Chemical Engineering Science 65 (2010) 3341–3351

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Constitutive model to predict flow of cohesive powders in bench scale hoppers

AbdulMobeen N. Faqih [a], Bodhisattwa Chaudhuri [b], Amit Mehrotra [c], M. Silvina Tomassone [d], Fernando Muzzio [d,*]

[a] Wyeth Pharmaceuticals, Pearl River, NY, USA
[b] Department Pharmaceutical Sciences, University of Connecticut, Storrs, CT, USA
[c] Glaxo Smith Kline, Raleigh, NC, USA
[d] Department of Chemical and Biochemical Engineering, Rutgers University, USA

ARTICLE INFO

Article history:
Received 23 September 2009
Received in revised form
25 January 2010
Accepted 15 February 2010
Available online 6 March 2010

Keywords:
Granular materials
Pharmaceuticals
Powder technology
Mathematical modeling
Discrete element modeling
Powder flow

ABSTRACT

This communication empirically correlates flow in two systems; an instrumented rotating drum (GDR) and a set of bench scale hoppers. A flow index obtained from measurements in the GDR is directly correlated to the flow through hoppers, providing a predictive method for hopper design and a convenient experimental test for screening materials and determining their suitability for specific hopper systems. Simulations were performed to understand the dynamics of flow in hoppers by using the same flow parameters in hoppers and rotating cylinders. Simulations showed that as cohesion increased it becomes harder for the particles to flow through the hoppers, in good agreement with the experiments. The effect of hopper angle also yields similar findings to experiments for Avicel, $K=60$, where the powder does not flow through the 45° hopper but flows well in a 75° hopper. Simulations were also used to calculate the normal forces on the walls of the hopper and the wall pressure distributions in both hoppers. As depth increases, the wall pressure increases for all cases. Finally, the simulations also helped understand the different flow behaviors (funnel and mass flow) that take place in a hopper. The simulated dynamics of flow in the rotating drum and in the hopper correlate very closely to experiments, indicating that the model cohesion parameters are, as desirable, material-specific but independent of geometry.

1. Introduction

Granular materials exhibit a wealth of interesting phenomena, including heaping under vibration, segregation, convection, fluidization, and density waves in pipes or hoppers. They are also very important from technological and industrial points of view. Many examples of important granular flows can be found in both industry and nature. Hoppers, chutes, and conveyor belts are used when transporting particulate materials such as food stuffs, pharmaceuticals, and coal. Other industrial applications include packing of granular materials, particulate segregation and mixing, and particulate drying. In nature, examples of granular flows include snow and mud avalanches, river sedimentation, dune formation, planetary ring dynamics, soil liquefaction, and ice flow mechanics. Clearly, characterization of the behavior of granular materials is essential to scientific community with significance to the pharmaceutical industry for downstream processing of solid dosage forms. However, most of the research has been focused on cohesionless materials, which tend to segregate when used with a poly-dispersed particle size distribution (Savage et al., 1983; Savage, 1984; Savage and Hutter, 1989), but that otherwise, provide relatively simple flows.

There has been some research work in the last few years on the much more complex field of cohesive powders (Adams and Perchard, 1985; Lian et al., 1993; Bocquet et al., 1998; McCarthy et al., 2001) however, the flow of cohesive powders is still poorly understood. Knowledge of powder flow properties is very important when developing manufacturing processes and handling procedures such as flow from hoppers and silos, transportation, mixing, compression and packaging (Knowlton et al., 1994; Peleg, 1978). Powder flow characteristics are commonly investigated under gravity loading conditions (Carstensen, 1974). The compressibility of a powder is a commonly used indicator of flowability and is often expressed using the Hausner Ratio, which is the ratio between the tapped and the loose-packed bulk densities of the powder (Hausner, 1967). Compressibility is also one of the tests proposed by Carr (1965) for the assessment of powder properties. Another commonly used flow indicator is the time it takes for powder to flow out of a funnel with a standard orifice size (Staniforth, 2002). Such measurements have

* Corresponding author.
E-mail address: fjmuzzio@yahoo.com (F. Muzzio).

0009-2509/$ - see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ces.2010.02.028

demonstrated the dependence of powder flowability on particles shape and size distribution (Baxter et al., 2000), instantaneous degree of consolidation, and relative humidity (Coelho and Harnby, 1978; Stanford and DellaCorte, 2006).

A key situation where flow is critical is the filling and emptying of hoppers. Despite their common use and deceptively simple design, one of the major industrial powder problems is obtaining reliable and consistent flow out of hoppers. These problems are usually associated with the flow pattern inside a hopper. An intriguing property of granular flow from a hopper is that in certain situations the flow rate is largely dependent on the diameter of the orifice, and weakly on the particle size and head of the material. Mass flow is an ideal flow pattern where the bulk is in motion and moving downwards towards the opening. The other common case is called *funnel flow*, where the powder starts moving out through a central ''funnel'' that forms within the material, leading to the powder collapsing and moving through the funnel. Most flow problems are caused by a funnel flow pattern and can be cured by altering the pattern to mass flow (Purutyan et al., 1998; Savage, 1965). The worst case-scenario is *no flow*, which can occur when the cohesive powder forms an arch across the opening, which provides sufficient strength to support itself. In order to prevent these problems, measurement of powder flow properties is necessary for design of mass flow hoppers.

In the last 45 years, significant improvements have been proposed to the mathematical models that quantify the flow of granular material through hopper. In 1964 Jenike utilized the radial solutions of Sokolovsky to quantify some aspects of granular flow, but as the solution lacked inertial terms, the granular flow discharge rate could not be predicted. Savage (1965) constructed the earliest model that accounted for inertial terms by setting the internal friction and the friction with the wall to zero. Later in 1967, Savage added wall friction but maintained gravity in the radial direction (Tomas and Schubert, 1979). Sullivan, Davidson and Nedderman et al. (1982), Nedderman (1992) applied these results to the Hour-Glass theory. In 1992, Thorpe (1992) showed that the earlier models assumed constant bulk density, which would overestimate the discharge rates. As the material flows through the hopper, the stress changes from zero at the top surface, reaches a maximum and falls to zero on the free-fall arch. Thus in the upper part of the hopper, the material is compressed and the interstitial air must be expelled, whereas in the lower part, the material dilates as air is being drawn in. As a result, elevated pressures occur in the upper part and sub-atmospheric pressures occur in the lower part. The most appropriate model that describes this change in stress behavior is the critical state theory (CST) (Bak et al., 1987), which assumes a logarithmic relationship between pressure and density (so that density is not defined when pressure equals to zero). However the CST, which is derived from soil mechanics, cannot be necessarily applied to extreme cases of failure for hopper flow.

In spite of the existence of predictive models and techniques to improve flow of free-flowing materials through hoppers, there lacks a general understanding of the flow behavior of powders as a function of cohesion. Cohesion clearly plays an important role in affecting flow properties and is a key target of flow property characterization. During the last few decades a variety of methods for assessment of cohesive powder flow properties have been developed using some type of a ''shear cell'' where the force required to initiate (or maintain) movement in a standard geometry is measured. The area was pioneered by Jenike (1964) who also developed the theoretical framework that became the field standard. In conjunction with the measured property data, he applied two-dimensional stress analysis in developing a mathematical methodology for determining the minimum hopper angle and hopper opening size for flow from conical and wedge shaped hoppers (Jenike, 1964).

Besides the Jenike tester, some other commonly used shear testers include the ring shear testers (Schulze, 1994), the Johanson (1992, 1993) indicizers, uniaxial, biaxial, and triaxial testers (Maltby and Enstad, 1993; Maltby, 1993), and Jenike and Johanson's quality control tester. While these methods have been useful for many purposes such as building roads and bridges, they have some shortcomings regarding processing of cohesive powders. The most salient drawback is that flow characteristics of powders are highly dependent on their densification (consolidation) states, i.e. powders can be more or less expanded or contracted when stressed, thus leading to a large variety of inter-particle forces and flow behavior (a phenomenon commonly referred to as ''jamming''). For small scale systems, powders often flow in a fully dilated state. Shear cells can approach the dilated state only asymptotically, and are affected by considerable experimental error for cohesive materials exhibiting a non-linear relationship between consolidation and flow.

The complex constitutive behavior makes accurate powder flow measurements difficult. Various modeling scales are commonly used to simulate granular materials. Understanding and modeling the dynamic behavior of particulate systems has been a major research focus worldwide for many years. Models of granular flows can be broadly divided into three categories: continuum, kinetic theory and discrete. When continuum approach fails or when no appropriate constitutive relations exist, the discrete element modeling (DEM) has proven tremendously useful. Molecular dynamics models are broadly classified by the contact model and integration method, as either hard-sphere, in which collisions are instantaneous and binary, and soft-sphere, in which collisions can be lasting and multiple. Here, the particles are permitted to suffer minute deformations, and these deformations are used to compute restoring elastic, plastic and frictional forces. The discrete element method (DEM), originally developed by Cundall (1971), Cundall and Strack (1979), has been successfully used to simulate chute flow, heap formation (Luding, 1997), hopper discharge (Ristow and Herrmann, 1994; Thompson and Grest, 1991) and flows in rotating drums (Rosato et al., 1986; Khakhar et al., 1997; Wightman et al., 1998).

In this article we investigate the flow and pressure dependence as a function of cohesion in two different geometries (rotating cylinder and hopper) using discrete element methods (DEM) and experiments. We test the parameters developed for simulating cohesive flow in a rotating drum by using the same parameters to simulate flow in hoppers of varying angle. DEM simulations are used to describe the behavior of granular materials after the initial filling stage (static state) and during the discharge (dynamic state) as a function of cohesion. These DEM results are compared with experimental studies for bench scale hoppers. In essence, the goal is to determine whether the parameters introduced from the rotating drum and applied to simulation studies in hoppers are independent of the geometry of the system.

The article is organized as follows: Section 2 lists the materials used in the experimental study and describes the experimental setup for the gravitational displacement rheometer (GDR) and bench scale hoppers. In Section 3, we report a DEM based constitutive model to compare the dynamics of the flow in the two geometries considered. Section 4 describes the experimental and simulation method for correlations between geometries and between experiment and simulations, Section 5 describes the experimental and computational results for flow dynamics in a rotating cylinder, and flow through hoppers of varying angle. Finally, in Section 6 we present our conclusions and outline directions for future work.