INSTANTANEOUS AEROSOL DYNAMICS IN A TURBULENT FLOW

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Short paper
DOI: 10.2298/TSCI1205492Z

Dibutyl phthalate aerosol particles evolution dynamics in a turbulent mixing layer is simulated by means of direct numerical simulation for the flow field and the direct quadrature method of moments for the aerosol evolution. Most particles are nucleated in a thin layer region corresponding to a specific narrow temperature range near the cool stream side. However, particles undergo high growth rate on the hot stream side due to condensation. Coagulation decreases the total particle number density at a rate which is highly correlated to the instantaneous number density.

Key words**:** *aerosol, direct quadrature method of moments, direct numerical simulation*

Introduction

Aerosols are ubiquitous both in nature and in industrial products. Aerosol dynamics involves various processes: nucleation [1], condensation [2], coagulation [3], collision [4], and transport [5]. Aerosol particles evolution is extremely sensitive to the history of temperature and vapor concentration that these particles undergo. Therefore it is very difficult to investigate the complex interaction between turbulence mixing and aerosol growth processes. Dibutyl phthalate (DBP) as condensate has been used in various studies [6-9] on aerosol dynamics. Other than solving the particle size distribution (PSD) evolution equation, method of moments solves only a set of moments. The moments set represents the most important fundamental information about the PSD function, such as total number density, average diameter, volume fraction, *etc*. [10, 11]. In this work, direct numerical simulation (DNS) combined with the direct quadrature method of moments (DQMOM) [12] is used to simulate DBP aerosol evolution in a turbulence mixing layer. Lin *et al.* [13] have performed numerical simulation on the nanoparticle nucleation and coagulation in a mixing layer. While only instantaneous aerosol dynamics are investigated in this article. Statistics on turbulence and aerosol dynamics can be found in another relevant work [9].

Models and equations

The DNS is performed by solving the unsteady, incompressible Navier-Stokes equations. The numerical scheme and boundary conditions can be found in [9]. Figure 1 shows a

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simulated temperature field. A plate (for *y* from 0 to 0.055) is placed at the inlet. Aerosol particles are generally described by the PSD function, which is governed the general dynamic equation (GDE) [14]. The GDE is solved with the DQMOM method.

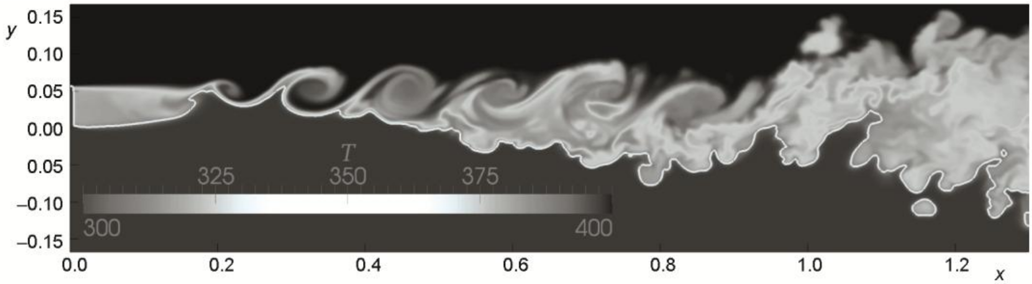

Figure 1. Snapshot of temperature field (clipped in *y* direction), with unit K. The hot stream has higher speed than the cool stream. The iso-contour line corresponds to *T* = 317 K

Results and discussion

Figure 2 shows a snapshot of M_0. The highest number density appears in the wake region. Air flow circulates in the wake region, with much lower speed than elsewhere. A parcel of air experiences much longer residence time in the wake region. Therefore, vapor nucleation continues to generate new particles and increases the local particle number density substantially. In the turbulence transition region $0.2 < x < 0.5$, particles are all confined in the roller structures. In this simulation, particles diffusion has been neglected because the Schmidt number is very large. The transport of particles is only due to flow convection. In the downstream region, particles are spread over due to turbulent diffusion.

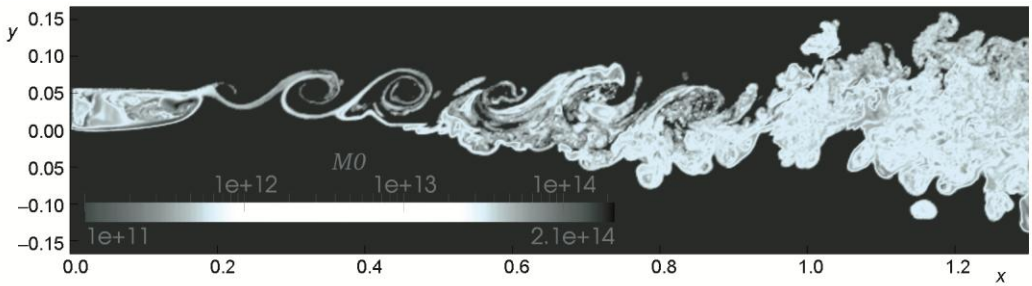

Figure 2. Snapshot of the zeroth moment M_0, the total particle number density [particles m^{-3}]

Figure 3 shows a snapshot of the nucleation rate. Nucleation takes place in a very narrow region. In fact, under the condition of unit Lewis number, the vapor concentration is linear to the temperature, and the nucleation rate function can be simplified to a function of temperature along The nucleation rate will obtain its maximum at specific temperature [8]. For the present simulation, the temperature corresponding to the maximum nucleation rate is around 317 K. Figure 4 shows a snapshot of the coagulation rate. Coagulation would reduce the total particle density, which is a counter process of nucleation on this regard. The highest coagulation rate appears in the wake region, where the number density obtains its maximum. By comparing the total particles number density (fig. 2) and the coagulation rate (fig. 4), they are found strongly correlated. It is found that the volume fraction in the wake region is much higher than that in the mixing layer. This is because particles stays in the wake region for long time, their size grows very fast due to condensation. Besides, the particles number density has highest value in this region. However, careful investigation of the number density and the volume fraction in the wake region shows that the highest volume fraction is not obtained at the region where the number density reaches its maximum. That is because the nucleated particles are very small. Although most particles are generated in the wake region around x = 0.15, particles grow faster at region around x = 0.05. This fact can be clearly seen from the distribution of the particles average diameter (fig. 5).

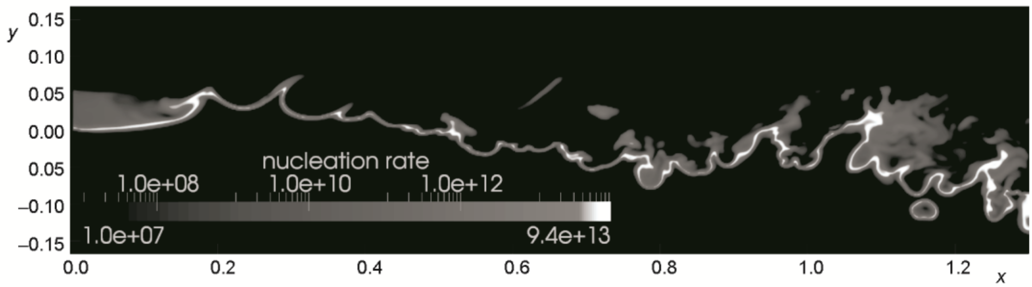

Figure 3. Snapshot of the nucleation rate [particles $m^{-3}s^{-1}$]

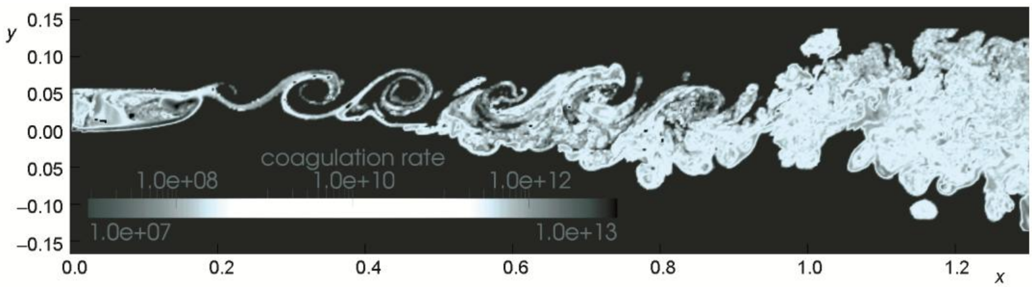

Figure 4. Snapshot of the coagulation rate, which is defined as the particle number density decreasing rate due to coagulation [particles $m^{-3}s^{-1}$]

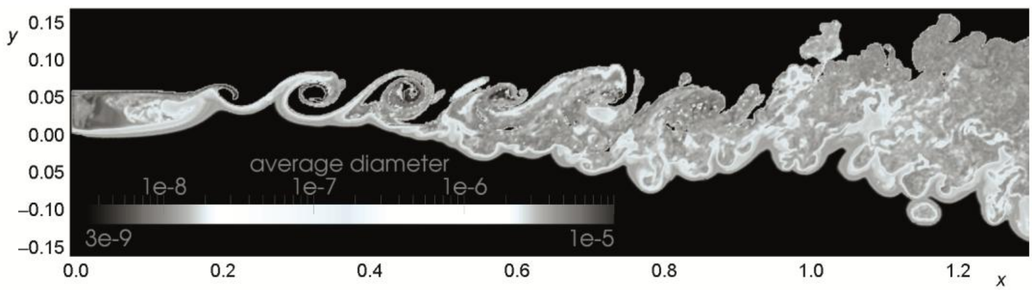

Figure 5. Snapshot of the average diameter ($d = M_1/M_0$), with unit m

It is shown that particles are actually larger in the region around x = 0.05 than those around x = 0.15. Another finding is that particles are smaller on the cool lean vapor side, because most particles are generated on that side due to nucleation. Apart from that narrow layer region of small particles, all particles have almost the same size.

Conclusions

In this work, the nucleation and growth of dibutyl phthalate particles in a turbulent mixing layer has been simulated through the combination of direct numerical simulation for the flow field and the direct quadrature method of moments for aerosol dynamics. A plate is placed in the inlet to speed up the flow transition to turbulence. A wake region is formed near the plate, which exhibits every different characteristics of aerosol dynamics from that in the mixing layer region.

The particles number density obtains its maximum value at the wake region, because fluid circulates in the wake region and the number of nucleated particles accumulates over time. Most particles are nucleated on the cool lean vapor side in the mixing layer. And the high nucleation region is limited around a filament layer corresponding to specific temperature (here around 317 K). The instantaneous coagulation rate is found to be closely related to the local number density, because coagulation is a function of the number densities of the corresponding coagulating particles. Particles growth rate due to condensation is found smaller on the cool lean vapor side than that on the hot rich vapor side. Particles have small average diameter on the cool lean vapor side, because of nanometer size particles are nucleated on that region, and the subsequent condensation growth rate is small. The highest particles volume fraction is observed in the wake region, due to the high nucleation rate, low turbulent diffusion, and long residence time there for particles to grow. Apart from the wake region, the volume fraction is found to increase along the steamwise direction.

Acknowledgment

Dr. Fabrizio Bisetti and Dr. Antonio Attili also have valuable contribution to this work.

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Paper submitted: August 1, 2012
Paper revised: September 6, 2012
Paper accepted: September 12, 2012