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Three-dimensional simulation of micrometer-sized droplet impact and penetration into the powder bed

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HIGHLIGHTS

- We propose a numerical method to model micron-sized droplets impacting on the powder bed.
- The Cartesian grid based volume-of-fluid method is used to track the liquid-air interface.
- A contact angle model is proposed and implemented on the embedded solid objects.
- The impact velocity has strong effect on the droplet-powder interaction.
- Our method can be used to determine the optimal printing conditions in the inkjet-assisted 3D printing.

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ABSTRACT

In recent years, various drop-on-demand inkjet technologies capable of precisely delivering micron-sized droplets have been adopted in a few novel powder-based 3D printing processes. The droplet-powder interaction is an important step in these 3D printing technologies. In this paper, we propose a direct numerical simulation method to study the micron-sized droplets impacting on the powder bed. Since the powder particle size in our study is comparable to that of impacting droplets, the powder bed is modeled with a large number of rigid solid spheres fixed in their positions during the droplet impact. A set of important dimensionless parameters and scaling arguments is presented to elucidate the underlying physics involved in the micron-sized droplets impacting on powder. The Cartesian grid based volume-of-fluid method is used to track the immiscible liquid and air interface during the droplet-powder interaction. A contact angle model is proposed to include the wetting effect of the liquid agent on powder particles. The proposed numerical methods are implemented in an open-source code *Gerris*. Two numerical tests relevant to our study are conducted to validate the modified simulation code. Finally, we carry out simulations of a micrometer-sized droplet impacting on the powder bed with three different impact velocities. For low impact velocity, the droplet can even gain the momentum in the early stage due to strong capillary forces at contact lines compared to inertial force. The large impact velocity results in a wider spread and deeper penetration, however the liquid distribution inside the powder bed can be segmented because of high impact energy. The numerical method proposed in our study can be used to design suitable droplet-powder systems as well as determine optimal printing conditions in the inkjet-assisted powder-based 3D printing technologies.

1. Introduction

Droplets impacting on a loosely packed powder bed is a ubiquitous phenomenon in many engineering and natural processes including powder-binder based 3D printing, wet granulation, spray drying, powder coating, agricultural sprays, water erosion of soil, and raindrops landing on sand or soil. Fundamental understanding of this phenomenon is crucial to achieve the desirable outcomes in a wide range of industries such as inkjet-assisted additive manufacturing, pharmaceuticals, food engineering, and agricultural chemicals.

Interaction between droplets and powder material is a complex physico-chemical process that involves many phenomena such as the kinematic impact, spreading over the powder surface, displacement of powder particles due to impact force (e.g. crater formation), capillarity-induced particle movement (e.g. granulation), droplet penetration into the powder bed due to capillarity of menisci in pores of powder beds, and evaporation of liquid. Although droplets impacting on powder surface attracts much less

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attention of researchers than those impacting on rigid solids (Josserand and Thoroddsen, 2016, Rein, 1993, Yarin, 2006), there is still a sizable amount of research work being done in this field. Popovich et al. (1999) investigated the penetration time of sessile droplets on carbon black powders and found that the droplet penetration rates do not show a direct correlation with fluid viscosity. Hapgood et al. (2002) also studied the penetration time for droplets deposited on several powder materials with no impact velocity and proposed a Washburn equation (Washburn, 1921) based model to predict the absorption time with reasonable accuracy. Hapgood and her team (Nguyen et al., 2009) later reported a strong effect of the hydrophobicity of powder particles on the penetration time. Holman et al. (2002) examined simultaneous spreading and infiltration of inkjet-printed droplets on ceramic powders in the context of 3D printing. Ghadiri (2004) investigated crater formation in soil, sand, and pastes from the impact of rain drops. He measured crater shapes and sizes, and related the crater volume to the surface shear strength and drop impact impulse. Charles-Williams et al. (2011) carried out experiments of drop impact on both dry and pre-wetted powder with small impact velocity and identified the competitive spreading versus capillary infiltration mechanisms in the formation of granules after impact. Marston et al. (2013, 2010) used high-speed photography to study the dynamics of liquid drop impact on powder. Their scaling analysis of experimental data indicated that the observed spreading, rebound and splashing can be broadly characterized in terms of the Weber number. A number of researchers (Katsuragi, 2011, Nefzaoui and Skurtys, 2012, Zhao et al., 2015) also used scaling analysis to correlate the spreading ratio, crater size, drop absorption time with non-dimensional numbers including the Weber number and Reynolds number. Lee and Sojka (2012) studied the influence of impact conditions on nucleus formation due to capillary forces of liquid menisci between particles. Emady et al. (2013a, 2013b, 2011) published a series of studies on droplet impact on a powder bed with a focus on wet granulation. They identified tunneling, spreading, and crater formation as three different granule formation mechanisms that occur when droplets impact loose powder beds.

So far good progress has been made in fundamental understanding of drop-powder interaction, however, we notice that in all above studies except (Holman et al., 2002) droplet volumes are on the order of microliter (i.e. drop diameter $\sim$mm). There is extremely limited research on picoliter droplets (i.e. drop size $\sim\mu$m) impact on granular materials. In recent years, various drop-on-demand (DOD) inkjet technologies (Basaran et al., 2013, Derby, 2010) capable of precisely delivering pico-amounts of liquid have been adopted in a number of novel powder-based additive manufacturing processes such as powder-binder 3D printing (Seyed et al., 2015), high speed sintering (Ellis et al., 2014), multi jet fusion of Hewlett-Packard Company (2014), and selective inhibition sintering (Khoshnevis et al., 2012). In powder-based 3D printing technologies, droplet diameter varies from 20 μm to 55 μm. Droplet impact speed is usually in the range from 3 m/s to 9 m/s. In order to have a good jettability using DoD inkjet devices, the viscosity of solutions is usually less than 10 centipoise. So far, a variety of materials including metals (e.g. steels, alloys), ceramics (e.g. alumina), and polymers (e.g. nylon, polycarbonate) has been used in the inkjet-assisted powder-based 3D printing. Depending on the specific technology, particle size of the powder bed varies from sub-micrometer to tens of micrometers.

The interaction between micrometer-sized droplets and powder plays a significant role in the quality (e.g. surface roughness, dimensional accuracy, strength, toughness) of products made by these 3D printing technologies. As the droplet size decreases from millimeter to micrometer, the droplet surface and kinetic energies can become very comparable. The droplet size also becomes comparable to the powder particle size or even the dimensions of interstitial spaces between powder particles. As a result, learnings from the impact of mm-sized droplets cannot be completely applied to micron-sized droplets. The time scale for the dynamics of micron-sized droplets impacting on powders is of the order of microsecond, which makes the experimental visualization of such fast event with high spatial resolution very challenging. Although modern high-speed imaging technology is capable of capturing the ultra-fast fluid phenomena at a temporal resolution of one million frames per second or even higher (Hutchings et al., 2007, Thoroddsen et al., 2008, Versluis, 2013, Visser et al., 2015), there are still limitations with experimental methods. For example, it is extremely difficult to measure the liquid profile inside the powder bed immediately after the droplet impact. Therefore, we propose to use the computation fluid dynamic (CFD) as an instrumental tool to obtain the insights into the liquid evolution of micron-sized droplets impacting on powder surface.

The objective of the study is to develop an accurate and reliable modeling tool to simulate the micron-sized droplets impacting on powder beds. Since the size of the powder particle in our study is comparable to that of impacting droplets, we model the powder bed with a large number of rigid solid spheres. Our focus is the initial phase of droplet-powder interaction such as spreading and penetration. We assume the powder particles are fixed in the space despite the impact force acting on particles during the impact. First, a set of important dimensionless parameters and scaling arguments is presented to elucidate the underlying physics involved in the micron-sized droplets impacting on powder and highlight the relevance of each important factor (e.g. impact velocity, liquid properties, powder properties) to the phenomenon. Thereafter, governing equations with proper boundary conditions are proposed to describe the fluid flow. Since droplet impact phenomenon is an immiscible two-phase flow involving moving contact lines on solid surface (Sui et al., 2014), we use the volume-of-fluid (VoF) method to track the sharp liquid-air interface. An open-source adaptive-meshing-refinement (AMR) based CFD code *Gerris* (Popinet, 2003, Popinet, 2009) has been modified to model the interaction between droplets and powder. Using the same modified code, we have successfully simulated the micron-sized droplet ejection process in thermal inkjet devices (Tan, 2016). To test the proposed numerical methods and their implementation in the simulation code, we carry out two numerical tests relevant to our study including capillary rise in a cylindrical tube and liquid capillary bridge between solid spheres. Finally, numerical examples of a micrometer-sized droplet impacting on the powder bed with different impact velocities are presented. The effect of impact velocity on liquid profile inside the powder is discussed as well. Although our example involves only one configuration of the powder bed (e.g. particle size, distribution, and pack density), our modeling approach can be easily applied in a parametric study involving different parameters for powder bed as well as liquid.

2. Dimensional analysis of microscopic droplet impact on powder

The fundamental behavior of fluids at the micron scale is both complex and distinct from our daily experience (Purcell, 1977, Squires and Quake, 2005). The essential fluid physics of microscopic flows is governed by a competition between various physical phenomena, which can be captured by nondimensional groups. A list of important dimensionless parameters relevant to the droplets impacting on powder beds is presented in Table 1. The droplet volume produced from the DOD inkjet devices usually varies from a few picoliters to hundreds of picoliters (Derby, 2010). Inkjet droplets usually travel at a speed of a few meters per second