Liquid Entry of Dry Powders: Particle-resolving Direct Numerical Simulations

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1. Introduction and Background

When a dry powder enters a body of liquid through its free surface, the resulting three-phase flow field frequently displays a rich dynamical behavior. Depending on the governing parameters such as particle shape and porosity, impact velocity and angle, surface tension, wettability, viscosity, density ratio and others, gas cavities can form and penetrate deeply into the liquid, where they may remain trapped in the powder, or escape from the powder and break up into small bubbles. These dynamics can be further complicated by such mechanisms as dissolution and/or particle swelling. The basic process of solid objects entering a liquid has been studied in some detail for the idealized configuration of an individual spherical, disk-like or projectile-shape object, as reported by, for example, Aristoff *et al.* (2010); Gonzalez-Gutierrez *et al.* (2014); Watson *et al.* (2021). The state of the art of this field of research is succinctly summarized in the comprehensive reviews by Truscott *et al.* (2014) and Magnaudet & Mercier (2020). Several researchers have extended these fundamental investigations to pairs of spherical particles that enter the liquid in parallel (Akbarzadeh *et al.* 2023; Wang *et al.* 2024), and recent years have seen a couple of initial studies of granular jets entering a body of water (Cervantes-Alvarez *et al.* 2020; Saingier *et al.* 2021). However, the situation of particles with more complex shapes, porosities or permeabilities, and pronounced wettability heterogeneity has not been investigated systematically in any detail, in spite of its relevance to a range of environmental scenarios and industrial applications, for example in the area of powder reconstitution, which is the primary focus of this proposal.

To achieve progress towards developing accurate models for powders composed of thousands of complex-shaped aggregates, the initial phase of the proposed investigation will concentrate on an individual particle with complex shape as well as heterogeneous porosity and wettability. When such a particle enters a body of fluid, its dynamics will be crucially affected by the interstitial gas trapped in its pore spaces. Depending on its entry velocity and angle, surface tension, solid volume fraction, solid-to-fluid density ratio, fluid viscosity, and other features, the interstitial gas may be carried deep into the liquid, where it can significantly modify the formation and breakup of particle aggregates. Our goal is to develop a first-principle understanding of the ensuing evolution of this complex multiphase flow process, and to derive quantitative relations for its evolution. At the present time, we do not have accurate predictive tools at our disposal that would allow us to optimize an industrial process in order to achieve certain outcomes, such as the complete breakup of any particle clusters, the homogeneous distribution of the particles within the liquid, or the expulsion of all gas from the liquid.

In order address this shortcoming, and to facilitate the development of quantitative, predictive tools that accurately describe the processes ensuing when a powder enters a liquid, we propose to conduct a series of first-of-a-kind, direct numerical simulations. These simulations will fully resolve the flow around complex particles as they enter liquids with a wide range of viscosities, including the dynamics of the interstitial gas as it either remains trapped or escapes from the pore spaces. As a starting point, we will investigate individual aggregates of complex, fractal geometry with prescribed porosity and permeability distributions and wettabilities across the entire range from hydrophobic to hydrophilic, including cases where the wettability varies with surface location. This computational research will be carried out in close collaboration with a corresponding experimental program in the group of Prof. Alban Sauret, who is already being funded by IFPRI, and who has a successful track record of studying the water entry of granular jets experimentally (Cervantes-Alvarez *et al.* 2020; Saingier *et al.* 2021), as shown in figure 1c. Prof. Sauret's group has the ability to create particles of complex shape and heterogeneous properties (porosity, wettability, roughness etc.), which has already been serving as basis for an ongoing collaboration between our groups (Maches *et al.* 2024).

By combining the above computational and experimental efforts, we expect to create the fundamental physical understanding that can serve as basis for modeling and quantifying the entry process of complex particles into liquids. During a potential follow-up project, we would then extend this analysis to entire clusters of particles, in order to arrive at a continuum-level description for the entry of powders into liquids, in a wide range of applications of importance to IFPRI members.

The **central, underlying hypothesis of the proposed project** assumes that direct numerical simulations that resolve the flow around each particle as well as the sharp gas-liquid interface will enable us to identify and validate scaling relationships that capture the entry of a granular material into liquids of different viscosities at the microscale. These scaling relationships can subsequently serve as the basis for developing predictive quantitative tools that accurately describe the macroscale evolution of this three-phase flow process.

2. Simulation Approach

2.1. *Fluid equations*

The numerical methodology for simulating the dynamics of a rigid aggregate embedded in a fluid is discussed in our earlier publications (Biegert *et al.* 2017; Biegert 2018; Deepwell *et al.* 2021; Maches *et al.* 2024). It considers an aggregate comprised of many individual spherical particles connected by rigid bonds, in a fluid based on the incompressible Navier-Stokes equations

$$\nabla \cdot \boldsymbol{u} = 0, \tag{2.1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\, \boldsymbol{u} = -\frac{1}{\rho_\mathrm{t}} \nabla p + \frac{\rho - \rho_\mathrm{t}}{\rho_\mathrm{t}} \boldsymbol{g} + \nu \nabla^2 \boldsymbol{u} + \frac{1}{\rho_\mathrm{t}} \boldsymbol{f}_\mathrm{IBM} \,. \tag{2.2}$$

Here, t denotes time, $\boldsymbol{u}$ the fluid velocity, p the pressure, ρ the possibly variable fluid density, $\boldsymbol{g}$ the gravity vector, $\nu = \mu/\rho$ the kinematic viscosity of the fluid, and $\boldsymbol{f}_\mathrm{IBM}$ the distributed force caused by the aggregate's action on the fluid, which is evaluated using an immersed boundary method (IBM) scheme.

The individual solid, finite-size particles are governed by the momentum equations

$$m\frac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \oint_{\Gamma_i} \boldsymbol{\tau}\cdot\boldsymbol{n}\mathrm{d}A + V\left(\rho_{\mathrm{p}}-\rho_{\mathrm{t}}\right)\boldsymbol{g} + \boldsymbol{F}_{\mathrm{b},i}\ , \tag{2.3}$$

$$I\frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \oint_{\Gamma_i} \boldsymbol{r}\times\left(\boldsymbol{\tau}\cdot\boldsymbol{n}\right)\mathrm{d}A + \boldsymbol{M}_{\mathrm{b},i}\ . \tag{2.4}$$

For these equations, $\boldsymbol{u}_i$ refers to the translational velocity of the i-th particle, $\boldsymbol{\omega}_i$ to the angular velocity, m to the mass, $I = \frac{1}{10}mD_{\mathrm{p}}^2$ to the moment of inertia, V to the volume, Γ_i to the surface, $\boldsymbol{\tau} = -p\boldsymbol{I} + \mu\left[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right]$ to the hydrodynamic stress tensor, $\boldsymbol{I}$ to the identity tensor, μ to the dynamic viscosity, $\boldsymbol{n}$ to the outward normal vector on Γ_i, and $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{x}_i$ to the position vector from the particle center $\boldsymbol{x}_i$ to the surface point $\boldsymbol{x}$. The rigid bond between particles is applied through $\boldsymbol{F}_{\mathrm{b},i} = \sum_{j=1}^{N}\boldsymbol{F}_{\mathrm{b},ij}$ and $\boldsymbol{M}_{\mathrm{b},i} = \sum_{j=1}^{N}\boldsymbol{M}_{\mathrm{b},ij}$, which represent the sum of all bond forces and moments, respectively, acting on particle i, where $\boldsymbol{F}_{\mathrm{b},ij}$ is the bond force and $\boldsymbol{M}_{\mathrm{b},ij}$ is the bond moment acting on the i-th particle from the j-th particle. These bonds hold the particles together such that the aggregate behaves as a single rigid body.

2.2. *Gas/liquid interface treatment*

In order to capture the evolution of the fluid/gas interface, we will utilize the volume-of-fluid method outlined in O'Brien & Bussmann (2020), which is coupled to the immersed boundary method for the moving particles and allows for the appropriate boundary conditions to be specified at the particle surface, in terms of liquid/gas/solid contact angle. Specifically, this contact angle can vary as a function of location along the surface of the particles, which allows for the simulation of multicomponent particle assemblies. For validation purposes we will perform numerical simulations of both static and moving boundary problems, and compare the numerical results with experimental data and theoretical models available in the literature.

2.3. *Generating particle aggregates*

We will represent the particle aggregates as fractal structures, i.e., as self-similar bodies that satisfy the relation

$$N = k_{\mathrm{f}}\left(\frac{D_{\mathrm{g}}}{D_{\mathrm{p}}}\right)^{n_{\mathrm{f}}} \tag{2.5}$$

where N is the number of individual particles making up the aggregate, n_{f} is the fractal dimension, k_{f} is a fractal prefactor, and D_{g} is the gyration diameter of the aggregate where $\boldsymbol{x}_{\mathrm{c}}$ denotes the center of mass. The fractal dimension is related to the overall shape of the aggregate. Aggregates will be generated using a Particle-Cluster Aggregation scheme outlined in detail in Skorupski *et al.* (2014). In this method, for predetermined values of n_{f}, k_{f}, D_{p}, and N, an initial particle is seeded and new particles are added to the aggregate such that equation (2.5) holds. Starting with two particles in contact at a single point, new particles are added to the aggregate at random locations until the complete aggregate has been constructed (fig. 1a). We note that the primary spherical particles can have different sizes and densities, thereby allowing for the creation of highly heterogeneous aggregates. Here we would hope for input from IFPRI members, in terms of desirable aggregate sizes, shapes, wettabilities and porosity distributions.

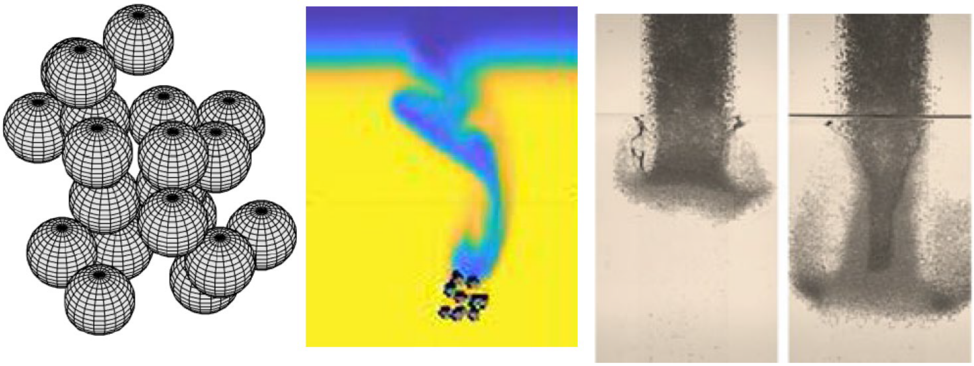

FIGURE 1. Left: a) Complex aggregate constructed by rigidly connecting 20 individual spherical particles. The aggregate shown has a fractal dimension of $n_f = 2.5$. The planned simulations will consider complex aggregates consisting of hundreds of primary spherical particles. Middle: b) A rigid aggregate settling through a miscible fluid/fluid interface that separates light (blue) fluid above from dense (yellow) fluid below. As the heavy aggregate settles through the interface, it traps light fluid in its pore spaces. This buoyant interstitial fluid initially slows down the settling of the aggregate, but it subsequently escapes from the pore spaces and is replaced by denser fluid, so that the aggregate's settling motion accelerates again. Right: c) Granular jet entering a body of water (Saingier *et al.* 2021).

3. Preliminary Results

Results for individual spherical particles settling through a miscible fluid/fluid interface were presented in our earlier publication (Deepwell *et al.* 2021). More recently, we have extended these simulations to complex particle aggregates settling through fluid/fluid interfaces (Maches and Meiburg 2024, in preparation), cf. fig. 1b.

4. Proposed Research

In order to gain fundamental insight into the liquid entry process of complex particles, we propose to proceed in a series of increasingly complex steps, so that we can clearly identify, distinguish and quantify the respective roles played by such features as particle shape, porosity distribution, entry velocity and angle, surface tension, density ratio, wettability, contact angle and others. In this process we will be able to build on our ongoing work on sedimentation of complex particles in stratified flows (supported by the U.S. Army Corps of Engineers), and on the mixing of stratified fluids by active swimmers (supported by NSF). The series of steps we propose to take are outlined in the following:

- **Year 1:** Implement the liquid/gas interface by means of the volume of fluid method, based on the methodology proposed by O'Brien & Bussmann (2020). Validate the implementation with known results for the water entry of single spherical particles.
- **Year 2:** Extensive parametric study for individual aggregates of complex shapes where we vary a) particle shape, b) porosity distribution, c) entry velocity, d) surface tension, e) homogeneous and heterogeneous wettability, f) fluid viscosity, and g) particle/fluid density ratio. Clarify and quantify the role of the interstitial gas, e.g. under what conditions does it get trapped so that it remains attached to the aggregate, when is it able to escape, and to what extent does it modify the liquid entry process in terms of the resulting aggregate deceleration and rotation? Formulate the relevant scaling laws describing this liquid entry process.

- **Year 3:** Extend the parametric study to several interacting aggregates of complex shapes that enter the liquid within close proximity of each other. Conduct preliminary simulations to quantify the interaction between neighboring aggregates and their respective cavities, in order to progress towards the development of models for the liquid entry of powders consisting of many individual aggregates of complex shapes.

During a potential follow-up project, we would then plan to conduct a systematic simulation campaign for hundreds of interacting aggregates entering the liquid within close proximity of each other, in order to derive quantitative models for the collective behavior of these aggregates that can be upscaled to larger, continuum scales.

5. Expected Outcomes

The grand challenge in developing reliable quantitative continuum-level models for the liquid entry of powders consisting of heterogeneous particles and aggregates is twofold: (i) we need to obtain a comprehensive quantitative understanding of the basic three-phase flow physics at the level of the individual particle or aggregate, and how it depends on the particle features (shape, porosity distribution, wettability heterogeneity etc.) and process characteristics (entry velocity and angle, fluid viscosity, interfacial tension etc.), and (ii) the three-phase flow dynamics at the individual particle level has to be upscaled to the continuum level, in order to capture the collective dynamics of many thousands of interacting aggregates constituting the powder. This two-step process will result in the development of predictive tools for the evolution of the particle, liquid and gas velocity and concentration fields when a powder enters a liquid. The first three years of the proposed projects will address the particle-scale phenomena under (i) above, while a potential follow-up project would focus on the topic of collective dynamics and upscaling. In this way, the proposed project will result in key fundamental advances of our understanding of the liquid entry of complex, heterogeneous particles, and in the development of quantitative models for powder reconstitution.

6. Potential Risks and Contingency Plans

The simulation campaign to be undertaken is of a highly multiscale nature, as the dimensions of the computational domain are several orders of magnitude larger than the individual complex particles. The simulations are also multiphysics, as they involve three phases and include additional complex features such as moving contact lines and heterogeneous wettability properties. These aspects will require a high degree of numerical resolution, which increases the computational expense. If necessary, it may be possible to use a simplified representation of the smaller grains, so that they do not require as many grid points to be adequately resolved. This would require additional computational tests for validation purposes. The planned simulations will be large-scale, i.e., massively parallel, and they will generate large amounts of data, thus requiring substantial amounts of storage resources at large, NSF-supported supercomputing centers. As our research group has a long, successful track record of obtaining such resources via competitive proposals, we do not expect this to represent a serious hurdle.

7. Relevance to IFPRI Members

IFPRI members routinely face the task of powder reconstitution, for example in the food, medical or chemical industries. Achieving uniform solutions in these applications can pose serious challenges, so that it is essential to have accurate predictive tools for the purpose of modeling and optimizing the underlying processes. The proposed research will advance the state of our current understanding, and establish quantitative relationships that can serve as basis for the formulation of models that capture such complex, multiphase flow processes.

8. Broader Educational Impacts

The day-to-day computational research will be carried out primarily by a Ph.D. student under Prof. Meiburg's guidance, who will learn a wide range of advanced skills, including scientific computing, data analysis, and complex physical modeling approaches. In addition, our research group regularly employs international exchange students as well as undergraduate research students, to assist with the data analysis, physical interpretation and visualization. Prof. Meiburg furthermore serves on the Board of Directors of the Engineering Academy Foundation at the local Dos Pueblos High School in Goleta, a highly successful program that provides about 400 public high school students per year (half of them female, and a significant fraction Latino students) with advanced training in science, mathematics, engineering, and art. We plan to offer a summer internship position to one of these high school students.

9. Budget

The budget for the amount of $42,000 per year over a three-year period is attached.

REFERENCES

Akbarzadeh, P., Krieger, M., Hofer, D., Thumfart, M. & Gittler, P. 2023 Parallel water entry: Experimental investigations of hydrophobic/hydrophilic spheres. *Phys. Fluids* **35**, 103301.

Aristoff, J.M., Truscott, T.T., Techet, A.H. & Bush, J.W.M. 2010 The water entry of decelerating spheres. *Phys. Fluids* **22**, 032102.

Biegert, Edward, Vowinckel, Bernhard & Meiburg, Eckart 2017 A collision model for grain-resolving simulations of flows over dense, mobile, polydisperse granular sediment beds. *Journal of Computational Physics* **340**, 105–127.

Biegert, Edward K. 2018 Eroding uncertainty: Towards understanding flows interacting with mobile sediment beds using grain-resolving simulations. PhD thesis, UC Santa Barbara, copyright - Database copyright ProQuest LLC; ProQuest does not claim copyright in the individual underlying works; Last updated - 2021-07-31.

Cervantes-Alvarez, A.M., Escobar-Ortega, Y.Y., Sauret, A. & Pacheco-Vazquez, F. 2020 Air entrainment and granular bubbles generated by a jet of grains entering water. *J. Coll. Int. Sci.* **574**, 285–292.

Deepwell, D., Ouillon, R., Meiburg, E. & Sutherland, B. R. 2021 Settling of a particle pair through a sharp, miscible density interface. *Phys. Rev. Fluids* **6**, 044304.

Gonzalez-Gutierrez, J., Carrillo-Estrada, J.L. & Ruiz-Suarez, J.C. 2014 Penetration of granular projectiles into a water target. *Scientific Reports* **4**, 6762.

Maches, Z., Houssais, M., Sauret, A. & Meiburg, E. 2024 Settling of two rigidly connected spheres. *J. Fluid Mech.* **to appear**.

Magnaudet, J. & Mercier, M.J. 2020 Particles, drops, and bubbles moving across sharp interfaces and stratified layers. *Ann. Rev. Fluid Mech.* **52**, 61–91.

O'Brien, A. & Bussmann, M. 2020 A moving immersed boundary method for simulating particle interactions at fluid-fluid interfaces. *J. Comp. Phys.* **402**, 109089.

Saingier, G., Sauret, A. & Jop, P. 2021 Falling jet of dry granular material in water. *J. Fluid Mech.* **916**, A34.

SKORUPSKI, K., MROCZKA, J., WRIEDT, T. & RIEFLER, N. 2014 A fast and accurate implementation of tunable algorithms used for generation of fractal-like aggregate models. *Physica A: statistical mechanics and its applications* **404**, 106–117.

TRUSCOTT, T.T., EPPS, B.P. & BELDEN, J. 2014 Water entry of projectiles. *Ann. Rev. Fluid Mech.* **46**, 355–378.

WANG, X., LYU, X., SUN, R. & TANG, D. 2024 Numerical study on the cavity dynamics for vertical water entries of twin spheres. *Defence Technology* **32**, 459–472.

WATSON, D.A., BOM, J.M., WEINBERG, M.P., SOUCHIK, C.J. & DICKERSON, A.K. 2021 Water entry dynamics of spheres with heterogeneous wetting properties. *Phys. Rev. Fluids* **6**, 044003.