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A new framework for population balance modeling of spray fluidized bed agglomeration

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ABSTRACT

Previous work (Hussain et al. (2013). *Chemical Engineering Science*, 101, 35) has pointed out that the conventional, one-dimensional population balance equation for aggregation can be expanded to accurately reproduce the results of discrete simulations of spray fluidized bed agglomeration. However, some parameters had to be imported from the discrete simulation (Monte-Carlo). The present paper shows how the expanded population balance can be run without importing parameters from the Monte-Carlo simulation. The expanded population balance still reproduces the results of Monte-Carlo simulations accurately, taking into account key micro-scale phenomena (sessile droplet drying, efficiency of collisions), but with much lower computational cost. Required input parameters are just the drying time of sessile droplets (calculated in advance), and the pre-factor of an equation that correlates particle collision frequency with fluidized bed expansion. In this way, the expanded population balance is, apart from autonomous, also (nearly) predictive. Its performance is demonstrated by comparisons with both Monte-Carlo results and experimental data for various operating conditions (binder mass flow rate, gas temperature). Despite formally being a one-dimensional expression, the expanded population balance captures additional properties, such as the number of wet particles and the number of droplets in the system, which are even difficult to measure in experiments.

Introduction

Particulate processes such as crystallization, aerosol formation, precipitation, polymerization, agglomeration, etc. appear in many branches of engineering and science. One of such processes is spray fluidized bed granulation (SFBG) which is widespread in industry because the products produced in a fluidized bed granulator have typical properties such as good flow behavior, excellent wetting and solubility behavior and very low dust content. Furthermore, SFBG offers an optimal choice to enhance the size of the particles by providing a compact design of the apparatus, intensive mixing, high heat and mass transfer rate and simultaneous wetting and drying of particles. Many daily life products such as instant milk, coffee beans, fertilizers, pharmaceuticals, etc. are produced by means of fluidized beds.

In SFBG, particles are fluidized by pumping hot air from the bottom of the granulator. To initiate the aggregation process, liquid binder is sprayed on the particles in the form of small droplets to make them wet and sticky. Particles move in a more or less random manner in the granulator and encounter collisions with each other. Due to collisions, a liquid bridge may be created if particles collide at wet spot/s. The liquid bridge further turns into a solid bridge due to hot and dry air passing through the granulator and an agglomerate is formed, provided the bridge withstands the impact from subsequent collisions. Hence, particles (agglomerates) grow by going through many micro-processes in SFBG. The present work focuses on population balance modeling of the most relevant micro-processes that affect the aggregation kinetics.

On a macroscopic scale, particulate processes such as SFBG are modeled by means of population balance equations (PBEs); see, e.g., Ramkrishna (2000). The one-dimensional (1D) PBE for pure agglomeration in a batch system with a homogeneous

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Nomenclature

a	base radius of spherical cap (m)
A	surface area (m)
$\bar{A}$	mean surface area (m)
B	birth rate (s^{-1})
d	diameter (m)
D	death rate (s^{-1})
e	restitution coefficient
f	frequency per particle (s^{-1})
F	pre factor
h	height (m)
k	mass transfer coefficient (m/s)
M	mass (kg)
$\bar{M}$	average mass (kg)
$\tilde{M}$	molecular weight (kg/kmol)
$\dot{M}$	mass flow rate (kg/s)
n	number density of particles ($1/m^3$)
N	number
$\dot{N}$	number flow rate
$\tilde{N}$	reduced number
P	system pressure (Pa)
P^*	saturation pressure (Pa)
St	Stokes number
t	time (s)
T	temperature (°C)
T^*	saturation temperature (°C)
u	velocity (m/s)
u, v	sizes (volumes) of particles (m^3)
V	volume (m^3)
x	mass fraction (wt%)
Y	moisture content (g/kg)
$\tilde{y}$	molar fraction of vapor

Subscripts

0	at initial time
a	asperities
b	binder
c	collision
coal	coalescence
drop	droplet
dry	dry
drying	drying
exp	expanded bed
fix	fixed bed
g	gas
l	liquid
p	particle
pp	primary particle
pos	position
tot	total
v	vapor
w	water
wet	wet
wd	wet–dry
ww	wet–wet

Superscripts

agg	aggregation
crit	critical
dry	dry
in	inlet
s	sector

Abbreviations

CNMC	constant number Monte-Carlo
CVMC	constant volume Monte-Carlo
MC	Monte-Carlo
PSD	particle size distribution
PBE	population balance equation
PBM	population balance model
SFBG	spray fluidized bed granulation

Greek letters

β	aggregation kernel (s^{-1})
β^*	size dependent part of aggregation kernel depends on structure
β_0	aggregation efficiency depends on β^*
ε	porosity (voidage)
η	wet surface fraction per wet particle/probability of collision at wet surface
θ	constant angle of droplet with particle surface degree
μ	viscosity (Pa s)
ρ	density (kg/m^3)
τ	drying time of a droplet (s)
ϕ	solid volume fraction
ψ	average success fraction due to dissipation of kinetic energy

distribution of particles and using particle volume as the internal coordinate is given by, e.g., Hulburt and Katz (1964) as

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v \beta(t, v-u, u)n(t, v-u)n(t, u)\,du - \int_0^\infty \beta(t, v, u)n(t, v)n(t, u)\,du, \quad (1)$$

where u and v are particle volumes, n is the number density distribution of the particles and β is the aggregation kernel.

The integro-differential nature of the PBE makes the equation difficult to solve analytically. Hence, many numerical schemes have been proposed in the literature to obtain the solution of the PBE (Hounslow, Ryall, & Marshall, 1988; Kumar & Ramkrishna, 1996; Kumar, Peglow, Warnecke, Heinrich, & Mörl, 2006; Kumar, Peglow, Warnecke, & Heinrich, 2008; Litster, Smit, & Hounslow, 1995). Despite the availability of good solvers, a primary challenge in using the PBE for simulation of SFBG is to model the kinetics of the process in the form of an aggregation kernel β. The right choice of $\beta(t, u, v)$ is probably the main and the most difficult part for the application of a PBE to analyze and understand the agglomeration process. Over the years, many aggregation kinetic models have been proposed in the literature; see, e.g., Sastry (1975), Hounslow, Pearson, and Instone (2001), Peglow, Kumar, Warnecke, Heinrich, and Mörl (2006), Abberger (2006, Chap. 24), and Rajniak et al. (2009). However, a model correlating the process conditions and material properties in rather general terms is not yet available.

The aggregation kernel is usually partitioned as a product of two factors, namely the size-independent term and the size-dependent term (see, e.g., Abberger, 2006, Chap. 24; Hounslow et al., 2001; Peglow et al., 2006; Rajniak et al., 2009; Sastry, 1975):

$$\beta(t, u, v) = \beta_0(t)\beta*(u, v). \quad (2)$$

The size-independent part $\beta_0(t)$ can be thought of as a collision/aggregation efficiency and depends on the time, operating conditions, moisture distribution, binder properties, etc. Whereas