Conference abstract LPES03

LBM Simulation of Pharmaceutical Particles in Laminar Air Flows

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Sci Pharm. 2010; 78: 564 doi:10.3797/scipharm.cespt.8.LPES03

Porous particles are present in various technical applications as well as in the field of medical treatment. The latter involves amongst others the production of highly porous and respirable particles to serve as solid inhalants and substitute intestinal medication. One promising way of manufacturing such biotechnological therapeutic agents is the lyophilisation of single drops or sprays – a complex technological approach that still requires research and process layout.

Besides experiments, numerical flow simulations are capable of providing insight into the physics that influence the transport and mass and heat transfer related to porous particles. Predicting the corresponding multiphase flows requires knowledge of the behaviour of porous particles in comparison to solid ones. By performing fully-resolved direct numerical simulations (DNS) of single complex particles correlations between particle properties and their fluid dynamic behaviour are to be established.

In this work, the Lattice-Boltzmann method (LBM) is used to simulate the flow around virtual lyophilisates and to calculate drag, lift and torque coefficients [1]. A future aim is to perform simulations of the sublimation process of frozen spray droplets which are numerically realized in form of heterogeneous particles. In a first approach, the highly-porous lyophilisates are modelled by creation of simplified aggregates consisting of spherical primary particles (Fig. 1, left). This base structure is covered by a mutable hull-shaped matrix to represent the second phase of the frozen solution of the medical agent which is shrinking due to sublimation (Fig. 1).

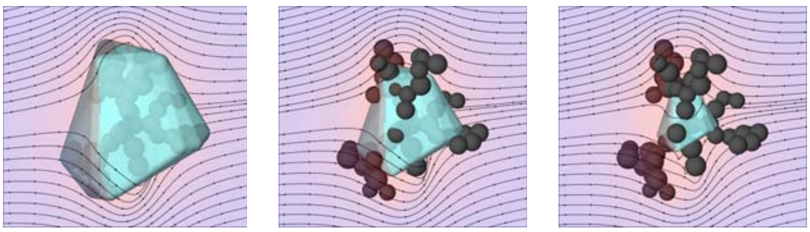

Fig. 1. Flow around a heterogeneous particle with shrinking second phase

This work was supported by Deutsche Forschungsgemeinschaft (DFG grant SO 204/36-1, SPP 1423).

[1] Hölzer A, Sommerfeld M. Lattice Boltzmann simulations to determine drag, lift and torque acting on non-spherical particles. Comput Fluids. 2009; 38: 572–589. doi:10.1016/j.compfluid.2008.06.001