SPH-DEM simulations of grain dispersion by liquid injection

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Abstract.
We study the dispersion of an initially packed, static granular bed by the injection of a liquid jet. This is a relevant system for many industrial applications, including paint dispersion or food powder dissolution. Both decompaction and dispersion of the powder are not fully understood, leading to inefficiencies in these processes. Here we consider a model problem where the liquid jet is injected below a granular bed contained in a cylindrical cell. Two different initial conditions are considered: a two-phase case where the bed is initially fully immersed in the liquid and a three-phase case where the bed and cell are completely dry preceding the injection of the liquid.

The focus of this contribution is the simulation of these model problems using a two-way coupled SPH-DEM granular-liquid method [M. Robinson, M. Ramaioli, and S. Luding, submitted (2013) and http://arxiv.org/abs/1301.0752 (2013)]. This is a purely particle-based method without any prescribed mesh, well suited for this and other problems involving a free (liquid-gas) surface and a partly immersed particle phase. Our simulations show the effect of process parameters such as injection flow rate and injection diameter on the dispersion pattern, namely whether the granular bed is impregnated bottom-up or a jet is formed and compare well with experiments.

Keywords: SPH, DEM, Fluid-particle flow, Discrete Particle Model, Dispersion, PARDEM
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INTRODUCTION

Granular-Fluid systems are ubiquitous in nature and industry. Sediment transport, erosion, avalanches and debris flows are important environmental phenomena and the interaction between grains and interstitial fluid can compromise the stability of slopes, building foundations and dams. Industrially, the dispersion of solid particles in a liquid is of broad relevance for chemical and painting processing. Both decompaction and dispersion of the powder are not fully understood, leading to inefficiencies in these processes. A relevant application for the food industry is the dispersion and dissolution of a dehydrated food powder by adding water, which includes the additional complexity of powder dissolution.

Recent studies have investigated two-phase systems where a fluid is injected in a granular medium initially saturated by the same fluid, either in two [3] or in three dimensions [4], or the three-phase system in which air is injected below an immersed granular medium [5, 6].

EXPERIMENTS

This study considers the dispersion of poppy seeds contained in a cylindrical cell, by the liquid injected from a central bottom orifice. The liquid exits the system from the top surface, which is permeable to the liquid, but not to the grains. The total mass of grains was 4.0 g for all experiments (and simulations), which resulted in a bed height of about 14mm. The wetting properties of the grains play an important role in the dispersion process. However, we wish to focus in this work only on the case in which the liquid-solid interfacial energy is significantly lower than the air-solid interfacial energy (i.e. liquid-solid contact angle is lower than ninety degrees and the system is often termed as hydrophilic). To cope with the hydrophobic nature of poppy seeds, we therefore ran experiments using water-ethanol mixtures with physical properties similar to pure water.

The top left side of Figure 1 shows a snapshot of the early stage dispersion of the grains by a liquid flow rate of 400 ml/min from a 1mm orifice, resulting in the formation of a liquid jet which wets the granular bed from top to bottom. The bottom left side of Figure 1 shows that a liquid flow rate of 100 ml/min results instead in a bottom-up impregnation of the granular bed. The left side of Figure 2 shows two later snapshots of the same experiments taken when about 6.7ml liquid had been injected. The dry seed patches in the top left image suggest that the lower flow rate injection is more successful in wetting the grains than the higher flow rate. A wider injection orifice diameter (right side of Figure 2) results in a bottom-up impregnation also at a liquid flow rate of 400 ml/min. Two-phase dispersion experiments in which the grains are initially completed immersed were also performed and resulted always in the formation of a jet. These experiments are not reported to allow more room for discussing the simulation results which are the central focus of this contribution.

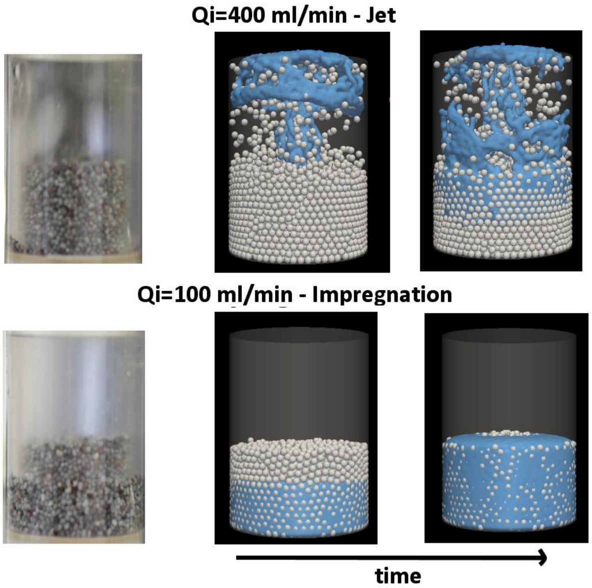

FIGURE 1. Dispersion of a dry granular bed of poppy seeds by a 1mm central injection hole. Left: Experimental dispersion patterns shortly after liquid injection starts. Center and Right: Pseudo-Three-Phase SPH-DEM simulations, two snapshots are shown in order of increasing time. Grains are represented using white spheres and the water free-surface is colored in blue. Top row: A 400 ml/min inlet flow rate generates a jet. Bottom row: A 100 ml/min flow rate induces a bottom-up impregnation.

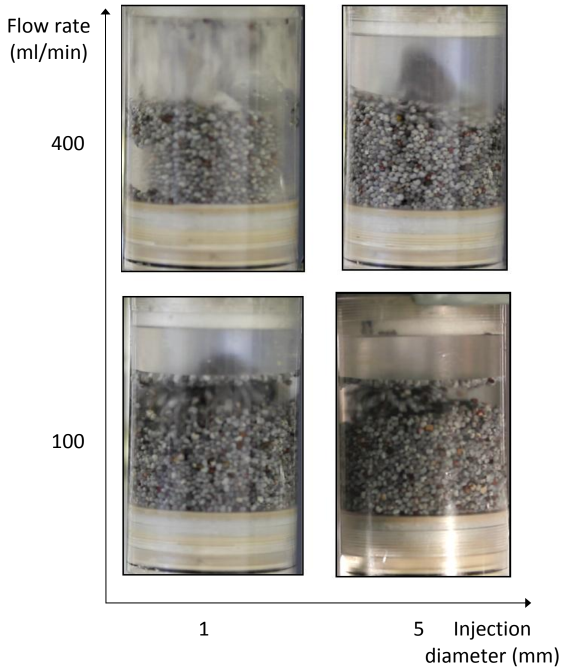

FIGURE 2. Effect of the injection diameter and flow rate on the experimental dispersion patterns of 4g dry poppy seeds. All images are taken after the injection of 6.7ml liquid. With high flow rate and small injection diameter a jet is formed and the granular bed is wetted from top to bottom, while in all other cases bottom-up impregnation occurs.

SPH-DEM MODEL

The dispersion cell simulations use SPH-DEM [1, 2], a granular-fluid simulation method previously developed by the authors. SPH-DEM couples Smoothed Particle Hydrodynamics (SPH) for the fluid phase and the Discrete Element Method (DEM) for the grains. In contrast to the more established CFD-DEM method, this is purely particle-based and enjoys the flexibility that comes from the lack of a prescribed mesh. It is suitable for problems such as free surface flow or flow around complex and/or moving geometries.

Rather than fully resolving the interstitial fluid, which is often unfeasible, the SPH model is based on the locally averaged Navier Stokes equations [7], which can be derived from the normal NS equations by the application of a smoothing operator. This separates the fluid variables into their large scale (i.e. resolved) and small scale (unresolved) components. The resolved components are discritised and integrated over time using a variable-resolution SPH implementation, which is coupled to the DEM particles/grains via a smooth porosity field (generated by applying the same smoothing operator to the DEM grain volumes) and the application of a drag force which is a function of the local porosity and superficial velocity difference between the two phases. This drag force models the influence of the unresolved fluid variables on the coupling.

The DEM model uses a linear spring dashpot contact model. Friction and lubrication forces between the grains are neglected in order to study the simplified model, but the influence of these forces on the simulation results is the subject of future research. For the coupling drag force we use the popular drag law proposed by Di Felice [8].

This two-way coupled SPH-DEM approach has been validated against several sedimentation problems [9].

SIMULATION SET-UP

The dispersion cell is simulated using a cylindrical no-slip boundary (same dimensions as the experiment), with cylindrical inlet/outlet, respectively at the bottom/top of the cell. The presence of the top filter is captured by including a top horizontal wall permeable to the fluid, but not to the grains.

The DEM granular particles were initiated at random positions within the cell and allowed to settle into a packed arrangement before the liquid injection was started, at $t = 0$. The poppy seed properties used in the experiments were measured and used in the simulations:

density is set to $\rho_p = 1160$ kg/m^3 and the diameter of all grains is equal to the poppy seed average diameter of $d = 1.1 \times 10^{-3}$ m. The total mass of grains was consistent with experiments.

Two different initial conditions were simulated. Pseudo-Three-Phase simulations were performed in which no water is present in the cell before liquid injection, which mimic experiments using dry grains in presence of interstitial air. The air was assumed to have no influence on the results and was modelled implicitly by the absence of fluid. The second initial condition was a two-phase simulation where the cell was completely filled with liquid/SPH particles and DEM grains, before liquid injection at $t = 0$.

In both cases SPH fluid particles were injected into the lower inlet at a constant velocity to simulate the jet, from $t = 0$ onwards. The fluid properties match that of water, with reference density $\rho_0 = 1000$ kg/m^3 and viscosity $\mu = 8.9 \times 10^{-4}$ Pa.

SIMULATION RESULTS

Pseudo-Three-Phase Dispersion Cell

Effects of Inlet Flow Rate

A range $50 \leq Q_i \leq 600$ ml/min of inlet flow rates were simulated with 1 mm injection diameter. For high inlet velocities $Q_i > 100$ the water jet fluidized a central column of grains and broke through the top of the bed. From here the cell filled with fluid from the top of the bed to the bottom, and then upwards from the top of the bed to the outlet. This behavior closely matched that of the experimental results, including the cut-off point at $Q_i = 100$ ml/min.

Below this cut-off point $Q_i \leq 100$ the jet failed to fluidize the bed and the dispersion cell filled with fluid from the bottom up to the outlet height. The movement of DEM grains was minimal until the bed had been completely immersed. Again this qualitative behaviours matched the experimental results.

The central and right images of Figure 1 show four snapshots from the Pseudo-Three-Phase simulation results. Grains are represented using white spheres and the water free-surface is colored in blue.

For $Q_i = 100$ ml/min the grains do not move significantly and the fluid free-surface height linearly grows over time from the bottom to the top of the cell. The fluid free surface is approximately constant over the horizontal width of the cell. For $Q_i = 400$ ml/min the jet quickly breaks through the centre of the grain bed, dispersing a large number of grains throughout the cell. Here the jet impacts on the top of the cell, but for smaller Q_i the jet did not reach the top. Once the jet breaks through, the cell fills with fluid from top to bottom until the DEM grains are fully immersed. For a more detailed analysis the reader should refer to [10].

Effects of Inlet Diameter

The diameter d of the inlet water jet was simulated at $d = 1, 2$ & 5 mm.

A cross section of the porosity field at $t = 1$ s is shown for the latter two diameters in Figure 3. In both these simulations the inlet flow rate is $Q_i = 400$ ml/min, and the inlet velocity is small enough (due to the larger inlet diameter) to avoid the formation of a strong central jet, such as the one obtained with 1 mm orifice.

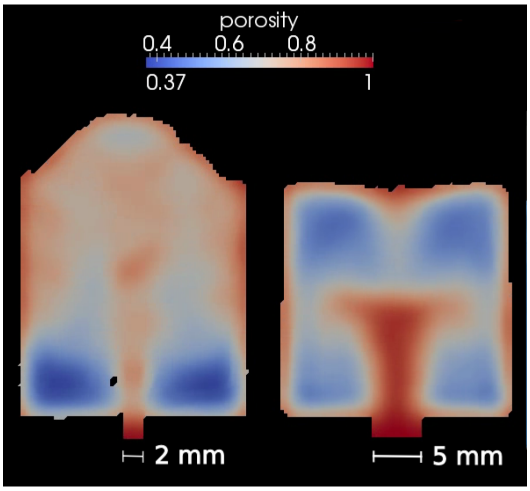

FIGURE 3. A cross section of the porosity field for simulations with inlet diameter $d = 2$ mm (left) and $d = 5$ mm (right), taken at $t = 1$ s. Red colours show areas of high porosity (i.e. the absence of grains), and the shape inlet jet can be seen in both cases as a vertically aligned red region extending up from the inlet. Blue colours indicate areas of high grain density. The black area above the porosity field defines the shape of the liquid free surface.

The jet with the smaller cross-section takes the form of a spout that breaks through the granular bed, leaving a relatively large annulus of static grains surrounding the inlet. This annulus is not completely saturated by the liquid which explains the higher liquid free surface height, with respect to the lower and flat liquid surface obtained in case of a 5 mm injection diameter. The reduced liquid inlet velocity generated by a 5 mm inlet does not produce a jet breaking through the bed. Instead, it lifts part of the grains, resulting in a large region of lower porosity half way through the granular bed. The top of the jet is characterized by an increasingly radial flow (rather than vertical) due to the vertical flow of water flow being halted due to the mass of grains above it.

Two-Phase Dispersion Cell

In the Two-Phase case, the grains are initially fully immersed in the liquid. The minimum fluidization velocity (proportional to the density difference between the phases for a 1D packed bed) is therefore significantly reduced, and in all the simulations performed ($50 \leq Q_i \leq 600$ ml/min) the liquid immediately fluidizes a central column of grains above the inlet forming a jet.

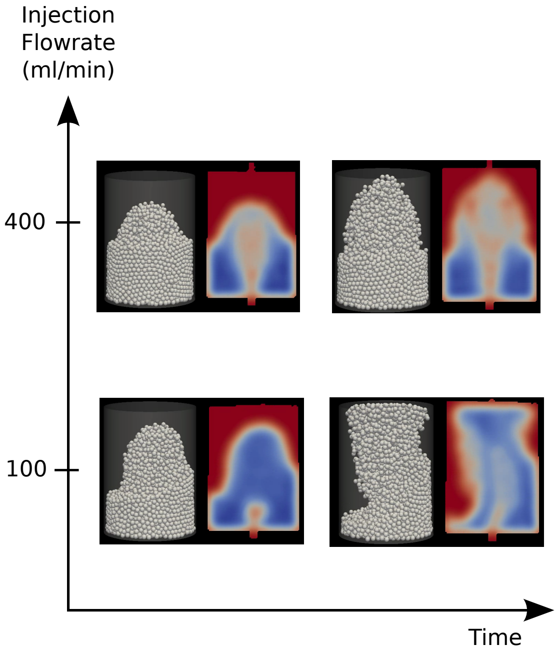

FIGURE 4. Two-phase SPH-DEM simulations with inlet flow rates $Q_i = 400$ (top row) and 100 ml/min (bottom row). For both cases two snapshots are shown in order of increasing time. Each subfigure shows the 3D distribution of grains on the left and a cross-section of the porosity field on the right. Red/blue colours show areas of high/low porosity.

The primary effect of the inlet velocity on the grain dispersion is on the cylindrical symmetry of the jet within the cell. For higher inlet velocities ($Q_i \geq 400$) the core of the jet is vertically aligned with the axis of the cell and is generally constant over time. See Figure 4 (top row) for an example of this type of behaviour. For lower inlet velocities ($Q_i \leq 100$), while the jet is initially vertically aligned, it quickly starts to randomly oscillate over time across the full horizontal width of the cell, occasionally becoming disrupted by the circulation of fluid and grains before reforming again. Figure 4 (bottom row) shows an example.

CONCLUSION

We have shown initial results from the study of the dispersion of a packed bed by the injection of a liquid jet. SPH-DEM simulations of the dispersion cell were performed over a range of jet flow rates and injection diameters, and compare qualitatively well with the experimental results. When the cell is initially filled with air, the same dispersion regimes of jetting vs. bottom-up impregnation are seen in both simulations and experiments at same flow rates, while the formation of a jet is always observed when grains are initially fully saturated.

While there is a qualitative match between simulations and experiments, more work is needed to establish a quantitative match, which is underway using high time-resolution, three-dimensional MRI measurements. Further model development is also planned to introduce a realistic description of liquid surface tension, which will enlarge the range of applicability of SPH-DEM simulations of grain dispersion.

These limitations notwithstanding, SPH-DEM is a powerful approach to access system variables which are difficult to access experimentally, such as the internal microstructure of the granular bed and the local degree of pore saturation by the injected liquid. Simulations thus represent a powerful complement to experiments in order to interpret the physical mechanisms at stake during grain dispersion by liquid injection.

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