

## Computational modelling of air suspension coating for bioencapsulation

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### INTRODUCTION

Air suspension coating is a common technique to encapsulate bioactive ingredients including pharmaceutical drugs, micronutrients and live micro-organisms, e.g. probiotics. A uniform coating is critical to maximise the biological functionality and shelf-life of the bioactive ingredients. The ability to apply a uniform coating within a minimum time is essential to minimise the loss of activity of the bioactive ingredients. However, air suspension coating is a complicated process involving control of over 20 variables, which affect the coating quality (Werner 2007). Many trial-and-error experiments are required to work out optimum coating operation, which is often a very costly exercise.

Here we describe a computational model using a coupled Discrete Element Method (DEM) and computational fluid dynamics (CFD) approach. Extensions to this model included simulation of the individual aerosol spray droplets, as well as simulation of collisions and spreading of spray droplets after impact with particles. To our knowledge, this is the first report of such a model that is able to track individual particle and spray droplet movement inside the fluid bed, map spray coating deposition on each particle surface and calculate the overall coating uniformity across the fluid bed. The application of the model is demonstrated using a top spray fluid bed coating process.

### MATERIALS AND METHODS

DEM is a Lagrangian approach for modelling granular systems, in which the positions and velocities of every particle is individually resolved. Particles in this system were simulated as frictional spheres, with a frictional coefficient of 0.5 and a density of 1000 kg/m<sup>3</sup>.

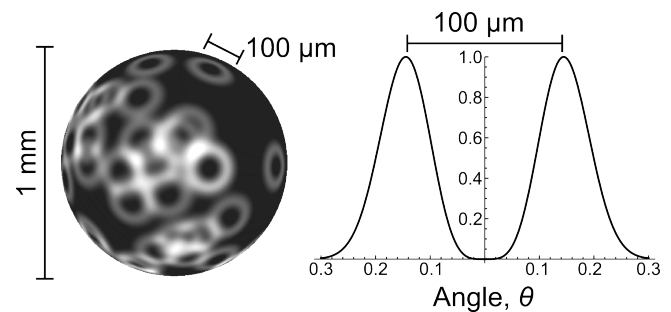
The CFD component used a formulation for incompressible gas flow in a porous media, first given by Kafui et al. (2002). The flow equations were discretised onto a regular Cartesian grid and solved using a variation of the pressure correction method (Hilton 2010). Turbulence was included using the WALE large eddy simulation method (Nicoud 1999). Drag forces between the gas and particles were used to dynamically couple the gas and particles. The coupling methodology has been applied and validated for a range of industrial gas-particle systems including fluidised beds (Hilton 2010), pneumatic conveying

(Hilton 2011a) and hopper discharge of fine powders (Hilton 2011b).

Spray droplets in the system were modelled as individual Stokesian particles. At each simulation time-step, the paths of each droplet were checked for collisions with particles. If a collision was detected, a splash pattern from the collision was mapped onto the surface of the particle. The splash pattern can be of various forms depending on the materials properties of the solid particle and spray droplets (e.g. surface tension and viscosity, etc.). In this study, the splash pattern from an individual droplet was modelled as a ring with a diameter of 100 µm based on detailed work by Karlsson et al. (2011). This ring-shaped splash pattern was modelled using a 'split Gaussian' function of the form:

$$g(\theta) = \exp\left(-\frac{\theta^k}{a}\right) (1 - \cos(2\theta))^2 \quad (1)$$

This function (normalised) is shown on the right hand side of Fig. 1. The left hand side of this figure shows an example of the coating built up on the surface of a particle from a series of randomly oriented splashes. Each ring on this particle is approximately 100 µm in diameter.



**Figure 1 : Coating distribution from multiple droplet impacts on 1 mm particle (left). Spherically symmetric coating function, Eq. 1 (right)**

The novel computational algorithm behind this mapping was developed specifically for this project. The algorithm is based on spherical harmonic expansions. These are defined over the surface of a sphere,  $f(\theta, \phi)$ , as:

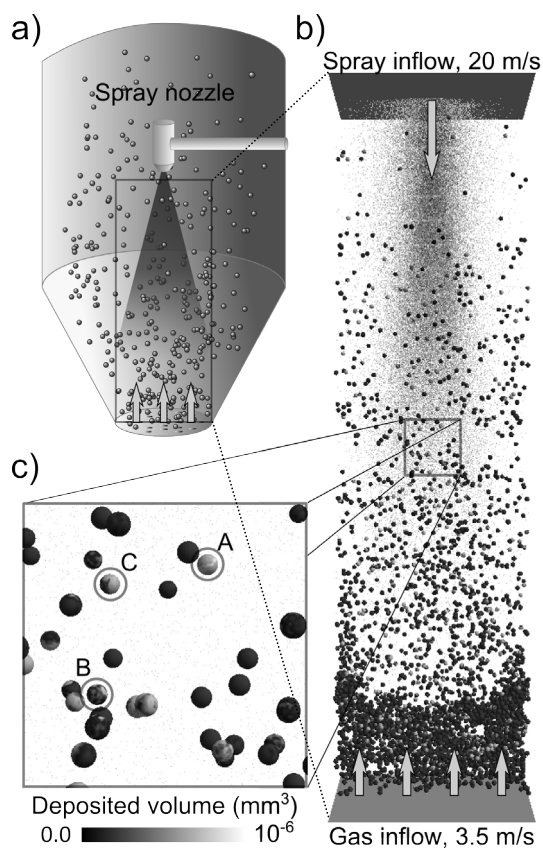
$$f(\theta, \phi) = \sum_{l=0}^N \sum_{m=-l}^l f_l^m Y_l^m(\theta, \phi) \quad (2)$$

where  $Y_l^m(\theta, \phi)$  are the spherical harmonic functions. A set of real coefficients  $f_l^m$  is stored for each particle.

The use of spherical harmonics allows circularly symmetric splash patterns to be efficiently mapped onto the surface of particles. Furthermore, spherical harmonics have a number of useful properties allowing metrics for the roughness (value: 0-perfect coating; 1-worst coating), distribution and volume of coating material to be rapidly evaluated.

## RESULTS AND DISCUSSION

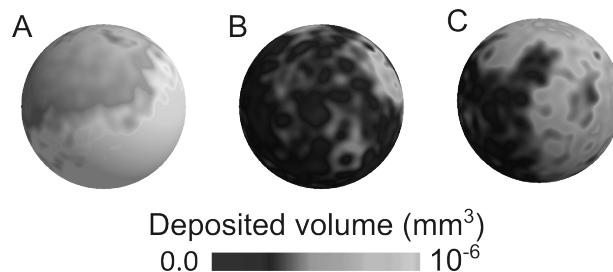
A schematic diagram of a top spray fluid bed coating set-up is shown in Fig. 2a. This consisted of a 15 cm tall domain with approximately 7500 particles of  $1.0 \pm 0.1$  mm. This was fluidised into a dilute gas-particle mixture by applying a gas inflow at 3.5 m/s at the base of the domain. Spray was injected into the top of the system at 20 m/s, with droplets of  $30 \pm 10$   $\mu$ m diameter distributed in a vertical cone with half-angle  $15^\circ \pm 2^\circ$  at a flow rate of 0.5 L/h.



**Figure 2 : (a) Schematic diagram of top spray fluid bed coater, with the simulation region shown as a rectangle; (b) Snap shot of the simulation at  $t = 10$  s; (c) Close-up of individual particles. Particles are shaded by coating distribution over their surfaces.**

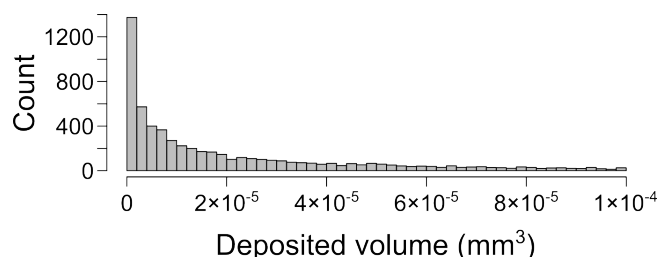
A snap shot during the coating process after 10 s of operation is shown in Fig. 2b. The lower part of the bed exhibited the typical bubbling behaviour found in fluidised beds. The upper part of the system contained a dilute mixture of gas and the particles that collided with the injected spray. Fig. 2c shows a close-up of the coating distributions over a section of the

particles. As an example of the high level of detail obtainable, three particles from Fig. 2c are shown in Fig. 3. The coating on particles A and C are highly non-uniform, whereas the distribution over particle B is more homogeneous. This is reflected in the roughness value obtained for these three particles, with A: 0.022, B: 0.004 and C: 0.046, showing that particle C has the most uneven distribution.



**Figure 3 : Detailed coating distributions for three particles, identified in Fig. 2c.**

The method allows metrics such as the coating volume on particles over the entire bed to be determined. A histogram of the deposited volume is shown in Fig. 4. This is heavily weighted towards zero, showing most of the particles in the bed have received no coating by 10 s, in agreement with Fig. 2.



**Figure 4 : Histogram of the column of coating material deposited on particles in the bed.**

## CONCLUSIONS

This computational model allows the evolution of coating distributions over the bed to be resolved at the individual particle level, which would be unobtainable by any other means. This model provides a fully integrated tool to optimise parameters required (hardware design, set up and processing conditions) to achieve optimum coating quality and efficiency without the need for costly experimental trial runs.

## REFERENCES

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