Population balance model for quality control of coating processes in fluidised beds

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Introduction

Fluidised bed coating is a technique which is used for the coating of solid particles and is often used in the food and pharmaceutical industry. A fluidised bed coating process consists of three different phases (solid particles, air, and droplets containing the coating material) which all interact with each other in a dynamical way inside a upside down truncated conical reactor (figure 1). The particles are fluidised by heated air that is coming from the bottom of the reactor. While travelling through the bed, the particles and the droplets exchange heat and water with each other, with the air and with the reactor wall. A nozzle placed above the fluidised bed sprays coating material towards the particles in the form of small droplets (diameter ~ 10 to 30 µm). F. Ronsse *et al.* (2005) developpped a dynamic heat and mass transfer model to describe the dynamic interaction between the different phases in the fluidised bed. The theory of population balance modelling was used for modelling the solid phase. The droplets were taken into account via an individual droplet submodel. The model as a whole showed good agreement with experimental thermodynamical data. The model, however, was not able to make detailed predictions about the quality of the coating process (agglomeration effects, spreading of the coating on the particles, etc…) and it had difficulties in predicting airflow (air bubbles and turbulence) . The objective of this study was to develop a new model that is able to accurately predict the quality of the coating process and the coated particles.

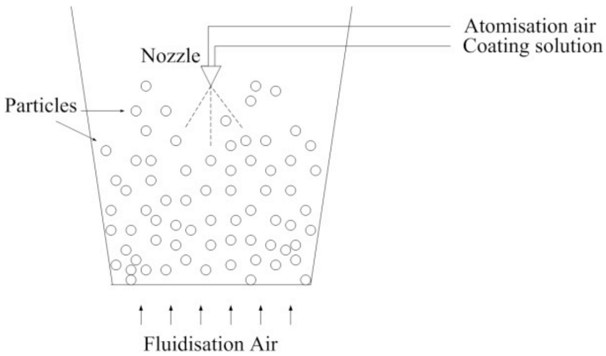

Figure 1. Fluidised bed coating reactor

Nomenclature

ρ	Liquid density $(kg\ m^{-3})$
μ	Viscosity $(kg\ m^{-1}s^{-1})$
σ	Surface tension $(N\ m^{-1})$
d_0	Initial droplet diameter (m)
w_0	droplet initial velocity $(m\ s^{-1})$
Oh	Ohnesorge Number $\left(=\frac{\mu}{\sqrt{\rho*\sigma*d_0}} \quad dimensionless\right)$
Re	Reynolds Number $\left(=\frac{\rho*d_0*w_0}{\mu} \quad dimensionless\right)$

Model

Population balances. In this study both the solid phase and the droplet phase were modelled by means of population balance modelling. In the application of population balances, one is interested in the distribution of particle populations and their effect on the system behaviour (D. Ramkrishna (2000)). The properties of the particles are represented by discrete (e.g. particle size) or continuous variables (e.g. temperature). Two types of variables can be distinguished: external variables, denoting the position of the particle, and internal variables, representing properties associated with the particle. The choice of variables must enable full specification of the rate of change of the particle state and birth and death processes of particles. A fundamental assumption in population balance modelling is that the rate of change of the state of a particle is a function only of the actual state of the particle and local variables of the fluidum. The population balance equation has the following general shape

$$\frac{\partial f_1}{\partial t} + \nabla_x \cdot \dot{\vec{X}} f_1 + \nabla_r \cdot \dot{\vec{R}} f_1 = h$$

The rate of change of the internal coordinates, $\dot{\vec{X}}$, can be interpreted as a motion through an abstract property space with dimension *n*. The rate of change of the external coordinates, $\dot{\vec{R}}$, can be interpreted as a motion through a 3D physical space. The average number density, $\boldsymbol{f_1}$, corresponds to the fraction of particles which have a certain particle state at time *t*. The net birth rate per unit volume of particle state space is represented by *h*.

Reactor. The fluidised bed, in which the particles and droplets move, was modelled as a 2D axisymmetric volume which is divided in conical control volumes. Thermodynamical behaviour (heat and mass transfer) in the fluidised bed was described by the equations developed by F. Ronsse *et al* (2005). A picture of a fluidised bed reactor is presented in figure 1. A flow chart of the model can be found in figure 2.

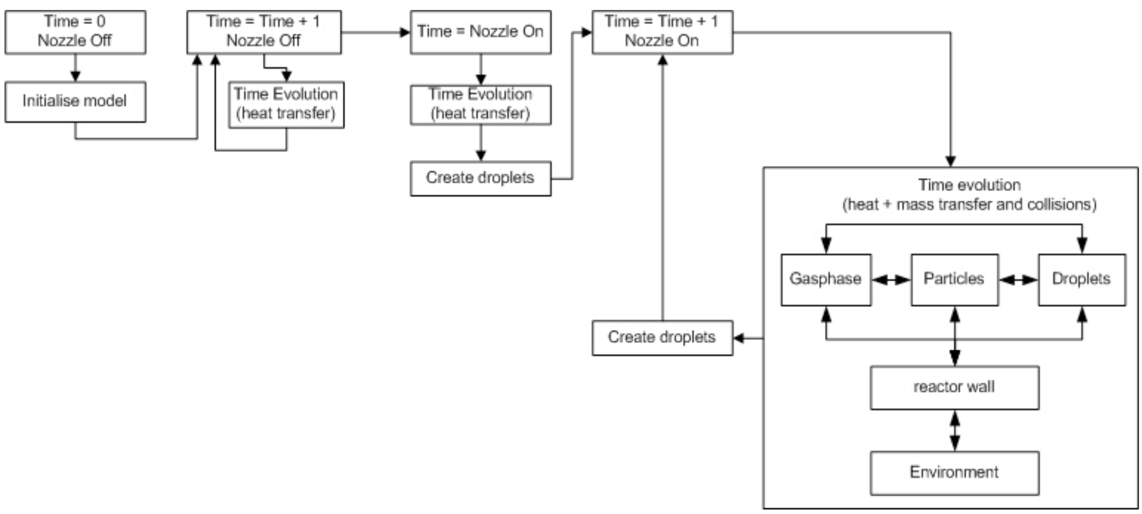

Figure 2 . Flow chart of the model.

Droplets. In the model, distinction was made between three different kinds of droplets.First, there are the droplets that move freely in the fluidised bed. They are characterised by temperature, velocity and diameter. The droplets move through the fluidised bed and interact with the air, the particles or the wall. The droplets originate from the nozzle with a predefined statistical distribution (diameter-, velocity- and starting angle distribution). Collision of the droplets with the particles can cause two possible events (1) spreading of the complete droplet on the surface of the particle or (2) splashing, *i.e.* part of the droplet spreads over the surface, the other part of the droplet bounces back and breaks up into secondary droplets which then move through the fluidised bed. Splashing will occur when the variable K in the relation

$$\mathrm{K} = \mathrm{Oh}\ Re^{1.25}$$

exceeds 57.7, whereas K lower numbers lead to complete deposition of the liquid on the surface (Mundo 1994). Splashing was not taken into account for droplets colliding with the reactor wall. Droplets that move outside the boundaries of the region of interest are also a source for spray loss.

A second series of droplets are the ones that have spread of the surface over the particles. They are characterised by temperature and height (figure 3.a).

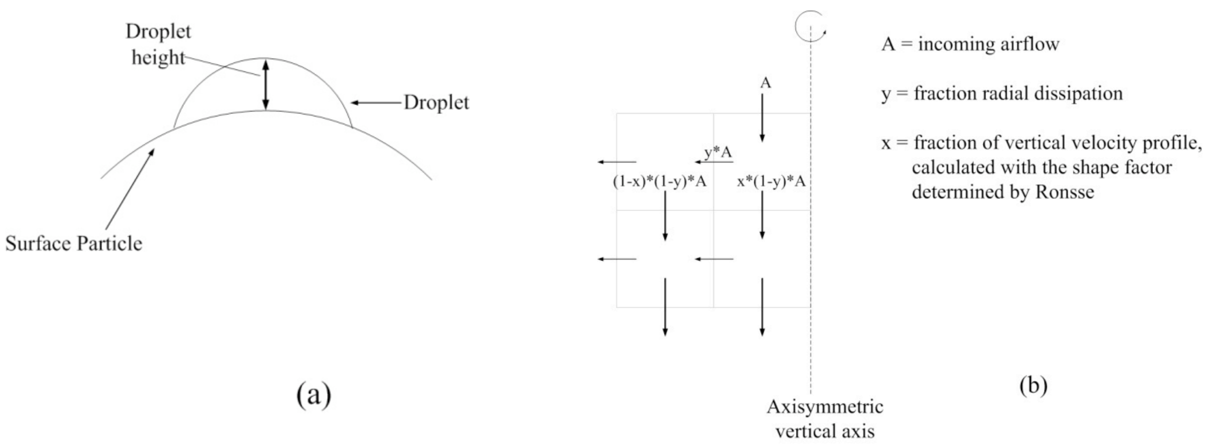

Figure 3. (a) Droplet on particle, (b) Modelled airflow pattern

The surface of each particle is divided into a certain number of zones on which droplets can collide. The surface of each zone is chosen in such a way that interaction between droplets that have collided on adjacent zones on the surface of the particle cannot interact with each other. This surface was determined by calculating the maximum spread a droplet can have. This is a reasonable assumption since there are a few hundreds of zones. Assuming typical fluidised bed coating conditions, the probability that two adjacent zones are both wet at the same time is thereby relatively small, as well as the probability that a zone is still wet when another droplet is colliding on that zone. The position of these droplets is determined by the position of the particle on which they reside.

Third, droplets that have collided with the reactor wall are to be considered. They are also characterised by temperature and height.

Particles. The particles are characterised by temperature and location in the fluidised bed. The surface of the particles is, as already stated before, divided in a certain number of zones. For each zone a log of two variables is kept: (1) the wetting and (2) the height of the deposed coating material.

The first variable*, i.e.* the local wetting of the particle, can be used to model agglomeration of the particles. If two particles collide with each other and if the contact area consists of two dry zones, no agglomeration will take place. On the other hand, if one of the particles collides with a wetted zone on another particle, agglomeration can occur with a certain probability which is a function of collision frequency, the probability that at least one of the contact zones is wet and the adhesion probability which represents the liquid bridge strength.

The second variable is needed to determine the thickness of the coating and the uniformity of the coating on the particle, two important quality parameters of the coating process.

Particle Movement. The positions that particles can take in the bed were discretisized based on the hexagonal closest packing of spheres. This means that particles will move in a lattice. For each position in the lattice, determination to which control volume that position belongs is needed in order to be able to calculate the thermodynamical behaviour. During the evolution of the system, an occupancy log for each position will be kept. The occupancy log enables to introduce air bubbles in the fluidised bed and prevents that two or more particles will cohabit a certain position in the bed.

Gasphase. Unlike in the work of F. Ronsse *et al.* (2005), the airflow in the fluidised bed was not modelled based on the gas velocity profile of a free axisymmetric jet (Schlichting *et al.* (2004)). The reason is that this velocity profile does not take into account any side effects at the wall, nor does it leave space to introduce air bubbles and turbulence, while it demands complex calculations for the air flow rates. Instead, a hypothetical airflow pattern was built based on conservation of mass in each control volume, airflow of the nozzle, airflow of the fluidisation air and a shape factor of the airflow from the nozzle determined by F. Ronsse *et al.* (2005) (figure 3.b).

The advantages of the use of this airflow pattern are: (1) The amount of radial dissipation of the airflow coming from the nozzle can easily be altered to fit the real decrease of the vertical component of the velocity, (2) determination of the air velocity profile from the airflow rates by means of interpolation, (3) turbulence and side-effects can easily be fit in the model in the future by introducing a random factor in the airflow.

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