different from the one used in simulations. In the experiments, two pressure transducers are used, and it is assumed that the pressure drop varies linearly with height, while in simulations, we perform spatial averaging inside the bed to obtain the bed voidage. We acknowledge that further improvement is required to achieve better quantitative agreement with the experiments.

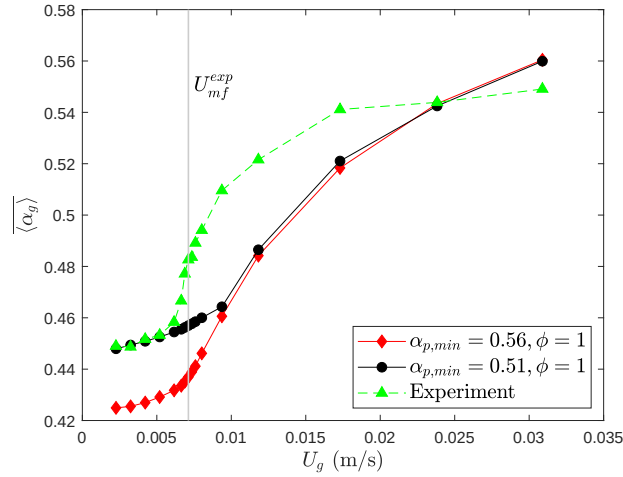


Figure D.3 Effect of threshold particle volume fraction for friction, $\alpha_{p,\min}$, on bed voidage.

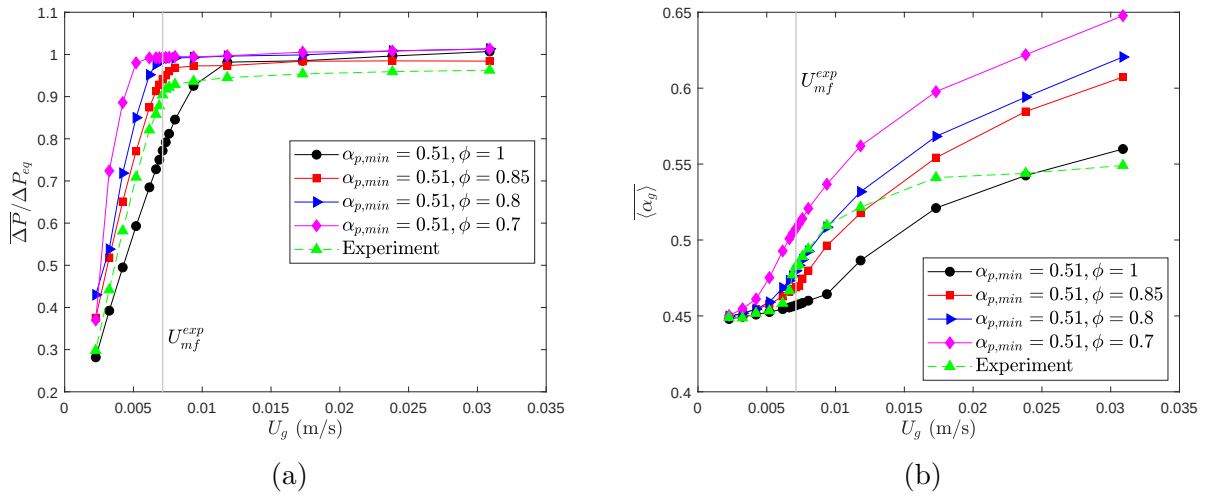


Figure D.4 Effect of sphericity coefficient, ϕ , on (a) pressure drop and (b) voidage profiles.

APPENDIX E CFD-DEM SIMULATIONS WITHOUT WALL EFFECTS

In this appendix, fluidization curves obtained from CFD-DEM tests without wall effects are presented. Figure E.1 shows that without both adhesion and particle-wall friction, no overshoot occurs. It also illustrates that accounting for interparticle adhesion and excluding particle-wall adhesion results in a smaller overshoot area compared to the simulation that considers both interparticle and particle-wall adhesion. Figure E.2 demonstrates that eliminating Van der Waals adhesion between particles and walls does not alter the homogeneous fluidization regime and the overall coordination number trend.

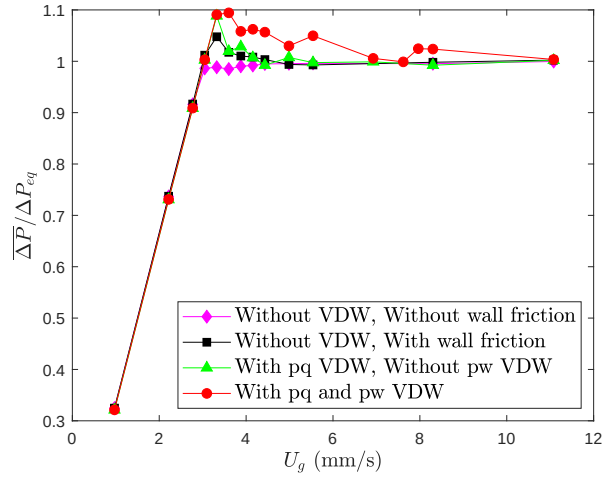


Figure E.1 Pressure drop curves for fluidization cycles with and without wall effects. VDW: Van der Waals adhesion, pq VDW: particle-particle adhesion, pw VDW: particle-wall adhesion.

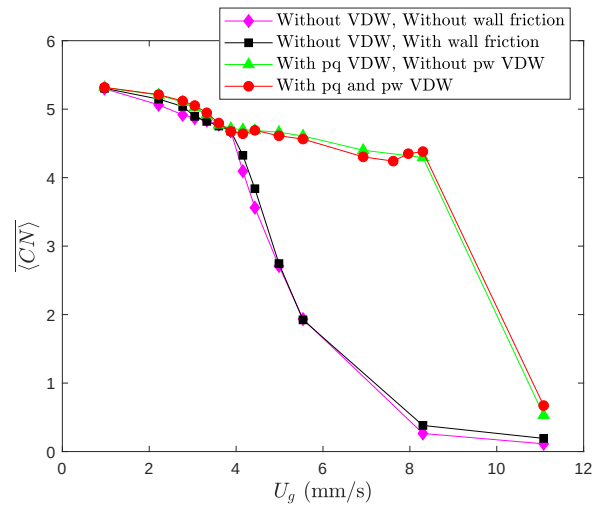


Figure E.2 Coordination number curves for fluidization cycles with and without wall effects. VDW: Van der Waals adhesion, pq VDW: particle-particle adhesion, pw VDW: particle-wall adhesion.