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International Journal of Pharmaceutics 320 (2006) 14–22
INTERNATIONAL JOURNAL OF PHARMACEUTICS
www.elsevier.com/locate/ijpharm

Characterizing powder mixing processes utilizing compartment models

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Received 24 January 2006; received in revised form 27 March 2006; accepted 28 March 2006
Available online 18 April 2006

Abstract

Powder mixing has been the subject of substantial research due to its importance in a variety of industrial sectors, including pharmaceuticals, food, and polymer manufacturing. Although a number of different models have been proposed in the literature, most of them are either empirical or require computationally intensive calculations that make them difficult to implement for realistic systems. The aim of this paper is to develop a simplified framework, based on compartment modeling that efficiently and accurately captures the system behavior. Using the V-blender as a model system, the compartment modeling approach was used to illustrate the effects of vessel loading on mixing as well as the impact of sampling methods on the accuracy of mixing characterization.

Keywords: Compartment modeling; Mixing models; Powders

1. Introduction

Many industrial sectors rely heavily on granular mixing to manufacture a large variety of products. In the pharmaceutical industry, it is very important to ensure homogeneity of the product. The pharmaceutical industry is one of the most representative examples, where homogeneity is very important to ensure product quality and compliance with strict regulations. Modeling can play an important role in improving mixing process design by reducing mixing time as well as manufacturing cost, and ensuring product quality. The main difficulty in modeling powder-mixing processes is that granular materials are complex substances that cannot be characterized either as liquids or solids (Jaeger and Nagel, 1992). Moreover, granular mixing can be described by multiple mixing regimes due to convection, dispersion, and shear (Lacey, 1954). Fan et al. (1970) reviewed a number of publications where powder mixing is modeled in an attempt to reduce the production cost and improve product quality. Although a complete literature survey is outside the scope of this paper, we will review the most relevant models in this introduction section.

The existing approaches used to simulate granular material mixing processes can be categorized as (1) heuristic models, (2) models based on kinetic theory, (3) particle dynamic simulations, and (4) Monte Carlo simulations (Ottino and Khakhar, 2000). Geometric arguments and ideal mixing assumptions are some common features of heuristic models. Although these models can generate satisfactory results, they are restricted to batch processes and are case dependent (Hogg et al., 1966; Thýn and Duffek, 1977). Kinetic-theory-based models are used to simulate mixtures of materials with different mechanical properties (size, density and/or restitution coefficient), where each particle group is considered as a separate phase with different average velocity and granular energy. These models typically address shear flow of binary and ternary mixtures based on the kinetic theory of hard and smooth spherical particles (Jenkins and Savage, 1983; Iddir et al., 2005; Lun et al., 1984). The main shortcoming of these models is that they focus on the microscopic interactions between particles, neglecting the effects due to convection and diffusion.

Particle dynamic simulations, which apply molecular dynamic concepts to study liquids and gases, are extensively used to simulate powder mixing (Zhou et al., 2004; Yang et al., 2003; Cleary et al., 1998). The main limitations of particle dynamic simulations are (a) the maximum number of particles required to model the system is restricted due to the computational complexity of the involved calculations, and (b) the lack of realistic particle morphology.

Monte Carlo (MC) simulations begin with an initially random configuration, which is driven to an energetically feasible

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doi:10.1016/j.ijpharm.2006.03.051

equilibrium. One limitation of such an approach is that it cannot provide information about time-dependent characteristics, since it does not follow a realistic dynamic trajectory (Steinbach, 2005).

In order to model granular mixing processes accurately and efficiently, in this paper we explore compartment modeling. Compartment modeling has been utilized in bioprocesses to study the effects of mixing in large-scale aerated reactors (Vrábel et al., 1999) and stirred reactors (Cui et al., 1996) with satisfactory results (both qualitatively and quantitatively). Curiously, this approach has not been used to model powder mixing. The main idea of compartment modeling is to spatially discretize the system into a number of homogeneous subsections containing a fixed number of particles. Discretizing also the time domain, a number of particles are allowed to flow from each compartment to the neighboring ones at each time step. The main advantages of compartment modeling are that (a) it incorporates all associated forces responsible for particle movement within the vessel, using a flux term that can be experimentally determined and (b) it allows the simulation of a large number of particles. Although the exact particle position cannot be determined the changes in composition can be captured by including the flow of particles entering and exiting each compartment.

In this paper, the aim is to demonstrate that compartment modeling can be used to characterize powder mixing. The paper is organized as follows. Section 2 describes the central concepts of compartment modeling and how it is used here to model a V-blender, which is used as a case study. Section 3 illustrates how compartment modeling is used to elucidate the effects of initial loading on the mixing process, and determine the optimal sampling protocol including the sampling locations, the number of samples, the number of particles per sample, and sampling time. Finally Section 4 presents the main conclusions and discusses future work directions.

2. Compartment modeling

Compartment modeling has been effectively used to model the mixing of fluids in reactors to incorporate micro-mixing effects. Correa (1993) and Shah and Fox (1999) have utilized this idea to model turbulence in chemical reactors. Specifically, the fluid is represented by a large number of particles. At each time step a certain number of particles enter the reactor, while particles randomly selected from the ensemble exit the reactor at the same mass flowrate. The interactions between particles are represented by random collisions based on the mixing regime.

Compartment modeling of solid mixers is applied by spatially discretizing the system into a number of subsections that are assumed to be perfectly mixed locally (in good agreement with experimental observations) and contain a stipulated number of particles. By also discretizing the time domain, a number of particles are allowed to flow from each compartment to the neighboring ones at each time step defining the particle flux, F. The number of particles transferred account for the convective and dispersive mixing occurring throughout the vessel. Following the ideas of Fan et al. (1970), who described solid mixing as a random process, the particles selected to enter and leave each compartment are randomly selected. The change in the number of particles of species j, in compartment i, at time step k, is denoted as $\Delta\phi_{ijk}$. All of the particles in the entire mixer are represented by the sum of all the interconnected compartments (w). Thus, the change in each species j throughout all compartments at every time step must equal zero as dictated by Eq. (1):

$$\sum_{i=1}^{w} \Delta\phi_{ijk} = 0 \tag{1}$$

Compartment modeling can in principle be applied to any mixing process as long as there is enough information regarding fluxes to identify different mixing regimes, define the number of compartments needed, and model the particle flux between neighboring regions. A V-blender is considered in this paper as an illustrative case study (Fig. 1a). The V-blender rotates around the x-axis from the upright position to the downward position. The details of the process are given in Brone et al. (1998). Following the experimental observations of Brone et al. (1998), this blender can be modeled with five compartments as shown in Fig. 1b. We identify each compartment as V_1, V_2, V_3, V_4, and V_5. The particle flux between compartments V_1 and V_2 is defined as F_1, and the flux between V_2 and V_3 is defined as F_2, as illustrated in Fig. 1b.

3. Mixing analyses

3.1. Vessel composition (initial load)

Several studies show that mixing performance can be improved by perturbing the symmetry of the mixer (Cahn et

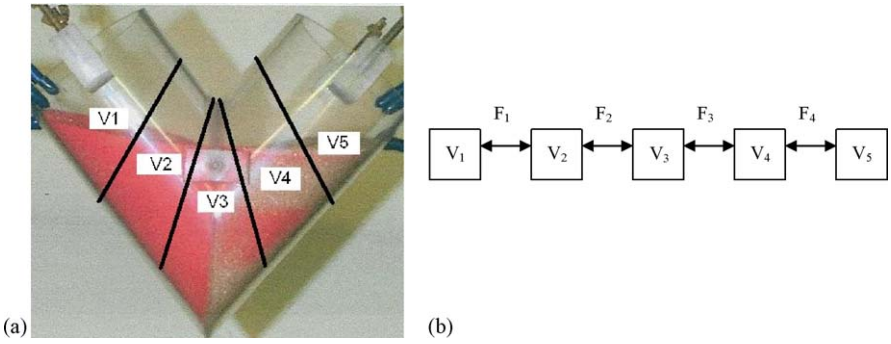

Fig. 1. (a) A discretized V-blender (b) compartment model of V-blender.