Introduction of a simple Markov chain particle growth model

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For the simulation of coagulation simple models can reproduce the qualitative behaviour of the particle size number distribution of nanoaerosols. A simple Markov chain model has been implemented with a Mathcad® simulation and a comparison with the nodal GDE code of Prakash *et al.* (2003) has been made.

The Markov Chain Model makes use of the transition probabilities and allows for growth or decay of particles for the whole particle size distribution. The advantage in the simple Markov chain is that only the probability matrix and the initial concentration is necessary to calculate the following state. The probability matrix can be simplified further by taking the coagulation constant. The preceding size distribution is independent due to the Markov chain relation. Each state as a function of time can be gained by a matrix potency (Durett 1999, Heiden et al. 2004).

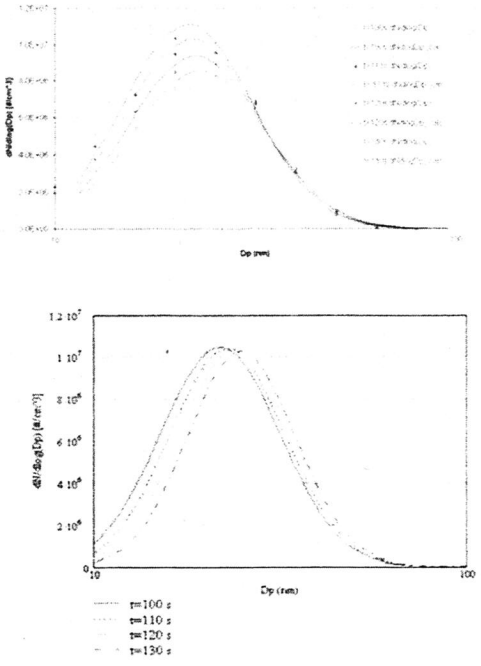

Figure 1. The figure above shows a simulation with the nodal GDE code (Prakash *et al.* (2003) that one below the Markov chain model presented for the same initial state (t=100s).

The application of the Markov chain can be imagined as stochastic process where the particles enter in a flow through the matrix. Primary particles enter and build small aggregates. The primary particles "diffuse" from smaller to bigger aggregates, till they leave at the upper end of the observation window. In the simplified case the growth is described by the diagonal and the above diagonal elements only.

The result of the comparison of the Markov chain model and the nodal GDE code of Prakash *et al.* (2003) is shown in Figure 1. Only coagulation was investigated. The nodal GDE code begins with a monodisperse aerosol, which was initialized with 10 nm and a particle number concentration of 10xE8 particles/cm^3. The self preserving size distribution is reached after 113 s. The Markov chain model is started for synchronization at the same values of the logarithmic size distribution for 100 s. There can be seen a different evolution of the particle diameter with the total number concentration approximately the same for both cases. As Friedlander (2000) states, the experiments and the theory show qualitatively different shapes for tobacco smoke. The theoretical results are similar to the nodal GDE code shown here whereas the Markov chain model comes nearer to the experiments.

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