



Prediction of porosity from particle scale interactions: Surface modification of fine cohesive powders



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ABSTRACT

Packing or powder bed porosity is a fundamental property of solid particulate systems and is of prime importance to many industries which handle or process such material. Inter-particle forces, which may couple with particle size and shape, can significantly affect porosity. For fine dry particles, the attractive van der Waals force is dominant and can prevent the packing of particles resulting in high porosity. This study investigates the effect of the van der Waals force on porosity of powder beds consisting of fine cohesive particles. Dry coating is utilized to modify the surface roughness of particles in order to further elucidate this effect. The results indicate that dry coating nano-sized particles onto coarser particles ranging in size from 5 μm to 223 μm can significantly reduce the van der Waals force resulting in reduced porosity. The granular Bond number, defined as the ratio of the cohesion force to particle weight was shown to accurately predict porosity, provided a multiple asperity particle contact model is employed. A subsequent theoretical investigation determined the effect of surface modification, specifically the size, surface energy, and surface area coverage of asperities on porosity. It showed that the surface roughness of non-surface modified particles may be poorly defined and may lead to erroneous calculation of inter-particle forces. Therefore, in addition to dry coating being a useful process to improve powder properties such as porosity, dry coating can be used to define surface properties to accurately predict bulk level powder properties from multi-asperity particle scale interaction models.

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1. Introduction

The packing of solid particulates is a practical concern for a variety of industries including the ceramic, mineral, and pharmaceutical in addition to being of great academic interest [1,2]. Powder bed porosity, along with the related parameters packing density and bulk density, is well studied and commonly utilized to characterize particulate packing [3]. It has long been established that under given packing conditions, porosity is mainly dependent on particle size, particle size distribution, and shape for dry coarse particles. Indeed, much of the earlier studies have focused on predicting porosity in consideration of these factors [4–6]. While the packing of dry coarse particles is mainly driven by the force of gravity, inter-particle capillary or van der Waals forces can have significant effects. Capillary forces can dominate wet systems and increase porosity by restricting the motion of particles [7]. Similarly, the inter-particle attractive van der Waals force can restrict the motion of fine dry particles (generally $<100 \mu\text{m}$) and form agglomerates thereby increasing porosity [8]. In fact, the porosity of nano-sized powders can be in

excess of 99% due to the formation of agglomerates [9]. Needless to say, these forces can complicate the modeling and prediction of particle packing [10,11].

While fine particles have a great utility in industry, their poor flow and packing behavior due to the van der Waals force can cause restriction or difficulty in their application. In order to improve the bulk powder properties of fine particles, surface modification techniques such as dry coating have been successfully used [12–15]. Dry coating alters surface properties by adhering or coating nano-sized particles onto larger micron-sized particles. By virtue of increasing the separation distance and decreasing the contact area of two contacting particles, nano-coatings acting as artificial surface asperities effectively reduce the van der Waals force resulting in improved powder flowability and packing. To account for the improvement in bulk powder properties caused by dry coating, particle scale force models have been used to show that applying nano-sized surface asperities can indeed decrease the van der Waals force by an order of magnitude or more [16]. Since bulk scale powder properties are derived from particle scale interactions, force models should offer some predictive capability for properties of particulate systems such as porosity. Likewise, the study of particle packing can offer better fundamental understanding of particle scale interactions.

This study investigates the effect of the van der Waals force on the packing, specifically powder bed porosity, of fine cohesive powders where such forces are dominant. Dry coating is utilized to alter the

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surface properties of particles in order to further elucidate the effect of the van der Waals force on porosity. It is shown that dry coating significantly decreased the porosity of fine particles. Using a multi-asperity force model modified from the Rumpf equation, the porosity is directly related to the granular Bond number which is defined as the ratio of the cohesion force, specifically the van der Waals force to particle weight. As a major novelty, the model enabled prediction of porosity for both non-surface-modified and surface-modified particles and allowed theoretical investigation into the effects of surface modification via dry coating. Further investigation showed that the surface roughness of non-surface modified particles may be poorly defined and may lead to erroneous calculation of inter-particle forces. Therefore, in addition to improving powder properties such as porosity, dry coating can also aid in determining particle scale interactions by defining surface properties in order to better predict bulk scale powder behavior.

2. Theoretical preliminary

In the absence of capillary or electrostatic forces, the van der Waals force can dominate the interaction between two particles in close contact when the particle size is small (<100 μm). The van der Waals force originates from the attractive nature between the two particle's constituent molecules and operates at very short distances [17]. The interaction potential between two molecules can be described by the Lennard-Jones potential where one may derive various expressions for the adhesion force between particles of various geometries. Because the van der Waals force is attractive, fine particles tend to agglomerate and are termed cohesive powders. While fine powders are advantageous for many applications, cohesive powders are known to display non-ideal processing properties such as poor flowability, low porosity, and high compressibility. Thus, for efficient powder handling and processing, improvement of these properties is paramount. Assuming that particle size and shape cannot be altered, the only practical method to influence strong inter-particle forces is through surface modification [12–15]. Surface properties of particles such as surface roughness and surface free energy can be modified and controlled through dry coating in order to reduce the van der Waals force between two particles at contact.

Dry coating methods coat nano-particles (guest particles) onto coarser micron-sized particles (host particles) through high intensity blending/mixing. As the guest particles are usually in a highly agglomerated state due to strong van der Waals forces, proper processing equipment is required to disperse the agglomerates which subsequently adhere to the surface of a host. Once the guest is coated onto a host, the guest remains adhered to the host surface also due to the van der Waals attractive force. The nano-sized guest particles act as artificial asperities on the host surface to increase surface roughness thereby decreasing contact area and increasing particle spacing between two host particles. The surface energy, which dictates the work of adhesion between two particles, can similarly be controlled by virtue of the guest's surface properties. A plethora of work on surface modification via dry coating has shown its usefulness in improving powder flowability, fluidization, bulk density, and compressibility to name only a few [12–15].

In order to more precisely account for the effect of the guest particles (i.e. artificial asperities) dry coated onto hosts, Chen et al. [15] modified the well-known Rumpf equation as shown in Eq. (1)

$$F_{vdw} = \frac{A}{16\pi} \left(\frac{1}{z_0^2} \frac{d_p}{2} + \frac{3}{z_0^2} \frac{d_p d_g}{d_p + d_g} \right) \quad (1)$$

where F_{vdw} is the van der Waals force between two spherical coarse particles (hosts) of diameter d_p coated with guest particles of diameter d_g . The first term on the r.h.s. of Eq. (1), known hereafter as the multi-asperity model, accounts for the van der Waals attractive force between

the two host particles while the second term accounts for the attractive force between the host and the guest. As opposed to the original Rumpf equation which only considers a single asperity separating two host particles by a distance of d_g , the multi-asperity model (Eq. (1)) accounts for the more realistic case of three asperities in contact defining the separation distance. As a result, the separation distance between the two host particles l_0 is given by Eq. (2)

$$l_0 = \sqrt{\left(d_p + d_g\right)^2 - \frac{1.21}{SAC} d_g^2 - d_p} \quad (2)$$

where SAC is the surface area coverage of guest particles on the surface of the host particle. The surface area coverage (i.e. number of guests on the host's surface) dictates the spacing between guest particles thus influencing the host–host separation distance. Furthermore, the surface area coverage determines the type of particle contact whether it is a host–host or host–guest contact. The former case is relevant for low guest loading where there is not sufficient number of guest particles to prevent host–host contact while the latter case is relevant for higher guest loadings where the primary contact is between host and guest. In the absence of any surface coating and assuming that the surface of the particle is perfectly smooth, Eq. (1) reduces to Eq. (3)

$$F_{vdw} = \frac{A}{16\pi z_0^2} \frac{d_p}{2} \quad (3)$$

where z_0 is the inter-atomic equilibrium distance (i.e. minimum separation distance) usually taken as 0.4 nm and A is the Hamaker constant which is related to the surface free energy and can be estimated by Eq. (4) [17]:

$$\Delta\gamma = \frac{A}{16z_0^2} \quad (4)$$

The multi-asperity model of Eq. (1) has been shown to predict fluidization behavior of fine dry coated powders [15] as well as the pull-off force of dry coated particles under consolidation [18]. Later developments of the multi-asperity model also incorporated the effect of particle deformation as well as the spatial and size distributions of asperities on the inter-particle force [16]. As a result, the multi-asperity model can offer a more precise calculation of the inter-particle force between particles having rough surfaces as compared to the Rumpf equation for single asperities or other common force models such as the modified JKR or DMT models [19] which like the Rumpf equation only account for a single contact.

While the multi-asperity model can determine the van der Waals force between two particles, it is not an absolute determination of inter-particle cohesiveness. Particles can experience a multitude of body or surface forces which will affect their interaction. Most common body forces relevant to particulate processing would include gravity, for example in particulate packing, or vibratory and centrifugal forces in certain powder processing equipment such as vibratory or rotating fluidized beds [20,21]. Surface forces acting on individual particles such as hydrodynamic drag in processes such as fluidization are also critical in affecting inter-particle cohesion and powder behavior [22]. Thus, to determine the inter-particle cohesion, the so-called granular Bond number evaluates the ratio of cohesive forces to non-cohesive body or surface forces as given in Eq. (5a):

$$Bo_g = \frac{F_{cohesion}}{F_{body/surface}} \quad (5a)$$

The granular Bond number of Eq. (5a) is the most general form as the cohesive force may include a combination of capillary, electrostatic, or van der Waals attractive forces and any relevant body or surface force. In this particular study, the unconsolidated packing of fine dry

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