Dynamics of highly concentrated, fresh aerosols during inhalation

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To assess health risks due to aerosol exposure, information on local particle as well as vapour deposition is crucial. Airborne particles that contain volatile substances are, in terms of mass transport, permanently interacting with the surrounding gas phase. Therefore, reducing aerosol dynamics to particle-particle interaction is not appropriate in many cases. While coagulation is basically a function of particle number and shape of the size distribution, phase transition also strongly depends on energy balances and composition of particle and vapour.

To simulate aerosol dynamics of a fresh and highly concentrated aerosol within the human respiratory system, we assumed that the incoming aerosol is in thermodynamic equilibrium with its surrounding. This assumption is necessary to assess the initial microscopic particle composition. Then aerosol dynamics, including coagulation, heat and vapour transport between the particulate and the vapour phase, and between the system boundary and the vapour phase, as well as phase transition, were computed. The effects of coagulation and phase transition as well as the superposition of both processes on the initial particle size distribution are depicted in figure 1, where phase transition implicitly shows the effect of heat and vapour transfer on the aerosol.

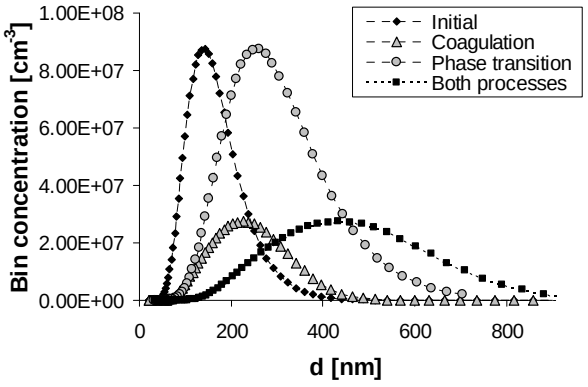

Figure 1: The influence of coagulation and phase transition on the initial particle size distribution.

As an example, we chose to simulate the evolution of a cigarette smoke particle size distribution measured by Ingebrethsen (2011). Further inputs are experimentally determined particle and vapour composition (Davies and Vaught, 2003; Lipowicz and Piadé, 2003). The initial particle size distribution has a concentration of 1.54 x 10^9 particles per cm^3. Its shape is lognormal with an average particle diameter of 150 nm and a geometric standard deviation of 1.44. Initial vapour humidity was assumed to be 75% in case of water and 7.9% in case of nicotine. Based on these assumptions initial water and nicotine fractions were computed for the particulate phase as a function of particle diameter.

The most important effect in the oral region is coagulation. Within a puffing period of 2 s and a subsequent 1 s breath hold, particles below 100 nm are almost reduced to zero, whereas particles larger than 250 nm are newly formed. Furthermore, the total particle concentration is reduced by about 70% from 1.54 x 10^9 cm^{-3} to 5.2 x 10^9 cm^{-3}.

Phase change strongly depends on the speed of water vapour transport from the system wall towards the vapour and on the removal of latent heat which is produced by condensation of water vapour on the particle surface. In the present simulation, phase change effects coagulation by a) reducing the diffusivity of the particles and by b) widening the particle size distribution. The reduced diffusivity is caused by the increasing particle diameter. This reduces thermal coagulation which was found to be the biggest contributor to total coagulation. On the other hand, phase transition widens the size distribution since the growth factor increases with increasing particle diameter. This has a positive effect on the thermal coagulation rate. The simulated net change of coagulation by phase transition is in the order of a few percent of the initial particle concentration.

Note that coagulation, phase transition and heat and vapour transport show strong interactions. Coagulation affects phase transition by changing particle composition particle number and the shape of the size distribution. Phase transition strongly depends on the supply of condensable vapour and the removal of latent heat. Heat and vapour transport also determines whether and where volatile substances are deposited.

This aerosol dynamics model, which in principle can be incorporated into any deposition model, will be implemented into the stochastic deposition model IDEAL (Koblinger and Hofmann, 1990), considering dilution, deposition, coagulation and phase transition.

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