Aerosol dynamics model for the hygroscopic growth of NaCl particles and resulting deposition in the human lung

R. Winkler-Heil, L. Pichelstorfer and W. Hofmann

Department of Chemistry and Physics of Materials, University of Salzburg, Salzburg, 5020, Austria
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Presenting author email: Werner.Hofmann@sbg.ac.at

Upon inhalation, hygroscopic particles will absorb water vapor from the warm and humid air in the human respiratory tract. Due the resulting increase in diameter, accompanied by a change of the density, particle deposition patterns in the human lung differ from those of non-hygroscopic particles of the same initial size. Since most inhalation experiments with hygroscopic particles in human volunteers were conducted with NaCl aerosols, the growth of these aerosols are simulated in the present study.

In a previous modeling effort, the hygroscopic growth model of Ferron *et al* (1988) was implemented into the stochastic asymmetric lung deposition model IDEAL (Winkler-Heil *et al*, 2014). In the present study, hygroscopic growth in the IDEAL lung model is described by the recently developed aerosol dynamics model ADiC (Pichelstorfer and Hofmann, 2015). The ADiC (Aerosol Dynamics in Containment) model simulates coagulation, phase transition, and heat/vapor transport. Deposition of inhaled particles in human lung airways is simulated for Brownian motion, inertial impaction and gravitational settling. Because of the stochastic nature of the deposition model, each inhaled particle follows a different path during inhalation and hence experiences a different growth.

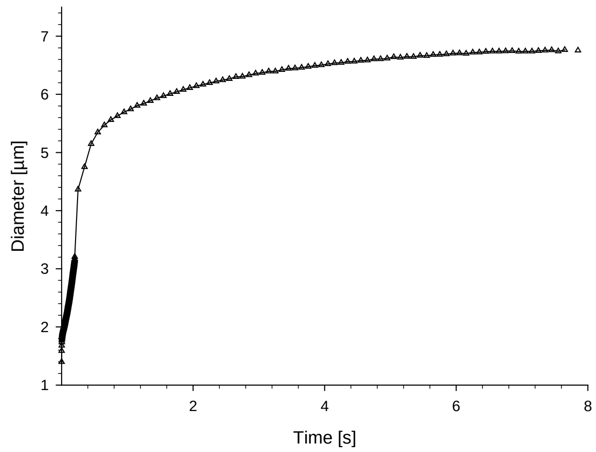

Figure 1. Hygroscopic growth of 1.4 µm geometric diameter NaCl particles during an 8 s breathing cycle.

Diameter growth curves of submicron and micron-sized NaCl aerosols as a function of time during a full breathing cycle were calculated for defined breathing parameters. For example, the growth curve for a NaCl particle with an initial geometric diameter of 1.4 µm, equivalent to initial aerodynamic diameter of 2.1 µm, inhaled through the mouth is plotted in Figure 1 for a flow rate Q = 250 $cm^3\ s^{-1}$ and a tidal volume V_T = 1000 cm^3, assuming symmetric breathing with no breath-hold period (Anselm *et al*, 1990). The plotted curve represents an average growth curve based on a few thousand individual growth curves. Diameters increase sharply in the first bronchial airways and continue to grow even during exhalation.

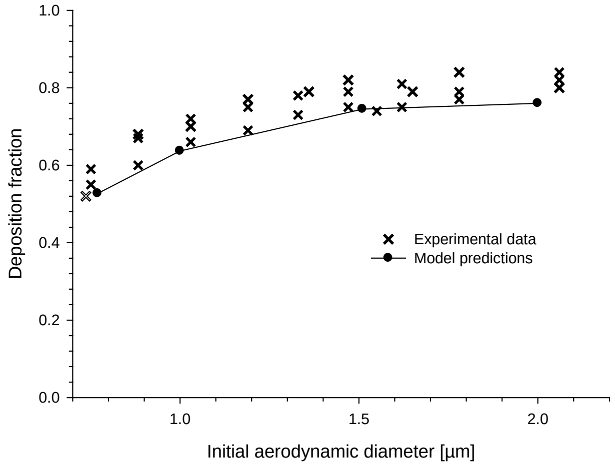

Figure 2. Comparison of predicted total deposition fractions for orally inhaled NaCl aerosols with the experimental data of Anselm *et al* (1990) and Gebhart *et al* (1990) as a function of initial aerodynamic diameter.

For model validation, simulation results are compared in Figure 2 with the experimental total deposition data of Anselm *et al* (1990) and Gebhart *et al* (1990) for three subjects inhaling dry monodisperse NaCl aerosols through a mouthpiece for Q = 500 $cm^3\ s^{-1}$ and V_T = 1000 cm^3. The comparison between predicted and measured total deposition fractions for initial aerodynamic diameters, ranging from 0.3 to 2.0 µm, indicates good agreement.

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