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THE EFFECT OF PHASE TRANSITIONS ON THE DROPLET SIZE DISTRIBUTION IN HOMOGENEOUS ISOTROPIC TURBULENCE

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Abstract. *We investigate the dynamics of an ensemble of discrete aerosol droplets in a homogeneous, isotropic turbulent flow. Our focus is on the stationary distribution of droplet sizes that develops as a result of evaporation and condensation effects. For this purpose we simulate turbulence in a domain with periodic boundary conditions using pseudo-spectral discretization. We solve in addition equations for the temperature and for a scalar field, which represents the background humidity against which the size of the droplets evolves. We apply large-scale forcing of the velocity field to reach a statistically steady state. The droplets are transported by the turbulent field while exchanging heat and mass with the evolving temperature and humidity fields. In this Euler-Lagrange framework, we assume the droplets volume fraction to be sufficiently low to allow one-way coupling of the droplets and turbulence dynamics. The motion of the droplets is time-accurately tracked. The Stokes drag force is included in the equation of motion of the individual droplets. The responsiveness of the droplets to small turbulent scales is directly related to the size of the individual spherical droplets. We perform direct numerical simulation to ultimately obtain the probability density function of the evolving radius of the droplets at different points in time with characteristic heat and mass transfer parameters. We determine the gradual convergence of the distribution function to its statistically stationary state for forced homogeneous, isotropic turbulence.*

1 INTRODUCTION

The interaction of droplets that undergo phase transition with a turbulent flow is encountered in many areas of engineering[1]. It is also of special importance in meteorology, e.g., in cloud physics[2]. In the context of cloud physics droplets are generated by the heterogeneous nucleation of water vapor on aerosols. Typically, the size of these aerosol droplets is of the order of 0.1 μm. The evaporation and condensation of water vapor from and to the droplets is the governing process for the growth of the droplets from sub micron size up to a size of around 20 μm, after which they grow mostly by coalescence until they become large enough to fall as a rain drop under gravity. Experimental evidence[3] also suggests the presence of a fairly wide size distribution $1-20$ μm of droplet radii in clouds. In fact, the size distribution that is generated has a strong influence on the coalescence rate of droplets which ultimately determines the time associated with the initiation of rain.

Much pioneering work has been done on the theoretical and numerical investigation of the influence of turbulence on evaporation and condensation associated with aerosol droplets[1,2,4]. The wide range of length and time scales of turbulence makes direct numerical simulation (DNS) of the evolution of the flow in combination with the droplets very costly. In Celani et al[4]. the authors used DNS focusing mainly on the large scales of turbulence. Emphasis has been given to resolving only the small scales[5] where it was found that a rather narrow distribution of droplet radii emerges. This was associated with the relatively small size of the computational domain.

In this paper we consider the situation of water droplets undergoing phase change and moving in air. Air also advects the vapor concentration field. We compute the natural size distribution of the droplets that arises as a result of the interaction between the droplets and the transporting turbulent flow. We assume the turbulent flow to be homogeneous and isotropic. We will perform DNS of the velocity field and the passively advected vapor and temperature field. The droplet trajectories are computed time-accurately in a domain with periodic boundary conditions.

From our simulation results we inferred the dynamical behavior of inertial particles moving in a homogeneous, isotropic turbulent flow. We have computed the probability density function (PDF) of the distribution of the droplets radii at various points in time. Starting from an ensemble of equal-sized small droplets, it was observed that the distribution becomes wider as time increases, while the location of the peak gradually increases. It is seen that these PDFs resemble locally a Gaussian distribution. The full convergence toward a statistically stationary state is seen to be a flow process.

The paper is organized in the following way. In Section 2 we will introduce the mathematical models that we have used for the air flow, droplets trajectory and the passive scalars. In Section 3 we focus on the details of the numerical tools that we have used for the simulation. Statistics regarding the droplets size are discussed in Section 4. Concluding remarks are collected in Section 5.

2 MATHEMATICAL MODELS

In this Section we first present the fluid mechanical model for the flow field in Subsection 2.1. The Lagrangian particle tracking is described in Subsection 2.2. In Subsection 2.3 we present the treatment of the evaporation and condensation processes and finally in Subsection 2.4 we present the equations of the dispersed phase in dimensionless form.

2.1 Governing equations for the flow field

Our principal goal here is to model the turbulent velocity field $\mathbf{u} = (u, v, w)$ which is advecting both the droplets and the vapor. The flow field we consider is assumed to be homogeneous and isotropic. We model the three dimensional velocity field $\mathbf{u}$ in dimensionless form by the incompressible Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial \mathrm{t}} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\bigtriangledown p_g + \frac{1}{\mathrm{Re}} \bigtriangledown^2 \mathbf{u} + \mathbf{f} \qquad (1)$$
$$\bigtriangledown . \mathbf{u} = 0$$

where p_g is the pressure of the gas, $\mathbf{f}$ is the external forcing term and Re is the Reynolds number based on a reference length, a reference velocity and the kinematic viscosity of the fluid.

The temperature of the gas is modelled as a passive scalar in the flow field and its transport is governed by the advection-diffusion equation. This implies that the temperature does not affect the flow. We decompose the temperature T_g of the gas into its mean value, denoted by $\langle \mathrm{T} \rangle$, and its fluctuating part $\tilde{\mathrm{T}}$. The mean temperature varies linearly and for our purpose it suffices to assume that the mean temperature varies linearly with x, thus $\langle \mathrm{T} \rangle = \alpha x$. Under these assumptions the resulting equation in dimensionless form becomes

$$\frac{\partial \tilde{\mathrm{T}}}{\partial \mathrm{t}} + (\mathbf{u} \cdot \nabla)\tilde{\mathrm{T}} - \kappa_t \nabla^2 \tilde{\mathrm{T}} = -\alpha u \qquad (2)$$

where κ_t is the thermal diffusivity, defined as $\kappa_t = 1/(\mathrm{Re} \cdot \mathrm{Sc})$ where Sc is the Schmidt number.

2.2 Lagrangian description of particle trajectory

Various forces affect the trajectory of droplets in the flow field. The dominant contribution to the force in the flow we consider is the drag force or Stokes drag. We neglect other forces as discussed in the seminal paper by Maxey and Riley[6], such as the Basset history effect and the added mass effect. We consider the volume fraction of the droplets in the domain to be small so collisions and coalescence among the droplets is neglected. Under these assumptions, the equation governing the particle position $\mathbf{x}$ and velocity $\mathbf{v}$

in dimensional form becomes:

$$\begin{aligned} \frac{\mathrm{d}\mathbf{v}}{\mathrm{dt}} &= \frac{\mathbf{u}(\mathbf{x},\mathrm{t})-\mathbf{v}}{\tau_v} \\ \frac{\mathrm{d}\mathbf{x}}{\mathrm{dt}} &= \mathbf{v} \end{aligned} \tag{3}$$

where we evaluate the fluid velocity $\mathbf{u}$ at the instantaneous location of the particle. Here τ_v is the inertial response time of the particle, and is defined in the following way:

$$\tau_v = \frac{\rho_d \mathrm{R}^2}{18\mu}$$

where R is the radius of the droplet, ρ_d is the density of the droplet and μ is the dynamic viscosity of the gas. In this paper we will consider the particles as water droplets and the gas to be air.

2.3 Equations for droplet evaporation and condensation

The focus in this paper is on the transport of dispersed droplets by a turbulent flow, in which phase transition through evaporation and condensation takes place. There are a number of phenomenological models that describe the change of mass of individual droplets. This directly affects the size of the droplets and hence their dynamic response time. The latter dependence is strong, given the quadratic dependence of τ_v on the radius. The translation from the mass of a particle to its size is by assuming the droplets to be strictly spherical.

We consider a droplet of instantaneous mass "m" moving in the turbulent velocity field $\mathbf{u}$ and let T_d be the absolute temperature of the droplet. The droplets are treated as point particles in the flow domain, and there is no temperature gradient across and within the particle. While investigating the motion of the small particles in the gas a quantity of relative importance is the Knudsen number (Kn), which is defined as the ratio of the gas mean free path to the characteristic radius of the particle. We are considering the situation when Kn is small ($\mathrm{Kn} \ll 1$), which means the radii of the droplets are larger than the mean free path of the carrier gas. The droplet size is quite large in the cases considered, so the change in size of the droplets by evaporation and condensation, which takes place as a result of exchange of vapor between the droplet surface and the surrounding, is governed by diffusion laws. Several authors[2,7] used the diffusion growth model for the droplets undergoing phase change. The rate of change of mass m of the droplet obeys the following equation[8],

$$\frac{\mathrm{dm}}{\mathrm{dt}} = \mathrm{Sh}\pi\rho_g\kappa_v\mathrm{R}(\mathrm{C}_{v,b}-\mathrm{C}_{v,d}) \tag{4}$$

In this expression Sh is the so-called Sherwood number, which is defined as the ratio of the convective to the diffusive mass transfer coefficient. In addition, κ_v is the diffusion

coefficient of the vapor and $\mathrm{C}_{v,d}$, $\mathrm{C}_{v,b}$ are the mass fractions of the vapor on the droplet surface and in the background. These are described next.

The mass fraction on the droplet surface $\mathrm{C}_{v,d}$ can be expressed in terms of the ratio of the partial vapor pressure to the total pressure on the droplet surface. Now considering the total pressure to be constant, the partial vapor pressure on the droplet surface can be evaluated in terms of the temperature of the droplet by Antoine's equation; which is actually derived from the Clausius-Clapeyron saturation law[9].

The temperature evolution of the droplet is influenced by the change in mass of the droplet. The temperature equation of the particle can be expressed as

$$\frac{\mathrm{dT}_d}{\mathrm{dt}} \;=\; \frac{\mathrm{Nu}\;\; c_g}{3\mathrm{Pr}\;\, c_d}\,\frac{\mathrm{T}_d-\mathrm{T}_g}{\tau_v}+\frac{h_L}{\mathrm{m}c_d}\frac{\mathrm{dm}}{\mathrm{dt}} \tag{5}$$

where h_L is the latent heat and c_d and c_g are the specific heat of the droplet and the gas respectively. Nu and Pr are respectively the Nusselt and Prandtl number. The vapor field for the background $\mathrm{C}_{v,b}$ is assumed to be advected by the turbulent flow and the vapors are at sufficiently low concentrations not to affect the flow. Under these assumptions we model the vapor mass fraction $\mathrm{C}_{v,b}$ by the advection-diffusion equation

$$\frac{\partial \mathrm{C}_{v,b}}{\partial \mathrm{t}}+(\mathbf{u}\cdot\nabla)\mathrm{C}_{v,b}\;-\;\kappa_v\,\nabla^2\mathrm{C}_{v,b}\;=-\,\Sigma_i\;\delta_{x_i}(V)\frac{\mathrm{dm}_i}{\mathrm{dt}} \tag{6}$$

Here δ is the Dirac measure of the infinitesimal chosen volume V surrounding the point where vapor concentration is computed and x_i is the instantaneous location of the ith particle. The term on the right hand side of the equation accounts for the fact that evaporation and condensation locally affect the vapor concentration field. If a droplet evaporates then this increases the vapor concentration in the surrounding and vice versa.

2.4 Dimensionless formulation of the dispersed phase equations

In our simulation strategy we use the non-dimensional version of all the equations. In dimensionless form the equations governing the droplet motion can be written as,

$$\begin{aligned}\frac{\mathrm{d}\mathbf{v}}{\mathrm{dt}} &= \frac{\mathbf{u}-\mathbf{v}}{\mathrm{St}}\\ \frac{\mathrm{d}\mathbf{x}}{\mathrm{dt}} &= \mathbf{v}\end{aligned} \tag{7}$$

Here St is a dimensionless number called the Stokes number of the particle, which is the ratio of the inertial response time τ_v to some characteristic time of the flow. We choose our characteristic time as the Kolmogorov time scale τ_η, defined by $\tau_\eta=(\nu/\epsilon)^{1/2}$ where ν is the kinematic viscosity and ϵ is the energy dissipation rate. The rate of change of mass of the droplet in dimensionless form can be written as

$$\frac{\mathrm{dm}}{\mathrm{dt}}=\frac{\mathrm{Sh}\;\mathrm{m}}{24\mathrm{Sc}\;\mathrm{St}}(\mathrm{C}_{v,b}-\mathrm{C}_{v,d}) \tag{8}$$

Also we use the initial maximum temperature T_0 of the flow field as the reference temperature. Using this we can make the droplet temperature equation dimensionless in the following way,

$$\frac{\mathrm{dT}_d}{\mathrm{dt}} = \frac{\mathrm{Nu}}{3\mathrm{Pr}}\frac{c_g}{c_d}\frac{\mathrm{T}_d - \mathrm{T}_g}{\mathrm{St}} + \frac{h_L}{\mathrm{T}_0 c_d}\frac{1}{\mathrm{m}}\frac{\mathrm{dm}}{\mathrm{dt}} \tag{9}$$

In the above equations Nu and Sh express the effect of convection on phase transition, while Pr describes the effect of thermal over viscous diffusion rate.

3 COMPUTATIONAL MODEL AND NUMERICAL SIMULATION

In this Section we describe the basic numerical method that was adopted for the simulation of dispersed multi-phase flow with phase transition.

We use a de-aliased pseudo-spectral method for both the velocity and the passive scalars in order to perform direct numerical simulation for the turbulent flow. In this method the velocity and the scalar field in the Navier-Stokes and the advection diffusion equation are represented by their Fourier series. The numerical integration of the equations is done by the four-stage, second order, compact storage, Runge-Kutta method[10].

We consider the computational domain to be a cubic box with periodic boundary conditions in each direction. For an isotropic turbulent flow we adopt the same spatial resolution in each direction, and have in total N^3 computational points in our domain, where N is the number of grid points in each direction in the physical space. In wave number space, the wave vector $\mathbf{k}$ has three components given by $k_\alpha = (2\pi/L)n_\alpha$ where L is the length of the box and $n_\alpha = 0, \pm1, \pm2, \pm3, ..., \pm(N/2-1), -N/2$ for $\alpha = 1, 2, 3$.

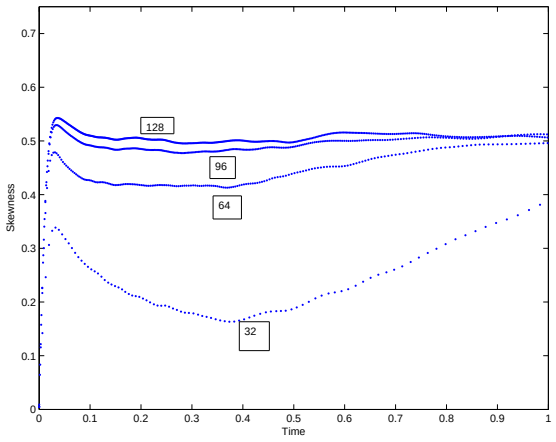

Figure 1: Convergence of skewness of the flow for different spatial resolutions N^3 with $N = 32, 64, 96, 128$ as indicated near the corresponding curves.

In order to resolve the smallest scales of the turbulent motion, which depend on the viscous dissipation rate, we retain the guiding criterion that $k_{max}\eta > 1$; where k_{max} is the cut-off wave number given by $k_{max} = \pi N/L$ and η is the Kolmogorov length scale of the turbulent flow. In Kuczaj et al.[11] the values of $k_{max}\eta$ associated with different spatial resolutions are presented for Reynolds number Re=1061 and Re=4243. We use large scale forcing for the flow field, which means that we inject energy in all the Fourier modes in the wave number space in the first shell. Full details can be obtained from Kuczaj et al.[11] In order to assess the accuracy of the simulations we include in Figure 1 predictions for the velocity skewness. It can be seen that for homogeneous isotropic turbulence the value of skewness is converging to 0.5 which is proved theoretically in the literature[12]. The figure also shows the convergence of our DNS results with the increasing grid resolution. Although the criterion $k_{max}\eta > 1$ is not strictly fulfilled for the lower resolutions, we observe that qualitatively the findings appear reliable.

The numerical treatment of the discrete droplet phase proceeds in a number of steps. We distribute the droplets initially randomly in space and provide as initial velocity the fluid velocity as found at the particle location. We assume that all the particles have initially the same radius. After a sufficiently long evolution the ensemble of droplets evolves into a statistically stationary distribution which is the result of evaporation and condensation in the forced turbulent flow. The initial temperature of the particle is set to be equal to that of the local temperature. In order to get information of the flow field such as velocity, temperature and vapor mass fraction at the location of a particle we perform trilinear interpolation. In the literature[1] trilinear interpolation was also used to get adequate results for the particle motion. The time integration of the particle trajectories was performed by the forward Euler method.

4 STATISTICS OF THE PARTICLE SIZE DISTRIBUTION

DNS of the flow of a dispersed ensemble of droplets undergoing phase transition in a homogeneous, isotropic turbulent flow requires the specification of a number of parameters. We assume our domain to be a cube having sides of length one. We introduce into the flow field an ensemble of 10^4 droplets all of which initially have a radius of 10^{-6}. In our simulations the Reynolds number is taken as 1061, which corresponds to a Taylor Reynolds number of 50.

We focus on the evolving radius of all the droplets and compute the corresponding distribution function. In Figure 2 we display the location of the peak of the distribution function as a function of time. Here by location we mean the radius at which the size distribution curve corresponding to a particular time has the highest peak. The initial condition corresponds to a sharply peaked PDF in which all droplets have the same radius. The location of the peak of this distribution is increasing with time. This growth gradually decreases as the statistically stationary state is approached. In order to achieve a more precise approximation of this ultimate PDF a longer simulation time is required.

The evolution of the PDF of the droplets size-distribution is displayed in Figure 3

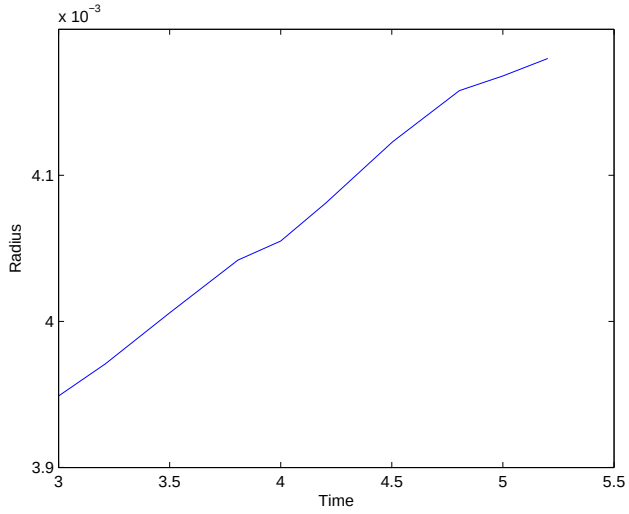

Figure 2: Evolution of the peak value of the distribution function as a function of time, indicating the gradual convergence of the PDF toward the statistically stationary state.

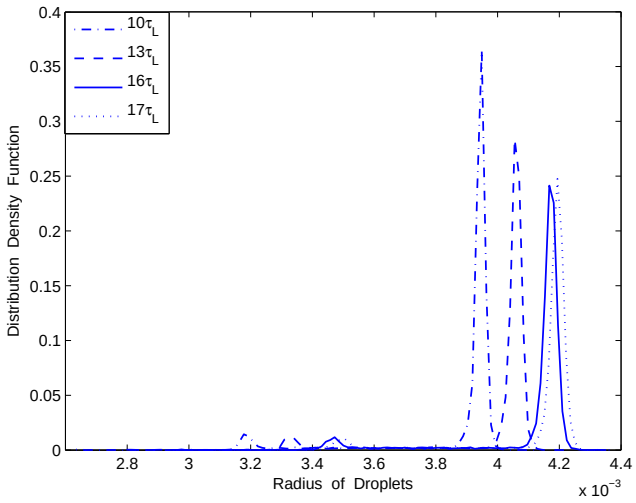

Figure 3: Probability density function of the droplet size distribution taken at times $10, 13, 16$ and $17\ \tau_L$ in which τ_L denotes the large-eddy turn-over time.

for a number of times. We notice that there is still quite some growth in the average droplets size as a result of condensation onto the droplets, for times $\geq 10\tau_L$, in which τ_L is the large-eddy turn-over time. The distribution functions are seen to have widened considerably, compared to the sharply peaked initial condition. The shape of the PDF

and its dependence on physical parameters of our model will be investigated numerically in the future and published elsewhere.

5 Concluding remarks

In this paper we have studied the turbulent transport of water droplets in air, that undergo phase transition represented by evaporation and condensation. The simulation was based on DNS using pseudo-spectral discretization. We have developed a two-way coupled mathematical model of the vapor concentration field with the change in mass of the droplets and observed the effect of turbulence on the size distribution of the droplets. From our simulation we observed that the PDF of the size distribution becomes wider as time increases. The convergence toward the statistically stationary state was followed for 10^4 droplets at a modest Reynolds number. In the future we will incorporate the effect of the droplet temperature on the gas temperature equation, and we will also compare our simulation results with experimental data.

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