

to characterize quality of fluidization of very cohesive systems, the notion of full-support velocity where the pressure drop is indeed commensurate with the weight of the bed has been introduced in the literature; this full-support velocity increases with degrees of wetness, or equivalently, the strength of cohesion^{48,51}. This is consistent with the increase in gas velocity required to sustain operation of a fluidized bed granulator with increased liquid loading⁵². From an operational perspective, it would be valuable to be able to predict this full-support velocity and the flow behavior in wet fluidized beds at even higher gas velocities.

1.3 Computational Study Of Wet Gas-Solid Systems

There is a long history of trying to exploit simulations of fluidized suspensions to gain insights at different scales that are difficult to extract from experiments^{53–56}. Computational methods to study fluidized suspensions fall into one of three categories: (i) Direct Numerical Simulation (DNS), (ii) Euler-Euler (EE), and (iii) Euler-Lagrange (EL) methods. In DNS, one solves Newton’s equations of motion for the individual particles and the Navier-Stokes equations of motion for the interstitial fluid, resolving the fluid flow around the particles completely⁵⁵; as such, this approach, requiring no constitutive postulates, is viable only for very small systems involving a few thousand particles, thus limiting its use to study of micro-scale flow features. In the EE approach, both gas and solid phases are treated as interpenetrating continua and locally averaged equations (commonly referred to as two-fluid model (TFM) equations) are employed to describe the spatiotemporal structures^{57–59}. This approach is, in principle, suited for the study of large scale flow characteristics, but it requires constitutive models for the fluid-particle interaction force as well as effective stresses in both phases. While considerable advances have been made in formulating the necessary constitutive models for dry systems^{53,54,57}, the field remains primitive for wet systems. In EL methods, the fluid phase is modeled via locally averaged equations, while the particles are treated as discrete objects subject to Newton’s equations of motion^{60–62}. Constitutive

models for the fluid-particle interaction force are needed for this approach, and it is uniformly assumed by all researchers that, at the scale of individual particles, the constitutive model for dry systems apply to wet systems as well. Deen et al.⁵³ provide a review of hard and soft-sphere approaches to model particle-particle interactions, which applies to both EL and DNS methods. The Discrete Element Method (DEM) of Cundall and Strack⁶³ is the most commonly used soft-sphere approach. Although EL simulations with several million particles can be handled today, industrial scale devices with billions of particles cannot be simulated unless one introduces some form of coarse-graining that cuts down the number of representative particles to be simulated (which introduces need for new constitutive models which are not yet well understood). Nevertheless, EL approaches are attractive to study meso-scale dynamics, requiring no more than a few million particles, and results from such studies can aid formulation of coarser EE and EL models⁶⁴. Treating particles as discrete objects is appealing for the study of meso-scale structures in wet systems as the formation and rupture of liquid bridges between particles can easily be incorporated in the models. The present study is concerned with EL simulations of meso-scale flow characteristics in wet systems.

1.4 Relevant Dimensionless Groups

A system and its behavior is often best described through key dimensionless groups, which collect the relevant physical parameters into a set of dimensionless quantities. The present problem involves multiple particle-scale dimensionless groups: the Bond number, Capillary number, Reynolds number, and Froude number. It is worth noting that another dimensionless group involving the liquid loading level is often referenced in this work. However, we reserve its discussion for Section 2.1.3.

Bond number

computational fluid grid length⁶⁸.

$$Fr = \frac{v_t^2}{d_p g} \quad (1.4)$$

1.5 This Work

The overarching goal of the thesis is to provide insight into the fluidization behavior of wet gas-solid flows. It is hoped that the understanding gained may then be used in the modeling and development of industrial applications. Current literature provides details regarding the effects of a liquid presence between small numbers of colliding particles^{27,69,70}, yet literature describing how these microscale effects influence the dynamics of meso-scale structures and macroscale characteristics, such as secondary flows and instabilities in fluidized beds, is lacking. Unlike previous computational work^{8,49,50} that concentrated on comparably large particles in dense flows, our work focusses on gas-particle systems typical for turbulent or circulating fluidized beds. Due to the ability to probe flow details that are difficult to measure experimentally, the study takes a computational approach to investigate the fluidized system, utilizing a Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) to simulate wetted particles suspended by a fluidizing gas phase. When wet particles collide, a liquid bridge is formed between the particles that provides a cohesive force. Wet particles continue to collide, resulting in the formation of agglomerates. While the system is dynamic, in that liquid bridges form and rupture, and agglomerates grow and break apart, a statistical steady state does eventually develop in which the time-averaged flow behavior of the system is unchanging. This statistical steady state yields data which form the basis of the results presented in this thesis.

The work first focuses on understanding how the wetting of particles affects agglomeration tendency within the fluidized bed. Snapshots of the system give a qualitative feel of wetting

effects, while the domain-averaged slip velocity provides a quantitative metric for assessing flow behavior within the bed. The domain-averaged slip velocity, which is the volume-averaged difference in gas and solid velocities in the bed, is used to measure the degree of inhomogeneity present. The agglomeration tendency within wet gas-solid fluidized beds is found to be described by a dimensionless parameter, referred to as a modified Bond number, that takes the form $Bo\Lambda^n$. Where Bo characterizes the cohesive surface tension force between bridges particles and Λ is a measure of the liquid content in the system. The origins of the modified Bond number are shown to stem from the average liquid bridge coordination number within the bed. The liquid bridge coordination number is simply the average number of bridges present on each particle in the system. As this value is not explicitly known, we present a means to express it as a function of the physical properties of the system.

Coarse fluid grids are required to simulate industrial scale units, such as fluidized beds, over practical time scales. Unfortunately, these coarse grids fail to capture microscale structures and thus overpredict the gas-solid drag force. To account for this shortcoming, filtered models are put into place that provide corrected drag coefficients. To this end, we propose a wet filtered drag coefficient as a function of the wetting properties within the bed. This wet filtered drag coefficient may be expressed as the product of a correction factor and the dry filtered drag coefficient. The accuracy of a coarse grid simulation with wet particles is shown to improve with implementation of a wet filtered drag coefficient.

The investigation concludes with probing the liquid distribution within an initially homogeneously wetted bed. The fraction of liquid on the particles or in the bridges, mean liquid content on the particles or in the bridges, and standard deviation of liquid in the bridges are expressed through the wetting properties. The fraction of liquid in the bridges is shown to be a function of the modified Bond number. Initially homogeneously wetted systems display flow behavior very much like those in which only liquid bridges of a set and constant volume were considered. Liquid spreading in inhomogeneously wetted systems is considered, in

subject to Newton's laws of motion. Interphase momentum transfer from the fluidizing gas phase to the solid particles is described by constitutive drag models. Here, we refer to a wet CFD-DEM. Wetness is introduced in the form of a liquid film that is uniformly distributed on the surface of the particles. Upon particle-particle contact, a cohesive liquid bridge forms and liquid is distributed from the particles to the bridge. At a critical separation distance, the bridge ruptures, and liquid is redistributed evenly between the particles. A wet CFD-DEM methodology is selected to study the system, as it is possible to directly model liquid bridge formation and rupture. In this way, agglomerates are permitted to form and break dynamically within the bed, and statistics regarding particle motion and bridge formation may be tracked directly.

2.1.1 Gas Phase

The fluidizing gas phase is modeled as an incompressible continuum and its motion is governed by the conservation of mass and momentum:

$$\frac{\partial}{\partial t} [(1 - \phi)] + \nabla \cdot [(1 - \phi)\mathbf{u}_g] = 0 \quad (2.1)$$

$$\rho_g(1 - \phi) \left(\frac{\partial \mathbf{u}_g}{\partial t} + \mathbf{u}_g \cdot \nabla \mathbf{u}_g \right) = -\nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \boldsymbol{\Phi}_d + \rho_g(1 - \phi)\mathbf{g} \quad (2.2)$$

Here, ρ_g is the density of the gas, ϕ is the solid volume fraction, \mathbf{u}_g is the gas velocity, p_g is the gas phase pressure, and $\boldsymbol{\tau}_g$ is the gas phase deviatoric stress tensor. The total gas-particle interaction force per unit volume of the mixture, exerted on the particles by the gas, $-\boldsymbol{\Phi}_d$, is composed of a generalized buoyancy force due to the slowly-varying (in space) local-average gas phase stress $(-p_g\mathbf{I} + \boldsymbol{\tau}_g)$ and the force due to the rapidly varying flow (in space) field around the particles. On a per particle basis, the total interaction force on the particle by the gas can be written as $\mathbf{f}_{g \rightarrow p, i} = -V_{p, i} \nabla p_{g, i} + V_{p, i} \nabla \cdot \boldsymbol{\tau}_{g, i} + \mathbf{f}_{d, i}$, where $V_{p, i}$ is the particle volume and $\mathbf{f}_{d, i}$ is the gas-particle force due to fluid flow around the particle. Subscript i indicates

interaction force on the particles due to fluidizing gas (as discussed above), I is moment of inertia, $\boldsymbol{\omega}$ is angular velocity, and \mathbf{q} is total torque.

Particle-particle interactions are modeled by a linear spring-dashpot model and frictional slider⁶³:

$$\mathbf{f}_{cont,ij}^n = -k_n \delta_{ij} \mathbf{n}_{ij} - \gamma_{d,n} \mathbf{v}_{ij}^n \quad (2.8)$$

$$\mathbf{f}_{cont,ij}^t = \begin{cases} -k_t \mathbf{t}_{ij} - \gamma_{d,t} \mathbf{v}_{ij}^t & \text{for } |\mathbf{f}_{cont,ij}^t| < \mu_{pp} |\mathbf{f}_{cont,ij}^n| \\ -\mu_{pp} |\mathbf{f}_{cont,ij}^n| \frac{\mathbf{t}_{ij}}{|\mathbf{t}_{ij}|} & \text{for } |\mathbf{f}_{cont,ij}^t| \geq \mu_{pp} |\mathbf{f}_{cont,ij}^n| \end{cases} \quad (2.9)$$

Here, k_n is the normal spring constant, δ_{ij} is the normal overlap between particles i and j , \mathbf{n}_{ij} is the unit normal vector pointing from particle i to collision partner j , $\gamma_{d,n}$ is the normal damping coefficient, \mathbf{v}_{ij}^n is the relative normal velocity of particles i and j , k_t is the tangential spring constant, \mathbf{t}_{ij} is the tangential overlap obtained from the integration of the relative tangential velocity between contacting particles, $\gamma_{d,t}$ is the tangential damping coefficient, \mathbf{v}_{ij}^t is the relative tangential velocity of particles i and j , and μ_{pp} is the friction coefficient. We note that parameters of the spring-dashpot model (shown in Table 2.1) are chosen such that the restitution coefficient of the dry particles (e_{pp}) is 0.9. Simulations here (and in most CFD-DEM studies) treat particles as having smaller spring constants (i.e. softer) than their physical values, as softer particles allow for longer time steps to be used, while still properly capturing collision dynamics. It is important to ensure that the flow structures and quantities extracted from the simulations are not dependent on the degree of softness. With this in mind, simulations were done with different spring constants and time steps to ensure that results were not sensitive to changes in these parameters. In order to fully capture the transfer and dissipation of momentum in each collision, the time step (shown in Table 2.1) was chosen to be between 1/50 and 1/100 of the binary dry collision time for all data

Here, \mathbf{n}_{ib} is the unit normal vector pointing from particle i to bridge b , \hat{h} is the surface to surface separation distance scaled by r where r denotes the particle radius, \hat{V} is the liquid bridge volume made dimensionless by scaling with r^3 ($\hat{V} = V_{lb}/r^3$), and θ is the contact angle which is assumed to be zero. As particles do not overlap in nature (this is only a consequence of soft-sphere modeling which models contacts more accurately than the hard sphere model), the cohesive force is finite at particle-particle overlap and is taken to be a constant equal to the cohesive force at zero surface-surface separation distance. When a liquid bridge reaches a critical distance, the bridge ruptures and liquid is redistributed. This critical liquid bridge rupture distance is given by Lian et al.³⁰:

$$\hat{h}_c = (1 + 0.5 \theta) \hat{V}^{1/3} \quad (2.14)$$

The liquid bridge force is present as long as a bridge exists. Particles are allowed to form multiple pairwise interactions via liquid bridges and in this way agglomerates form. As there is no size distribution of particles in our system, upon bridge rupture the liquid in the bridge is split evenly between the two particles.

Two methods are used in this study for determining the liquid bridge volume upon particle-particle contact:

- (a) *Constant liquid bridge volume.* We assume that liquid within the bed is distributed evenly throughout the particles. Upon particle-particle contact, a liquid bridge of set volume is immediately formed. The volume of the bridge, V_b , is predetermined and is given as an input to the simulation. For systems modeled in this fashion, the liquid loading, or degree of wetness in the system, is characterized by the parameter Λ , which is the ratio of liquid bridge volume to particle volume.

$$V_{lb} = \Lambda \frac{\pi}{6} d_p^3 \quad (2.15)$$

(b) *Liquid transfer.* In the physical system, when a liquid-coated particle surrenders some liquid to the bridge, it has less free liquid available to form new bridges with other particles with which it may collide. Upon particle-particle contact, a liquid bridge of set volume is immediately formed. The volume of the bridge is a function of the liquid on the contacting particles. We use the model from Shi and McCarthy³² to determine the liquid bridge volume, updating the available liquid on the particles as liquid is moved from the particle surface to the bridge.

$$V_{lb} = \frac{1}{2} (V_{lp,i} + V_{lp,j}) \left(1 - \frac{\sqrt{3}}{2} \right) \quad (2.16)$$

Here, $V_{lp,i}$ and $V_{lp,j}$ represents the liquid volume on the surface of particles i and j respectively. The liquid loading in these systems is described through the parameter Ψ , which represents the ratio of liquid to solid volume in the system.

2.2 System Studied

Euler-Lagrange simulations of uniformly sized particles fluidized by a gas have been performed in 3-D periodic domains. The domain takes the form of a vertically oriented rectangular prism, with a square base and aspect ratio of 4. Particles are spherical and identical in size. Contact interaction between particles (treated as soft spheres) are represented through a linear spring-dashpot model, supplemented with a frictional slider. Rolling friction is not taken into account in the present series of simulations. The discretized form of the locally averaged equations of motion describing the fluid phase are solved using cubic grids. This approach is often referred to in the literature as the Computational Fluid Dynamics and Discrete Element Method⁷².

The boundary conditions are such that the domain is periodic in all three directions. That is: 1) the distance between any two points in a given direction (of domain length Δ_y) is $\Delta_y - |y_2 - y_1|$ for cases in which $|y_2 - y_1| > \Delta_y/2$, and 2) particles leaving through one side of the domain enter in the opposing side with identical velocities.

To achieve fluidization, a mean pressure gradient that exactly balances the weight of the suspension per unit cross sectional area is imposed in the periodic domain. p_g in equation (2.2) contains two components: a periodic pressure gradient, and a linearly varying pressure component along the flow direction which balances the total weight of the suspension. The transient simulations are initialized with a nearly homogeneous distribution of particles in the domain. The fluid cells are given initial velocities such that the gas-solid slip velocity is that of the homogeneous steady state system and the momentum of the overall system is zero. There is a transient period after initialization in which inhomogeneities arise as particles fluidize, collide, and form or break liquid bridges. Eventually, the system reaches a statistical steady state in which fluidization behavior fluctuates around a statistical average. Results show that the state in which the system is initiated does not affect the statistical steady state that the system eventually reaches, though the transient time required to reach that state may change.

Although all results will be presented in terms of dimensionless quantities, we provide in Table 2.1 values of various dimensional, physical, and computational parameters for a typical physical system.

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