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CAPTURING AEROSOL DROPLET NUCLEATION AND CONDENSATION BURSTS USING PISO AND TVD SCHEMES

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The formation of an aerosol is a complex physical phenomenon. Although an aerosol is often perceived as a uniform gaseous substance, it contains many small dispersed droplets or particles. The scales which govern the evolution of such an aerosol are not only macroscopic. For example, the interaction of individual molecules in a supersaturated vapor determines the homogeneous nucleation rate, which, in turn, defines macroscopic properties of the aerosol, such as composition or surface deposition rate.

To describe the microscopic physics of aerosol formation using macroscopic quantities, classical nucleation theory (CNT) is adopted. CNT is sensitive to mixture properties such as temperature and saturation. A small variation in pressure or temperature may lead to a critically supersaturated state and results in rapid bursts of newly created aerosol droplets. Condensation of vapor onto these droplets subsequently decreases the saturation, thereby effectively stopping further nucleation. In the modeling of multiphase fluid flow, the occurrence of nucleation and condensation puts a stringent requirement on the accuracy of the numerical method. First, the environment in which nucleation is triggered should be well captured by the method. Moreover, the sharp gradients in the solution associated with nucleation, call for accurate numerical treatment.

In this work, a numerical study of a single-species two-moment Eulerian aerosol model (Ref. [1]) in a finite volume (FV) framework is presented. We adopt the PISO algorithm [2] for compressible flow. Whereas the original PISO algorithm was developed for transport of species from one phase to another by chemical reaction, we adapt the original method to treat transport between vapor and liquid phases by nucleation and condensation. Within this framework, we precisely assess how *numerical* aspects of the model affect the solution for the aerosol mass fraction and droplet concentration.

Numerical simulations were carried out for flow in a Laminar Flow Diffusion Chamber

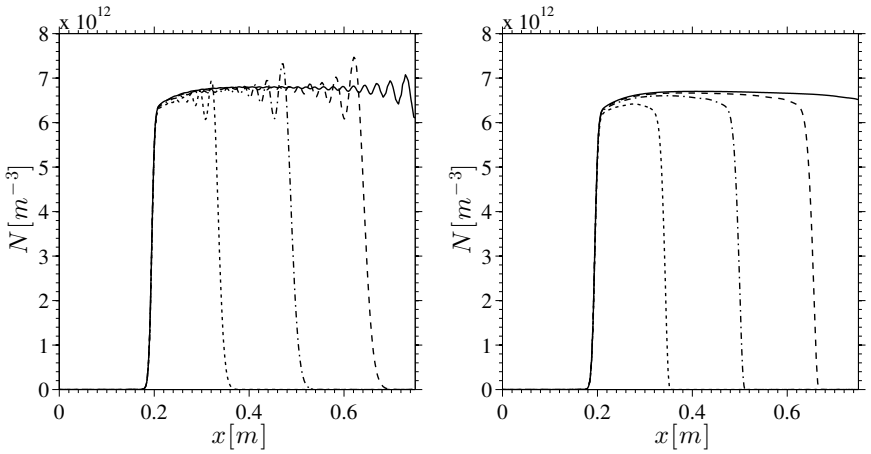

Figure 1: Droplet concentration N $[m^{-3}]$ along the LFDC centerline position x $[m]$ for (a) a central FV scheme and (b) a TVD (MUSCL) method, at times $t = 1$ (dots), $t = 1.5$ (dash-dot), $t = 2$ (dashed) and $t = 2.5$ (solid) in $[s]$.

(LFDC) [3]. A hot saturated vapor entering the cooled LFDC becomes critically supersaturated, leading to nucleation and condensation. In a transient FV simulation employing second order central discretization, the introduction of a saturated vapor front is shown to lead to unphysical numerical waves (Figure 1a) in the aerosol mass fraction and droplet concentration, which slowly decay in time while being advected outside the flow domain. We present and compare two approaches to address this problem:

1. A TVD interpolation scheme is applied to the convective terms, to preserve the monotonicity of the solution. An acceptable time-accurate transient solution is achieved on coarse grids, compared to a linear interpolation scheme (Figure 1b).

2. The amplitude and wave length of the numerical waves decrease linearly with increasing number of grid nodes along the chamber axis. For effective capturing, an adaptive grid refinement method is presented, which suppresses fluctuations while keeping computational cost reasonable.

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