Binary aerosol droplet formation

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One of our main goals in this work is to study the evolution of the aerosol drop size distribution and the droplet concentration distribution from the water/glycerol vapour mixture. A theoretical analysis of binary droplet formation from a water/glycerol vapour mixture has been performed using a "1.5"-dimensional population balance model to simulate the evolution of the aerosol drop size distribution as well as the mean droplet concentration. The simulation includes the relevant mechanisms nucleation, condensation, evaporation and coagulation.

The simulation model was developed and implemented in the commercial solver PARSIVAL. The self-adaptive numerical algorithms in PARSIVAL are based on the Galerkin h-p (h-p: Variable grid - variable order) method and a temporal discretization of Roth's type (Wulkow et al., 2001).

As expected, from these simulation results it can be seen that nucleation and condensation are strongly affected by the supersaturation. The properties of the droplets are investigated at different vapor compositions. At a higher glycerol concentration in the vapor despite higher nucleation rates larger droplet sizes evolve compared to low glycerol vapor pressure. The evolution of the mean droplets composition starts from almost pure glycerol, is then reduced quickly, passes a minimum before, finally increasing again towards equilibrium composition. Furthermore, the final mean droplet size depends on the mass of vapor at a constant vapor composition of water/glycerol.

The influence of the mechanisms in determining the droplet size is an important focus. At the beginning of the process, aerosol nucleation is playing a dominant role, with rather small droplet growth rates. Later on, the condensation process becomes more and more important and due to the increasing number of droplets and growing particle surface the condensing mass increases rapidly and the mean droplet size significantly increases. The coagulation process is becoming significant even later than the condensation. With severe reduction of the number of droplets coagulation leads to an even faster growth of droplet sizes.

However traditional dynamic simulation methods are at a disadvantage when modeling more than one internal variable, whereas. Monte Carlo methods easily can be extended to a multidimensional case. Monte Carlo simulation is based on the use of a particle ensemble representative for the whole system in order to calculate the properties of the system. Here we use event-driven Monte Carlo algorithm with a stepwise constant-volume method formulated for simultaneous nucleation, condensation and coagulation (Maisels et al., 2004). By using event driven time evolution, the problem of choosing a correct time step is removed. The accuracy of the Monte Carlo solver depends on the number of simulation particles. The droplet number changes according to the chosen mechanism. At each step of the simulation a mechanism is selected with a probability that is directly calculated with the rate of the three processes. The nucleation and coagulation processes result in increases or decreases of the drop concentration, respectively. However, condensation results in surface growth but does not effect the total drop number concentration. When the droplet number in the simulation volume increases or decreases by a factor of two of its initial value, the simulation volume is halved or doubled, respectively.

A systematic validation of the Monte Carlo algorithm with respect to simulation parameters (ensemble size, integration step size etc.) will be presented. Subsequently, a comparison of droplet size distributions and droplet composition resulting from Monte-Carlo and 1.5D-population balance, respectively, will be given. Furthermore, a parameter study using the Monte Carlo technique shows impressively the advantage of this new algorithm.

When nanoparticles are present in a moving fluid, they will be transported by the fluid. Nanoparticles can move in and out of fluid parcels and their location will differ from those of the fluid parcels due to random/Brownian motion. Thus, in future studies a method which allows combing Monte-Carlo based PBE modeling with CFD model will be developed (Kruis et al,. 2012).

The measurement of the particle size of the aerosol is by light scattering. A liquid mixture of glycerol and water is evaporated by heating and then condensed by cooling, thus the aerosol is produced. The experimental procedure used for the formation is designed and built. For the measurements a goniometer with a He-Ne laser is selected. Before measurement of the aerosol many preparation measurements are carried out to check the converted structure. Subsequently, the measurements with different parameters can be performed. Finally, the scattering intensity of the droplets is evaluated and compared with the theoretical values. Thus, the size of the particles is determined.

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