Mathematical modelling of nanoparticle formation using ANSYS/Fluent

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Nanoparticle formation in hydrodynamic flows is an often occurred process in atmosphere and industry. To predict the aerosol properties the researchers apply mathematical modelling that is based on solving the general dynamic equation (GDE)

$$\frac{\partial \rho n}{\partial t} + \nabla \cdot (\rho \bar{u} n) + \rho \frac{\partial (Gn)}{\partial v} = \nabla \cdot (D \nabla n) + \rho I(v^*) \delta(v - v^*) + \\ + \frac{1}{2} \rho \int_0^v \beta(v - v', v') n(v - v', t) n(v', t) dv' - \\ - \rho n(v,t) \int_0^\infty \beta(v, v') n(v', t) dv' \quad (1)$$

where ρ is the density of gas, $n(v, t)$ is the particle size distribution function (PSD), $G(v)$ is the rate of condensational growth in the particle volume interval $[v, v+dv]$, $\bar{u}$ is the velocity field of gas, D is Brownian diffusivity of particles, I is the rate of formation of new particles of critical volume v^* due to nucleation. The birth and loss of particles by coagulation in the interval $[v, v+dv]$ are determined by the last two terms in RHS respectively.

The method of moments is a widely used routine for numerical solving of the GDE. In this method the GDE is substituted by equations for the moments of the PSD. Moments of the PSD are scalars that characterize mean aerosol properties (total concentration, volume fraction). CFD packages such as ANSYS/Fluent provide an option to solve the transport equation for an arbitrary scalar φ

$$\frac{\partial \rho \varphi}{\partial t} + \nabla \cdot (\rho \bar{u} \varphi) = \nabla \cdot (D \nabla \varphi) + S_\varphi \quad (2)$$

where S_φ is the source term. User-defined scalars (UDS) should be defined for the moments of the PSD. To account the internal mechanisms of nucleation, condensation and coagulation the source terms should be implemented by user-defined functions (UDF).

In this work the moment method in conjunction with solving the Reynolds-averaged Navier-Stokes equations was applied to model of the formation of di-ethyl-hexyl-sebacate (DEHS) nanoparticles in the hot free axisymmetric turbulent jet due to nucleation, condensation and coagulation. In the assumption of the lognormal PSD [1] UDS with appropriate source terms were defined for the first three moments and vapor concentration to account gas-to-particle conversion. Three models of particle growth were realized: coagulation-controlled model, condensation-controlled model and full model that includes both processes.

The flow configuration was a steady axisymmetric non-isothermal free jet. The jet originates in a nozzle of diameter d=0.001 m. The exit velocity in nozzle was U_0=45 m/s (Re=2500). The saturation temperature of vapor was T_0=180°C, the ambient temperature was T_a=27°C. The standard k-ε model is chosen as a turbulence model.

The evolution of geometric mean particle diameter d_g on the jet axis is shown in Fig.1. The coagulation-controlled model gives polydisperse aerosol with d_g=32 nm. The pure condensational model gives monodisperse aerosol with d_g=31 nm. The full model shows that after initial condensational growth the particles grow additionally by coagulation and finally we have polydisperse aerosol with d_g=40 nm.

There were no problems with convergence in calculations by model with coagulation source terms. Decreasing under-relaxation factors is needed for the condensation-controlled model and full model because of high non-linearity of problem in this case.

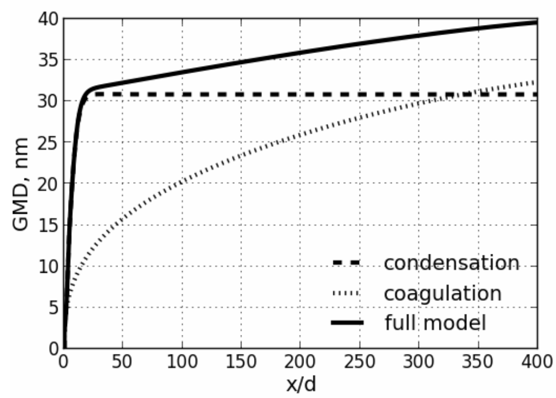

Fig.1. Profile of the geometric mean diameter on the jet axis.

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