Computers and Chemical Engineering 75 (2015) 1–13

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

A multi-compartment population balance model for high shear granulation

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ARTICLE INFO

Article history:
Received 17 November 2014
Received in revised form 9 January 2015
Accepted 14 January 2015
Available online 22 January 2015

Keywords:
Granulation
Stochastic weighted algorithm
Compartmental model
Breakage
Coalescence

ABSTRACT

This work extends the granulation model published by Braumann et al. (2007) to include multiple compartments in order to account for mixture heterogeneity encountered in powder mixing processes. A stochastic weighted algorithm is adapted to solve the granulation model which includes simultaneous coalescence and breakage. Then, a new numerical method to solve stochastic reactor networks is devised. The numerical behaviour of the adapted stochastic weighted algorithm is compared against the existing direct simulation algorithm. Lastly, the performance of the new compartmental model is then investigated by comparing the predicted particle size distribution against an experimentally measured size distribution. It is found that the adapted stochastic weighted algorithm exhibits superior performance compared to the direct simulation algorithm and the multi-compartment model produces results with better agreement with the experimental results compared to the original single-compartment model.

1. Introduction

Granulation is a size enlargement process to produce granules with desired properties. It is one of the key processes in the manufacture of fertilisers, detergents and pharmaceuticals. It is usually performed to reduce dustiness, which leads to improvements in powder handling and transportation.

Modelling approaches for wet granulation processes can be separated into two categories: population balance modelling and the discrete element method (DEM). The population balance approach tracks the change in the particle population with time through birth and death processes. For applications in granulation, these processes are usually the coalescence and breakage of particles (Braumann et al., 2007). On the other hand, in DEM, the motion of each particle and droplet is computed simultaneously using Newtonian equations of motion (Cameron et al., 2005). However, by itself, DEM does not consider the aggregation of granules and other processes (Barrasso and Ramachandran, 2014), and it is also usually very computationally expensive.

The current work involves modelling a high shear granulation process using a population balance model through a stochastic modelling framework. Stochastic particle methods are able to simulate a high number of independent particle properties, in the case of granulation, the properties included in the modelling framework are usually solid content, liquid content, as well as porosity (Barrasso and Ramachandran, 2014; Chaudhury et al., 2014; Darelius et al., 2006; Rajniak and Matsoukas, 2013; Oullion et al., 2009; Poon et al., 2008).

Currently, there are two popular stochastic particle methods available in the literature: the direct simulation algorithm (DSA) and stochastic weighted algorithms (SWAs). In basic implementations of the DSA involving coagulation, the particle ensemble may be depleted to the point that there is only one computational particle left in the ensemble and this is avoided by duplicating the ensemble when the particle count falls below 50% (Braumann et al., 2010b). Even then, it is often pointed out that the DSA produces unstable estimates of the concentrations of the rarer particles (Menz et al., 2013; Patterson et al., 2011). Weighted particle methods, or SWAs may be used to counter these problems. In SWAs, each particle is given a statistical weight which is proportional to the number of particles represented by the computational particle. Instead of depleting the particle ensemble, coagulation events in SWAs adjust the statistical weights (Patterson et al., 2011).

These stochastic particle methods are traditionally used to model processes without particle transport, implying that the

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http://dx.doi.org/10.1016/j.compchemeng.2015.01.009
0098-1354/

Nomenclature

a_P	constant for confidence intervals
d	mass fraction for an individual sieve class
e	particle coefficient of restitution
e_{coag}	coalescence coefficient of restitution
e_{l_i}	liquid coefficient of resistance
e_{s_o}	solid coefficient of resistance
e_{s_r}	reacted solid coefficient of resistance
F_c	ratio of normalisation parameters
g	breakage frequency (s^{-1})
H_a	height of asperities (m)
K	coalescence kernel ($m^3\,s^{-1}$)
k_{att}	attrition rate constant ($s\,m^{-5}$)
k_{col}	collision rate constant (m^3)
k_{comp}	compaction rate constant (s/m)
k_{pen}	penetration rate constant ($kg^{0.5}\,s^{-1.5}\,m^{-3.5}$)
k_{reac}	reaction rate constant ($m\,s^{-1}$)
L	number of stochastic runs
l_e	external liquid volume (m^3)
l_i	internal liquid volume (m^3)
M	calculated ensemble property
M_0	particle number concentration (m^{-3})
M_1	first volume moment
M_2	Second volume moment (m^3)
m	mass of particle (kg)
m_{total}	total normalised mass in the network ($kg\,m^{-3}$)
$N_{compartments}$	number of compartments
N_{max}	maximum number of computational particles
N_S	number of sieve classes
n	number of computational particles
n_c	number of copies to make
$n_{impeller}$	impeller speed ($rev\,s^{-1}$)
OF	objective function
P	confidence level
p	pore volume (m^3)
Q_3	empirical cumulative distribution function
R	particle radius (m)
R_{break}	rate of breakage (s^{-1})
R_{col}	rate of collisions (s^{-1})
$R_{droplet}$	number inflow rate of droplets ($m^{-3}\,s^{-1}$)
R_{incep}	rate of inception (s^{-1})
R_{inflow}	rate of inflow (s^{-1})
R_{out}	rate of particle outflow (s^{-1})
r_{pen}	rate of penetration ($m^3\,s^{-1}$)
$r_{reac,e}$, $r_{reac,i}$	rate of reaction ($m^3\,s^{-1}$)
s_o	volume of original solid (m^3)
s_r	volume of reacted solid (m^3)
s_r^*	critical amount of reacted solid (m^3)
t_{CPU}	CPU time (s)
t_f	simulation stop time (s)
U_{col}	particle–particle collision velocity ($m\,s^{-1}$)
U_{imp}	particle–impeller impact velocity ($m\,s^{-1}$)
$V_{droplet,mono}$	volume of droplets (m^3)
$\dot{V}_l$	binder flow rate ($m^3\,s^{-1}$)
V_N	normalisation parameter (m^3)
$V_{reactor}$	reactor volume (m^3)
v	total particle volume (m^3)
$v_{parent,min}$	smallest particle that can break (m^3)
w	statistical weight
Y	number of responses
y^{exp}	responses from experiments
y^{sim}	responses from simulations
z	state of the stochastic particle system

Greek symbols

$\alpha_{daughter}$	breakage; distribution
$\beta_{daughter}$	breakage; distribution
Δt	reactor time step (s)
ϵ	particle porosity
ζ	high-precision solution
η	binder viscosity (Pa s)
η_1	empirical mean of a measured functional
η_2	empirical variance of a measured functional
μ_{dsd}	droplet geometric number mean size (m)
μ_{psd}	powder geometric number mean size (m)
$\nu_{min,max}$	ratio of the biggest to the smallest possible fragment
ν_{max}	maximum fraction of the particle that can break
ρ_{l_e}, ρ_{l_i}, ρ_{s_r}	binder density ($kg\,m^{-3}$)
ρ_{s_o}	material density ($kg\,m^{-3}$)
σ_{dsd}	droplet geometric number standard deviation
σ_{psd}	powder geometric number standard deviation
τ	reactor characteristic residence time (s)
Ψ	parameter for breakage

system is perfectly mixed (Braumann et al., 2010b; Menz et al., 2012). However, in powder mixing process such as high shear granulation, advective or diffusive particle transport should not be ignored. Granulation processes usually proceed in three stages (Iveson et al., 2001): wetting and nucleation, consolidation and growth, and attrition and breakage. The nucleation stage is the process of bringing the liquid binder into contact with the powder and is often regarded as a very important stage in granulation processes (Faure et al., 2001). In the mixer used in this work, not all powder particles are wetted in the same way and the assumption of uniformity breaks down. It is clear this has to be included in the model.

To account for the heterogeneous behaviour of powder mixing processes, several compartmental models have been proposed and these models often involve DEM simulations to gain particle flow data as input to the population balance models (Bouffard et al., 2012; Freireich et al., 2011; Li et al., 2012; Sen and Ramachandran, 2013). However, not much attention is paid in implementing stochastic methods in compartmental models with particle transport. In most of the models, the transport of particles is included as an extra term in the population balance equations (Denis et al., 2003; Li et al., 2012; Maronga and Wnukowski, 1997). Just recently, Menz et al. (2014) presented a sequential modular approach to solve a reactor network with a multi-dimensional population balance model coupled to gas-phase chemistry using the stochastic approach. Irizarry (2012) presented the 'particle bundle flow' method which ensures that particles will not hop across two domains in a single time step. In granulation, the stochastic approach is used by Bouffard et al. (2012) to incorporate particle flow into their two-dimensional population balance model. The main purpose of this paper is to include spatial inhomogeneity into an existing granulation model (Braumann et al., 2007) with multiple compartments. In conjunction with this, a stochastic weighted algorithm (Patterson et al., 2011) which improves numerical stability is adapted to this model. This paper also presents a new method to transport computational particles across different compartments.

This paper is structured as follows. In Sections 2 and 3, the population balance model and compartmental model are described in detail. Section 4 presents the algorithms used to solve the compartmental model, which include an adapted stochastic weighted algorithm that is crucial in providing numerical stability. Sections 5 and 6 assess the numerical issues and convergence in the stochastic