



Statistical simulation of molecular diffusion effect on turbulent tetrad dispersion



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ABSTRACT

Molecular diffusion can significantly affect the dispersion and mixing processes at small temporal and spatial scales in turbulent flows, especially when differential diffusion among species is considered. Since species mixing takes place at the molecular level, it is very beneficial to study and model this phenomenon from a kinetic viewpoint. However, most molecular simulation methods, such as the direct simulation Monte Carlo (DSMC) method, are inefficient for high Reynolds or low Knudsen number flows. The diffusive information preservation (D-IP) method, which based on the Fokker–Planck model, can overcome this difficulty. In the current paper, we firstly validate the D-IP method by simulating the decaying homogeneous isotropic turbulence, and then apply it to investigate the effects of molecular diffusion in the turbulent tetrad dispersion. Two typical kinds of particles, i.e., the gas-phase molecules (Schmidt number, $Sc = 1$) and marked fluid particles (approximately to the soot particle, $Sc = \infty$), have been considered. The effects of differential diffusion are found to be closely related to the tetrad initial size and weakly dependent on the Taylor-scale Reynolds number. Although the discrepancy of the tetrad size and shape between the gas-phase molecules and marked fluid particles is more significant in the turbulent dissipation scale, this influence can extend to larger scales, i.e., the inertial range, due to the correlated fluctuations and intermittency of the turbulent flows. It indicates that the molecular diffusion as well as the differential diffusion cannot be neglected if interested processes belong to small scales, such as in the combustion.

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1. Introduction

Scalar dispersion and mixing in turbulent flows are closely related to many types of industrial and environmental processes, such as the atmospheric pollutant dispersion and combustion. Generally, turbulent scalar dispersion and mixing processes depend on both turbulent motions in the macro-scale and molecular transport in the micro-scale. For physical or chemical phenomena that take place at small temporal or spatial scales, molecular transport becomes more important compared to turbulent motions. An excellent example is the combustion, in which chemical reactions happen in the molecular collision scale and strongly interact with the molecular and turbulent transport [1]. As well known, the molecular transport, which determines the species mixing in combustions, can influence the flame instability and structure [2], while their differences among species can further affect the dynamic process of combustion and pollutant emissions [3–6].

Since species mixing as well as chemical reactions take place at the molecular level, it is very beneficial to study and model these phenomena from a kinetic viewpoint [7–9]. In recent years, several efforts have been made to numerically investigate combustion phenomena by using the direct simulation Monte Carlo (DSMC) method, such as for the spontaneous combustion [10,11] and the unstretched diffusion flame [12] of hydrogen oxygen mixture. Detailed reaction mechanism has been confirmed in these simulations, however the transport–chemistry interaction is rarely considered because of the limited computational size and time step of the DSMC method. Therefore, applying the DSMC method to the multi-scale problems such as combustions is still challenging [13].

Simulating molecular motions following the Fokker–Planck model instead of the Boltzmann equation [14–17] can break these limitations in the DSMC method. Since a continuous stochastic process replaces the binary molecular collision compared to the DSMC method, the numerical methods in the framework of the Fokker–Planck model are less restricted by the temporal and spatial scales and more efficient for small or moderate Knudsen number (Kn) flows. Therefore, they are feasible for simulating multi-scale

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problems. For example, the Fokker–Planck model has been verified both in the rarefied [15,16] and continuum gas flows [17]. In the continuum regime, the Fokker–Planck model would degenerate to a diffusive form, based on which, the diffusive information preservation (D-IP) method has been proposed [17]. In the previous papers, the D-IP method has shown advantages in simulating small Knudsen number gas flows [17], and has been further applied to the homogeneous isotropic turbulent (HIT) [18] and turbulent channel flows [19] at low Reynolds numbers.

Since the D-IP method simulates the turbulent flows and molecular motions from the kinetic viewpoint uniformly, their interactions, which determine the turbulent dispersion and mixing processes, can be directly computed and sampled. In direct numerical simulations (DNS), the turbulent dispersion and mixing processes are often investigated by the Eulerian approach [51,52]. However, as transport issues are addressed naturally from the Lagrangian viewpoint, the Lagrangian approach [53–55] has also been used by many authors dated back to the work of G. I. Taylor (1921) [20]. Afterwards, the molecular diffusion effects on turbulent dispersion processes have been studied starting from the pioneer work of Saffman (1960) [21], such as for the scalar dispersion in the isotropic turbulence [22] and the turbulent channel flows [23–25], the concentration fluctuation of pollutant [26,27] and the chemical reactions [28–30]. Most of the above literatures focus on the Lagrangian behavior of a single particle or particle pairs, which are closely connected to the average expansion and concentration fluctuations of a cloud of passive contaminants, respectively. Nevertheless, the geometric evolution of the particle cluster is also important to understand the physical mechanism of dispersion and mixing processes in turbulent flows, such as their statistical conservation laws [31]. The geometric evolution of a cloud of Lagrangian particles is preferable to be modeled through the multi-particle dispersion [32], where the study of tetrad (four-particle cluster) that is the minimum configuration to define a volume, is of special interest. Although many authors [33–37] have investigated the evolution properties of tetrads expansion and distortion in turbulence through DNS and stochastic models by tracking marked fluid particles, the effects of molecular diffusion on tetrad dispersion have been rarely discussed, which would be significant in the small-scale processes, such as chemical reactions and combustions [2–6].

Thus, in order to study the molecular diffusion effects on the tetrad dispersion by using a kinetic numerical scheme, we would first review and verify the Fokker–Planck model and the D-IP method in Sections 2 and 3 in this paper. Then, the D-IP method is applied to compute the temporal and spatial evolutions of the tetrad dispersion and their Lagrangian statistics in Section 4. As mentioned by Pitsch and Bisetti [38,39], the differential diffusion among soot particles (Schmidt number, $Sc \approx \infty$) and gas-phase species ($Sc \approx 1$) can cause soot to be transported towards the flame sheet where it is oxidized, which would influence the soot formation and evolution significantly. In analogy to the soot transport in combustions, two typical kinds of particles, i.e. the gas-phase molecules and the marked fluid particles, are considered in Section 4. In addition, their differential diffusion effects are going to be analyzed. Finally, conclusions and remarks of this paper are presented in Section 5.

2. Diffusive information preservation method

2.1. The linear Fokker–Planck model

The Fokker–Planck equation can be considered as an approximation of the Boltzmann equation for gas flows [56], where molecular binary collisions are replaced by continuous random

processes. When the external force is neglected, the Fokker–Planck equation can be written as,

$$\frac{\partial f(\mathbf{c}, \mathbf{x}, t)}{\partial t} + c_i \frac{\partial f(\mathbf{c}, \mathbf{x}, t)}{\partial x_i} = \frac{\partial}{\partial c_i} [\zeta(c_i - U_i(\mathbf{x}, t))f] + \frac{\partial^2}{\partial c_i \partial c_i} \left[\frac{\zeta k_B T(\mathbf{x}, t)}{m} f \right], \quad (1)$$

where c_i is the molecular velocity, $U_i(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$ are the mean velocity and temperature of the flow fields at location \mathbf{x} and time t ; k_B and m are Boltzmann constant and molecular mass, respectively; ζ is the friction coefficient which characterizes the time scale of the relaxation process for the velocity distribution function $f(\mathbf{c}, \mathbf{x}, t)$. In equilibrium, $f(\mathbf{c}, \mathbf{x}, t)$ relaxes to corresponding Maxwell distribution f_M ,

$$f_M = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp \left(-\frac{m}{2k_B T} (c_i - U_i)^2 \right), \quad (2)$$

where n is the number density.

In numerical simulations [14–17], the Fokker–Planck Eq. (1) is usually solved through the Langevin model by simulated particles (hereafter, referred to as simply “simulator”), i.e.,

$$\frac{dX_i}{dt} = c_i, \quad (3a)$$

$$\frac{dc_i}{dt} = -\zeta(c_i - u_i^{eq}) + \left(\frac{2k_B T^{eq}}{m} \right) \frac{dW_i(t)}{dt}, \quad (3b)$$

where \mathbf{X} is the position of the simulator; $\mathbf{W}(t)$ is a Wiener process with $dW_i(t) = W_i(t + dt) - W_i(t)$, $\langle dW_i(t) \rangle = 0$ and $\langle dW_i(t) dW_j(t) \rangle = dt \delta_{ij}$, where δ_{ij} is the Kronecker delta. The symbol $\langle \dots \rangle$ denotes an ensemble mean. Considering the location of simulators, we define the Lagrangian quantities $u_{k,i}^{eq}(\mathbf{X}, t)$ and $T_k^{eq}(\mathbf{X}, t)$ as the mean velocity and temperature of simulator k at the location \mathbf{X} and time t . They can be considered as the local values corresponding to the Eulerian quantities at field position \mathbf{x} , such as $U_i(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$, and $U_i = \langle u_i^{eq} \rangle$, $U^2/2 + c_v T = \langle u^{eq2}/2 + c_v T^{eq} \rangle$ in a computational cell, where c_v is the specific heat at constant volume. Additionally, we defined $c'_i = c_i - u_i^{eq}$ and $c''_i = c_i - U_i$ as the thermal velocity corresponding to u_i^{eq} and U_i , respectively, where $\langle c'_i \rangle = \langle c''_i \rangle = 0$. In Refs. [14–17] the molecular motions are calculated based on explicit solutions of the Langevin model (3), where the corresponding mean quantities of simulators are assumed to be constant during the molecular motion in a time step Δt , i.e.,

$$u_{k,i}^{eq}(\mathbf{X}, t_0 + t') = u_{k,i}^{eq}(\mathbf{X}_0, t_0) \text{ and } T_k^{eq}(\mathbf{X}, t_0 + t') = T_k^{eq}(\mathbf{X}_0, t_0), \quad (4)$$

where $t' \in [0, \Delta t]$, $\mathbf{X}_0 = \mathbf{X}(t_0)$ is the simulator's location at the initial time t_0 . Combining Eqs. (3) and (4), the molecular motion of the simulator k can be solved explicitly,

$$\Delta X_{k,i} = X_{k,i}^{t_0 + \Delta t} - X_{k,i}^{t_0} = u_{k,i}^{eq}(\mathbf{X}_0, t_0) \Delta t + \Delta X_{k,i}^D, \quad (5)$$

where $\Delta X_{k,i}^D$ is the thermal motion. Afterwards, by using the integral solutions of the Langevin model [14,17,40], the thermal motion and molecular velocities of simulators can be sampled as

$$\Delta X_{k,i}^D = c'_{k,i}(t_0) \frac{1 - e^{-\zeta \Delta t}}{\zeta} + F^{1/2} \tilde{\psi}_{1,i}, \quad (6a)$$

$$c_{k,i}(t_0 + \Delta t) - u_{k,i}^{eq}(t_0) = c'_{k,i}(t_0) e^{-\zeta \Delta t} + \frac{H}{F} F^{1/2} \tilde{\psi}_{1,i} + \left(G - \frac{H^2}{F} \right)^{1/2} \tilde{\psi}_{2,i}, \quad (6b)$$

with

$$F = \frac{k_B T^{eq}}{m \zeta^2} (4e^{-\zeta \Delta t} - e^{-2\zeta \Delta t} + 2\zeta \Delta t - 3), \quad (7a)$$

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