Modelling of Single Droplet Drying and Morphology Evolution using Meshfree Simulation Methods

W. Säckel*, F. Keller, U. Nieken
Institute of Chemical Process Engineering, University of Stuttgart, Germany
saeckel@icvt.uni-stuttgart.de and nieken@icvt.uni-stuttgart.de

Abstract

Spray drying is a widely used industrial process. However, in many cases process parameters need to be evaluated empirically in order to achieve the desired product properties. Common drying models of single droplets typically picture a spherical symmetric geometry and thus model radial distributions of a quantity. These are calculated according to effective transport parameters, which need to be fitted to experiments. The substructure and its morphology and properties inducing the transport behaviour cannot be predicted. However a more detailed insight into the drying process is very desirable.

The present contribution introduces a novel approach for single droplet drying models based on the meshfree method Smoothed Particle Hydrodynamics (SPH). In this technique the continuum is approximated using interpolation points, so called particles, which can move independently from each other according to a Lagrangian viewpoint. Due to the particle-based point of view meshfree methods are capable of handling phenomena occurring in morphology evolution like large material deformations and fractures.

In a first model the Smoothed Particle Hydrodynamics approach is validated in comparison to a common grid-based model using finite differences. The implementation of Nusselt and Sherwood boundary conditions requires more effort in the SPH model, when surfaces of arbitrary shapes need to be regarded. The conversion of area based fluxes into volume/mass based ones can be undertaken using the CSF approach. In a next step the model was enhanced to fluid dynamics incorporating the motion of an incompressible Newtonian liquid using a predictor-corrector projection method. Solids are modelled as a different particle/point class using a rigid body approach. Surface tension and wetting are implemented using forces between interpolation points. By applying different forces between different phases a wetting behaviour can be parameterised. Using this technique the first drying period regarding a suspension can be modelled in principle. In order to simulate the second drying period, where transport through a porous crust is taking place, diffusive vapour transport through the gas phase was implemented and tested for a porous structure containing fixed solids, a liquid and a gas phase.

Numerical results showed that the SPH approach is able to achieve the same results as grid based methods, when Nusselt and Sherwood boundaries are applied and radial distributions are calculated. Moreover the geometries can be arbitrarily shaped due to the CSF approach. Simulations for the drying of a suspension have been undertaken in a two-dimensional study. A variation of physical properties, the wetting behaviour and the size of solid particles, leads to different morphologies inside the droplet. Subsequently simulations of diffusive vapour transport and the receding liquid interface inside a fixed, porous structure were undertaken. The approach is capable of modelling the second drying period, too, so that a future drying model of a droplet can regard both drying periods on a detailed length scale.

The approach shows reasonable results and underlines the methods ability to study morphology evolution. However, the method is relatively new for this application, thus requiring further research. In the near future studies shall be undertaken using a finer resolution. A future perspective lies in multi-scale simulations, which may combine the potential of detailed approaches like the one presented here with the computational efficiency of coarser approximations.

* Corresponding author: saeckel@icvt.uni-stuttgart.de