Eulerian modeling of polydisperse aerosol deposition in a realistic cast of the human upper respiratory tract

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Inhaled aerosol droplets may deposit in the human respiratory tract by means of inertial impaction, interception, gravitational settling or diffusion. The importance of each of these mechanisms depends on the droplet size as well as on the flow conditions. Nano-sized droplets may deposit due to diffusion, whereas micron-sized droplets are more likely to deposit through inertial drift. To understand the impact of an inhaled aerosol on the respiratory system it is important to model these mechanisms accurately.

We adopt a sectional, compressible, internally mixed aerosol model for the description of the transport and evolution of a polydisperse aerosol (Frederix *et al* 2016). This model was shown to give accurate predictions for non-isokinetic aerosol sampling, driven by inertial droplet drift. Here, we extend the model to include droplet diffusion based on the Stokes-Einstein Brownian diffusivity model. Also, we develop a wall boundary condition to capture the deposition flux due to both Brownian motion and inertial drift.

Validation of the Eulerian aerosol model is based on the simulation of the evolution of a polydisperse aerosol in a bent pipe. The aerosol droplets, spanning a large size range $10^{-9} < d < 10^{-5}$ m with d the droplet diameter, deposit with a size-dependent deposition efficiency η. As a function of droplet size, η attains the familiar 'V-shape' curve, indicating that small droplets deposit due to diffusion and large ones due to inertia. In between these two regimes, there exists a droplet size for which deposition is at its minimum. Fig. 1 shows our predictions of η in two bent pipe geometries (Reynolds number Re=100, Dean number De=38 and Re=1000, De=419). We find good agreement with the predictions of a straight pipe diffusion deposition model (Ingham 1975) and an inertial deposition model (Cheng and Wang 1981), demonstrating the feasibility of the Eulerian approach. Enhanced deposition is shown for Re=1000 with respect to Ingham's predictions, illustrating the increased accelerations at elevated Reynolds number.

The model is also effective for the simulation of aerosol transport and evolution in a realistic cast of the human respiratory system. In (Nordlund *et al* 2016) an experimental study was presented of aerosol deposition in a human lung cast. Fig. 2 shows predictions of the deposition in this geometry using our model, for a monodisperse aerosol consisting of water droplets with size d=10µm. For these droplets, inertial deposition is dominant. Deposition hot-spots show near the first and the second generation branching. Droplets with, a relatively large momentum, drift away from carrier gas streamlines and impact on the inner surface of the cast. We compare experimental data against predictions of our Eulerian model for both the diffusion and inertial regimes.

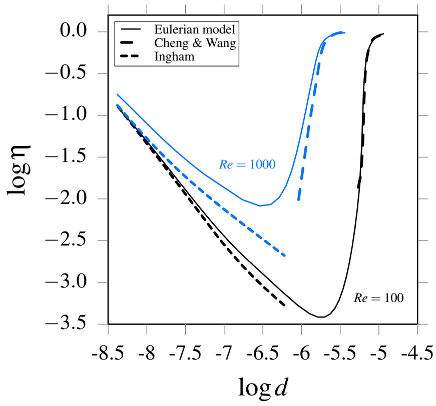

Figure 1. Predictions of bent pipe deposition efficiency for Re=100 (black) and Re=1000 (blue).

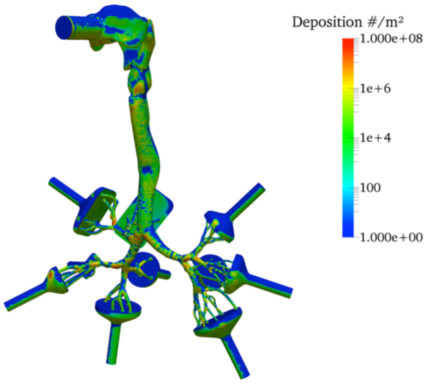

Figure 2. Deposition of d=10 µm water droplets in a realistic lung cast geometry.

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