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DNS of differential thermal and mass diffusions in free turbulent shear flows

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Abstract

The diffusion of scalars in turbulent flows is the combined effect of the molecular diffusion and the turbulent diffusion, and the latter usually dominates. We investigated the diffusion of scalars with different diffusivities through two canonical free turbulent shear flows, i.e., the mixing layer and the homogeneous isotropic flow, by means of direct numerical simulation (DNS). In the mixing layer, the molecular diffusion has a big impact on the diffusion of scalars in the laminar region where the scalar gradient is high. In the turbulent region, the molecular diffusion has a negligible effect on the diffusion. In the homogeneous isotropic flow, the higher molecular diffusivity strengths the dispersion of scalars of relatively smaller values. However, the molecular diffusion exhibits a counter effect on the scalar diffusion for the relatively larger value. This work is intended to figure out the feasibility of the assumption that the thermal and mass diffusions of a contaminated content are equal, in other words, unit Lewis number assumption, which is often adopted.

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1. Introduction

One of the most prominent features of turbulence is the strong mixing effect of contaminants contained in turbulent flows. When heating (or cooling) is relatively mild, the temperature field can be readily assumed to be a passive scalar. On the other hand, when the concentration of a species is not too high to affect the bulk density of the fluid significantly, the mass concentration can also be treated as a passive scalar. In turbulent flows, the turbulent diffusion is generally orders of magnitude higher than the molecular diffusion. Therefore the difference between the thermal diffusivity and the mass diffusivity is usually neglected when the mean values of temperature and the mass concentration are of interest. The assumption of unit Lewis number (the ratio of thermal diffusivity to mass diffusivity) has been adopted in many studies (combustion, aerosol, etc).

However, there are various situations that neglecting the difference between thermal diffusivity and mass diffusivity may cause large errors in evaluating a physical quantity which strongly depends on the actual probability distribution

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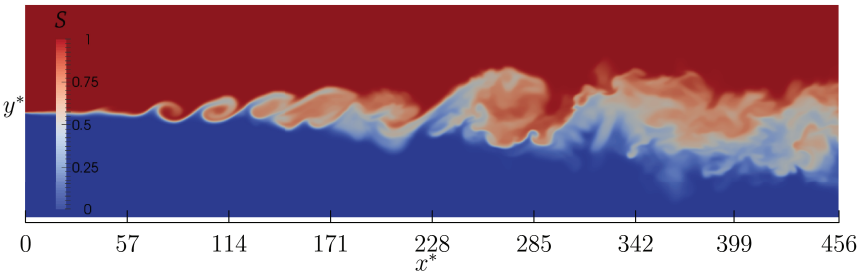

Fig. 1. A snapshot of the scalar concentration S.

functions (pdfs) of the temperature and mass concentration. One typical example is to determine the mean nucleation rate of aerosol particle in turbulent flows [1]. Nucleation refers to the process of gas-to-particle conversion, such as the formation of fog (fine water droplets) due to the supersaturation of water vapor. The nucleation rate (number of particle formed per unit volume per unit time) is an exponential function of temperature and vapor concentration, which is extremely sensitive to the small fluctuations of temperature and vapor concentration. Hence, it is important to quantify how big the error is when adopting the unit Lewis number assumption for such cases.

Direct numerical simulations were carried out to investigate the differential thermal and mass diffusions in canonical free turbulent shear flows, i.e., turbulent mixing layer and homogeneous isotropic turbulence. This research is a part of the project to determine the Lewis number effect on the aerosol nucleation rate in turbulent flows.

2. Methodology and Configurations

2.1. Numerical schemes

The numerical code adopts the finite difference scheme on structured grid, which was developed at Standford University [2] and was adapted by the authors for the current research.

Besides the Navier-Stokes equations, the control equation for a passive scalar is also solved

$$\frac{\partial S}{\partial t} + \nabla \cdot (\vec{u}S) = D\nabla^2 S \tag{1}$$

where S is a scalar value (which could be the temperature or the mass fraction), $\vec{u}$ is the flow velocity, and D is the diffusivity. In this work, three scalars with different diffusivities were simulated, i.e., $D_+ = 3.8 \times 10^{-5}$ s^2/m, $D = 1.9 \times 10^{-5}$ s^2/m, and $D_- = 8.4 \times 10^{-6}$ s^2/m. The corresponding scalars are denoted as S_+, S, and S_-.

The simulations were performed on a 64 cores workstation in parallel. More details about the numerical schemes can be found in Ref. [3].

2.2. Mixing layer

The computational domain is a canonical mixing layer with $768 \times 398 \times 16$ grid nodes. The streamwise velocities are $u_1 = 15$ and $u_2 = 5$ m/s for the top and bottom streams. The momentum thickness at the inlet is $\delta = 0.028$ mm, the normalized dimension is $456 \times 365 \times 9.5$ ($x^* = x/\delta$, $y^* = y/\delta$, and $z^* = z/\delta$).

Figure 1 is a snapshot of the scalar S on a 2d slice along the $x - y$ plane (clipped in the y direction), showing the configuration of the mixing layer. Three scalars with value 1 (for convenience) are injected along the fast stream at the the upper inlet simultaneously. Along the z direction, periodic boundary condition is used.

2.3. Homogeneous isotropic turbulence

The computational domain is a box of $256 \times 256 \times 256$ uniform grids with periodic boundary conditions in each direction. The velocity field is initialized by the Passot-Pouquet spectrum [4] with turbulent Reynolds number $\mathrm{Re}_t =$

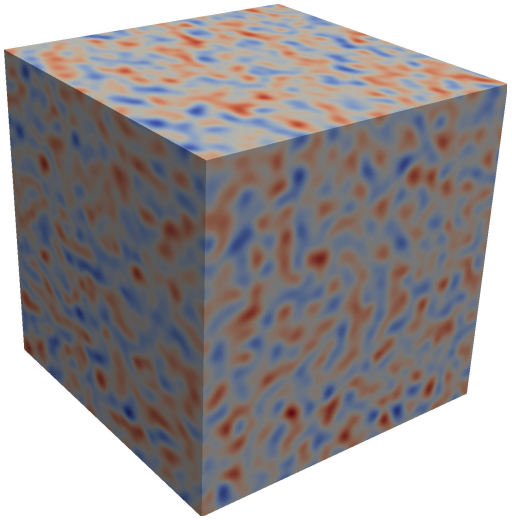

Fig. 2. Contours of initial velocity magnitude on the bounding box of the simulation domain for homogeneous isotropic turbulence.

247. Three blobs of scalars $S_+ = S = S_- = 1$ are released in the center of the domain at zero time. Figure 2 shows the contours of the initial velocity magnitude on the bounding box of the simulation domain.

3. Results and discussion

3.1. Mixing layer

Along the flow direction the mixing layer can be separated into three regions, i.e., the laminar region, the transition region and the turbulent region. The method to quantify the three regions can be found in Ref. [3]. Here, $x^* < 50$ is the laminar region, $50 < x^* < 230$ is the transition region, and $x^* > 230$ is the turbulent region.

Numerical simulation results show that the statistical mean cross profiles of the three scalars with different diffusivities are almost identical (not shown), which means that the mean value of a scalar is mostly determined by turbulent diffusion, and molecule diffusion has a negligible effect.

Figure 3 shows the scatter of scalars at various x^* locations, which describes the correlation between the scalars at various cross planes. In the laminar region (Fig. 3(a)), the scatter points collapse to two smooth curves (for S_+ vs S and S_- vs S, respectively). There is almost no randomness can be observed. At the cross plane $x^* = 30$, the scalar profile has a very sharp transition from 0 to 1, resulting a very high scalar gradient along the cross direction. The significant deviation from linear correlation (which should be a straight diagonal line) between the scalars comes from the high gradient. The scalar S_+ with a larger diffusivity has a lower value than S near 1, but a higher value than S near 0. That is because stronger molecular diffusion will make more scalars diffuse to the lower region from the higher region. And vice versa for S_-. At the cross plane $x^* = 60$ (Fig. 3(b)), scatter points show higher randomness than those at $x^* = 30$ due to the transition to turbulence. At $x^* = 120$ (Fig. 3(c)), even higher randomness is observed. However, the deviation from linear correlation becomes very small. At $x^* = 422$ (Fig. 3(d)) in the turbulent region, the randomness is small, and systematic deviation from the linear correlation is not existed. From these results, it can be concluded that the molecular diffusion dominates where the scalar gradient is high and the turbulence is weak. In the mixing layer configuration, molecular diffusion has a negligible impact on the scalar diffusion in fully turbulent region.

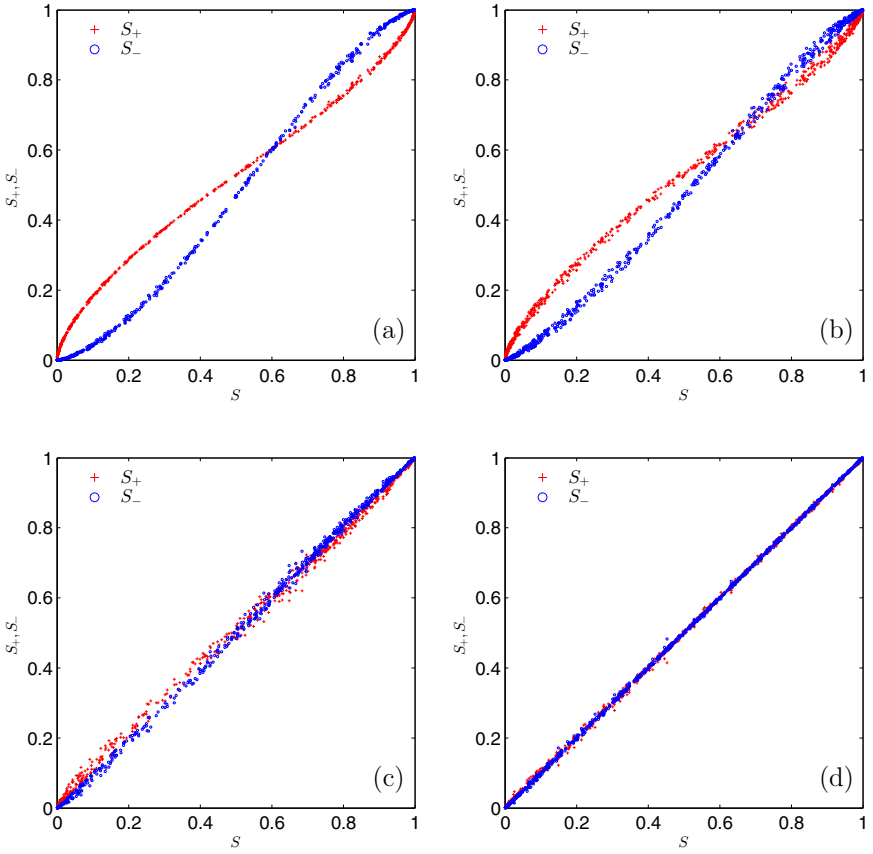

Fig. 3. Scatter of scalars at various x^* locations in the mixing layer. (a) $x^* = 30$; (b) $x^* = 60$; (c) $x^* = 120$; (d) $x^* = 422$.

3.2. Homogeneous isotropic turbulence

For the scalar blob diffusion in the homogeneous isotropic decaying turbulence simulated here, the maximum value of the scalar field decays exponentially with time. At the beginning, the flow distorts the scalar blob. Then the flow may tear the blob to parts, which may render islands or holes in the iso-contour of the scalar (not shown).

Figure 4 shows the scatter of scalars at different time. The patterns of the scatters are similar at different time, except for the decaying magnitude of the scalars. Overall, the spreading of the scatter points increases with time, which demonstrates an ever stronger effect of turbulent diffusion. For relatively smaller value of scalar, higher molecular diffusivity strengths the dispersion of scalars. However, molecular diffusion exhibits a counter effect on the scalar diffusion for a relatively larger value of scalar.

4. Conclusion

The diffusion of scalars with different molecular diffusivities in two free shear turbulent flows, i.e., the mixing layer and the homogeneous isotropic flow, was investigated by means of direct numerical simulation. In the mixing layer, the molecular diffusion has a big impact on the diffusion of scalar in the laminar region where the scalar gradient is high. In the turbulent region, the molecular diffusion has a negligible effect on the diffusion compared with the turbulent diffusion.

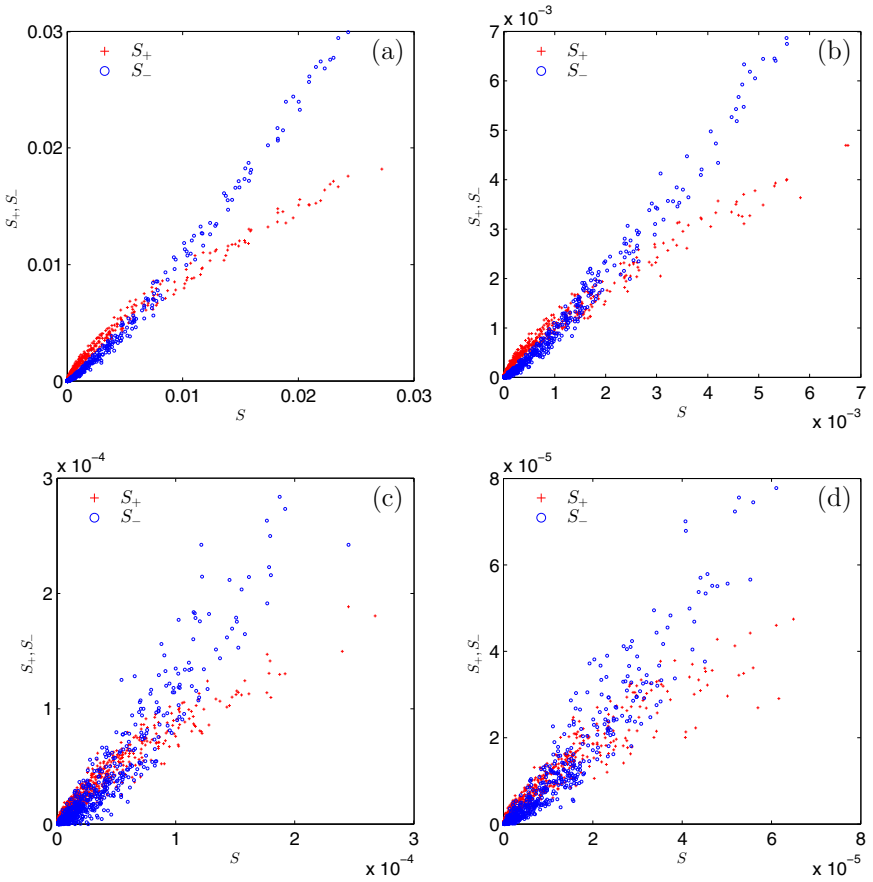

Fig. 4. Scatter of scalars at various time in the homogeneous isotropic turbulence. (a) 0.05 s; (b) 0.1 s; (c) 1.5 s; (d) 1.2 s.

In the homogeneous isotropic flow, higher molecular diffusivity strengths the dispersion of scalars of relatively smaller values. However, the molecular diffusion exhibits a counter effect on the scalar diffusion for the relatively larger value.

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