SIMULATION OF AEROSOL EVOLUTION IN A TURBULENT FLOW

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Summary The complex interaction between turbulent mixing and aerosol growth processes is investigated in a canonical turbulent flow configuration by means of direct numerical simulation. A cold gaseous stream mixes with a hot stream of vapor in a developing mixing layer. Nanometer sized droplets nucleate at the turbulent interface and subsequently grow as more vapor condenses on their surface. As the droplet number density increases, coagulation processes become important. The simulation results show that the mean aerosol number density reaches a maximum on the lean vapor side across the mixing layer, while the average droplet diameter peaks on the rich vapor side, where growth is more intense. It is also found that the size distribution function of the droplets exhibits self-similarity along the streamwise direction.

MOTIVATION, SCOPE, AND METHODS

Nucleation, condensation and coagulation of aerosol can be found in many fields, such as powder technology, cloud formation, and vehicular exhaust particulate evolution etc. Turbulence greatly affects aerosol dynamics [1, 2]. Yet, there exists little quantitative understanding about the complex interaction between turbulence and aerosols. This work investigates the aerosol evolution in a turbulent shear layer by integrating various advanced numerical methods from different fields, i.e., Direct Numerical Simulation (DNS) for flow field, Quadrature Method Of Moments (QMOM) [3] for aerosol dynamics, and Lagrangian particles method for convection of passive fields. It is intended to develop a new numerical tool to provide better understanding for the complex interaction between turbulent mixing and aerosol growth processes.

The control equations for aerosol evolution in fluid flow are the combination of the Navier-Stokes equations to describe flow field, the convection-diffusion equation for temperature and vapor concentration fields, and a population balance equation to model the evolution of aerosol particle size distribution (PSD) function $f(\vec{x}, t, \xi)$ [4]

$$\frac{\partial f}{\partial t} + \nabla \cdot (\vec{u} f) = \left[\frac{\partial f}{\partial t}\right]_{\text{nucleation}} + \left[\frac{\partial f}{\partial t}\right]_{\text{condensation}} + \left[\frac{\partial f}{\partial t}\right]_{\text{coagulation}} \tag{1}$$

where $\vec{u}$ is the fluid flow velocity. The right hand side includes nucleation, condensation and coagulation processes, which are modeled by classic physical models [4]. Directly solving the PSD equation is computational prohibitive when coupled with DNS. QMOM deals with the corresponding moments equations (6 moments in current work). It uses Gaussian quadrature to close the moments equations (owing to the nonlinearity of aerosol dynamics, the control equation for lower order moments contains higher order moments, i.e., the moments equations are not closed). Lagrangian particles method [5] is used to deal with the moments convection. There is no need to deal with the convection term within QMOM, and many difficulties therein can be circumvented.

RESULTS AND DISCUSSION

The flow configuration is shown in Figure 1. A hot stream carrying unsaturated vapor mixes with a cool stream. The vapor temperature decreases owing to turbulent mixing. When the vapor gets super saturated, nucleation takes place to generate nanometer droplets. These droplets can grow owing to vapor condensation on the surface or coagulation of two droplets. This work simulates the whole processes with high performance computing. It used 80M grid nodes to discretize the flow field, 2B Lagrangian particles to track the evolution of moments of the aerosol PSD. Around 2M CPU-hours were used for the simulation on the IBM Blue Gene/P supercomputer in KAUST, which has 65,536 independent processing cores.

Figure 2 (left) shows a snapshot of the aerosol number density. Lighter color region denotes higher number density. The filament-like structure shows nucleation takes place in the mixing front of passive scalar fields (temperature and vapor concentration). The aerosol volume faction (Fig. 2 right) obtains higher value in the down stream region and in the vortex cores, owing to longer residence time therein. Investigation on the streamwise profiles of mean number density and volume fraction indicates that both values increase along the streamwise direction. The crosswise profiles exhibit self-similarity, i.e., profiles at different cross sections all nearly collapse to the same curve after a linear transformation based on the mixing layer width. Another interesting finding is the differential transport of droplets across the mixing layer. Figure 3 shows the scatter plots of number density and average diameter across the mixing layer. It is found most droplets nucleate at the lean vapor side (small mixture fraction), while droplets grow faster to larger size at the rich vapor side (big mixture fraction).

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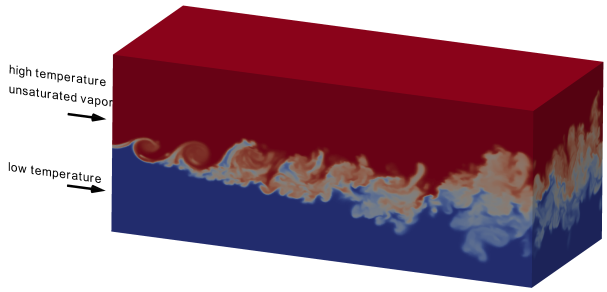

Figure 1. Configuration of the computational domain. The temperature contour is also shown.

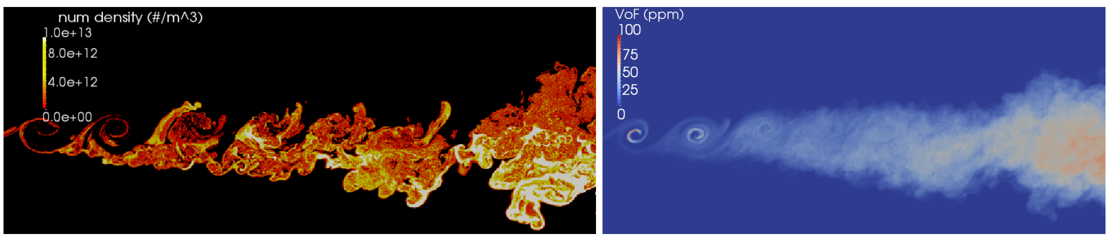

Figure 2. Left: Snapshot of aerosol number density. Right: aerosol volume fraction averaged along spanwise direction.

CONCLUSIONS

The aerosol evolution in a turbulent field is investigated by means of direct numerical simulation. The simulation results show that the mean aerosol number density reaches a maximum on the lean vapor side across the mixing layer, while the average droplet diameter peaks on the rich vapor side, where growth is more intense. It is also found that the size distribution function of the droplets exhibits self-similarity along the streamwise direction.

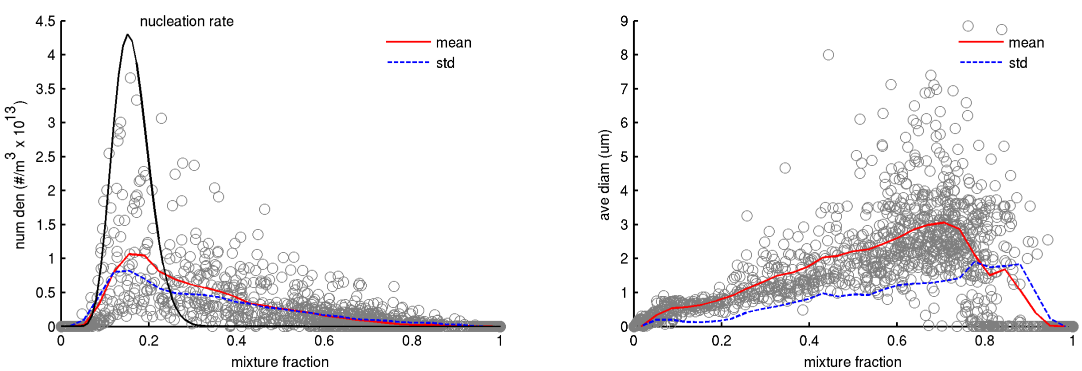

Figure 3. Scatter plots of number density and average diameter.

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