# Modeling Lagrangian sub-micro particles flow and deposition using LES

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## Abstract

Flow and deposition of air-born particles as well as medial sprays has been subject to computational as well as experimental research at the author's department for several years. We developed numerical model of particle deposition with full breathing cycle [1]. Lately our focus has been drawn to small micron and sub-micron particles and particles of irregular shape. OpenFOAM and its lagrangian classes has been extended to take into account forces important for small particles. Except Brownian diffusion it is namely van der Waals force between particles. This model has been coupled with lagrangian model for fiber transport and deposition. All these models has been implemented as an extension of *intermediate kinematic* lagrangian class.

For the van der Waals force collision model from spray class has been adopted to take into account attractive and repulsive forces. Trajectory collision model of Nordin [2] has been adopted to calculate the particles proximity in a time step. In a given range of distance van der Waals force has been applied on a particle couple. Although it is difficult to validate the model against experiments, computations of porous particle deposition in a airways are currently in progress to prove the concept.

To take into account non spherical particles, model for small fibers has been implemented. For each lagrangian particle its directional vector as well as torque and rotation is computed (following approach of Iacono [3]). The drag coefficient is computed with respect to the fiber orientation in the flow-field [4].

The resulting model is used for computation of fibrous particle deposition in the human airways. Small fibers tend to penetrate deeper into the lungs compared to the globular particles, hence the health risk is higher. Another application for the developed model is the computation of deposition of porous particles of micron size. These particles are used for drug delivery. It has been found that the flow pattern of these particles is influenced by non-sphericity as well as van der Waals forces. To take into account the effects of the drug release from the porous particle and interaction with the moist air in the human airways, tortuosity model has been implemented into the *intermediate thermo* class in lagrangian model. This thermo model has been also extended to take into account Soret effect of directional force on particles from the temperature gradient.

Results from these computation are going to be validated against the PDA/LDA measurements on a stand currently build at our laboratories.

**Key words:** aerosol, Lagrange particles, van der Waals, fibres

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