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Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation

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ABSTRACT

This paper is concerned with computational aspects of a multidimensional population balance model of a wet granulation process. Wet granulation is a manufacturing method to form composite particles, granules, from small particles and binders. A detailed numerical study of a stochastic particle algorithm for the solution of a five-dimensional population balance model for wet granulation is presented. Each particle consists of two types of solids (containing pores) and of external and internal liquid (located in the pores). Several transformations of particles are considered, including coalescence, compaction and breakage. A convergence study is performed with respect to the parameter that determines the number of numerical particles. Averaged properties of the system are computed. In addition, the ensemble is subdivided into practically relevant size classes and analysed with respect to the amount of mass and the particle porosity in each class. These results illustrate the importance of the multidimensional approach. Finally, the kinetic equation corresponding to the stochastic model is discussed.

1. Introduction

This paper is concerned with computational aspects of a multidimensional population balance model of a wet granulation process. Wet granulation is a manufacturing method to form composite particles, granules, from small particles and binders, using equipment such as rotating drums, fluidised beds and high-shear mixers [1]. These composites have enhanced handling properties over their raw components, and are used for a variety of products, ranging from fertilizers to drugs and detergents. In order to yield granules with a high product quality, a good understanding of the process is required, which may be obtained through modelling of the granulation process. The formation of granules can be described with population balances models, allowing the tracking of the number of particles with desired properties.

Since the 1960s one-dimensional population balance models, i.e., with one characteristic property, have been used to describe granulation processes [2,3]. A one-dimensional description of the granules was subsequently found to be insufficient [4,5], and models with three or more dimensions have been introduced [6–10]. Several approaches have been applied for the numerical solution of population balance models. These are for instance the method of moments [11], sectional methods [12–15], and finite element methods [16]. However, the computational effort for the solution of the models with these methods increases enormously, if the number of dimensions is changed from one to two, three, or even more. Stochastic particle methods offer an attractive alternative for the solution of multidimensional population balance models and have successfully been applied to granulation models [9,10]. Moreover, stochastic algorithms have not only been applied to models

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for particulate processes such as crystallisation [17], nanoparticle synthesis [18–22] and granulation [23,24], but also to those for chemical reactions [25], liquid–liquid mixing [26,27] and droplet coalescence in clouds [28]. Several studies investigated the stochastic treatment of aggregation processes for one- and two-dimensional models [29–33]. Despite this wealth of studies, it remains open how stochastic algorithms would perform for a model with a higher number of dimensions and additional processes, for instance breakage of particles. In addition, an assessment of the numerical approach with respect to the numerical errors is important, in particular, when the solutions for different models are computed in order to discriminate one over the other model. Another aspect in model development is the solving of the inverse problem, i.e., the estimation of model parameters using experimental observations. A detailed understanding of the numerical solution of complex, multivariate models is beneficial, given that surrogate models may be constructed and used for this task.

The purpose of this paper is to present a detailed numerical study of a stochastic particle algorithm for the solution of a five-dimensional population balance model for wet granulation. In particular, the influence of numerical parameters on the macroscopic properties of the particle ensemble is investigated.

A description of the stochastic particle model is given in Section 2. Each particle consists of two types of solids (containing pores) and of external and internal liquid (located in the pores). Several transformations are introduced that correspond to coalescence, compaction and breakage of particles. Numerical results are presented in Section 3. A convergence study is performed with respect to the parameter which determines the number of particles in the system. Several interesting properties of the system are computed, like the number of particles per unit volume and the mean particle porosity. In addition, the ensemble is subdivided into practically relevant size classes and analysed with respect to the amount of mass and the particle porosity in each class. These results illustrate the importance of the multidimensional approach. Finally, in Appendix A, the kinetic equation corresponding to the stochastic model studied in this paper is discussed.

2. Model

The mathematical model is a jump process characterised by the state space, the jump rates and the jump transformations. Its purpose is to describe the evolution of particles in a high shear granulation process. The particle vector

$$x = (s_o, s_r, l_e, l_i, p)$$

consists of non-negative internal variables, which are

- original solid volume s_o,
- reacted solid volume s_r,
- external liquid volume l_e,
- internal liquid volume l_i and
- pore volume p.

Note that

$$l_i \leqslant p \quad \text{and} \quad s_o + s_r = 0 \Rightarrow p = 0. \tag{1}$$

Several dependent variables are defined. The particle volume is

$$v(x) = s_o + s_r + l_e + p. \tag{2}$$

The particle radius is (assuming a spherical shape)

$$R(x) = \sqrt[3]{\frac{3}{4\pi} v(x)}.$$

With the assumption that the densities of the liquids and the reacted solid are the same,

$$\rho_{l_e} = \rho_{l_i} = \rho_{s_r}, \tag{3}$$

the particle mass takes the form

$$m(x) = \rho_{s_o} s_o + \rho_{l_e}(s_r + l_i + l_e),$$

where ρ_{s_o} and ρ_{l_e} are input parameters. The porosity is defined as

$$\varepsilon(x) = \frac{p}{v(x)}. \tag{4}$$

The external surface area is (spherical particle)

$$a_e(x) = \pi^{1/3}(6v(x))^{2/3}. \tag{5}$$

The internal surface area is