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A New Algorithm to Solve Condensation/Evaporation Growth and Coagulation of Nanoparticles

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We usually define as « nanoparticles », those particles which present at least one dimension less than 100 nm. Several studies have measured different emission sources of nanoparticles, for indoor and outdoor air. It is also known that these particles are likely to have multiple effects on human health. (Oberdörster et al.(2005)).

Aware of the risks related to nanoparticles, INERIS decided in 2009 to create a research program in order to develop a model that would be able to simulate the dynamics of nanoparticles in both confined and free atmospheres.

Unlike existing models, it is necessary to follow both numerical and mass concentrations of particles in order to correctly account for the time evolution of nanoparticles and their potential health effects, as the number concentration is much more relevant for nanoparticles. This study addresses condensational growth, evaporation and coagulation.

A comparative review of algorithms currently used in air quality models is presented as well as new algorithms adapted to nanoparticles. We use the sectional approach in which the size distribution is discretized into sections characterized by a fixed mean geometrical diameter, particles properties are assumed to be constant over each particle size section. Two different initial particle distributions are used, one from regional pollution in hazy conditions and another one from diesel engine emission measurements.

During the simulation of condensational growth, evaporation and coagulation, the size of the particles changes. In order to maintain the fixed mean geometrical diameter of each section, we have to proceed to a redistribution of the particle mass and number concentrations at each time step: particles are then transferred to the section which corresponds to their new diameter. It appears that some of the algorithms used for redistribution are better fitted for nanoparticles, among them we present a new hybrid algorithm based on number redistribution for small sections and mass redistribution for coarse sections.

Futur work will consist in including several physical processes specific to nanoparticles such as nucleation and wall deposition.