TRANSPORTATION PROPERTIES OF SCALAR TURBULENCE AT DIFFERENT MOLECULAR PRANDTL NUMBERS

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ABSTRACT

The transportation property of scalar turbulence is studied at various molecular Prandtl numbers in both homogeneous and inhomogeneous turbulence. The results show that the Reynolds averaged Prandtl number is a linear reciprocal function of molecular Prandtl number, whereas subgrid Prandtl number takes a minimum around Pr~1 in LES. The variation of turbulent Prandtl number with molecular Prandtl number can be well interpreted by the transportation mechanism at different molecular Prandtl numbers.

1. INTRODUCTION

The scalar flux in turbulence is of great importance to practical applications, both in engineering and in natural environment. The eddy diffusion model is commonly used in practice, where the Reynolds averaged scalar flux is characterized by means of turbulent Prandtl number Pr_T, i.e. the ratio of eddy viscosity to eddy diffusivity. For simplicity, the turbulent Prandtl number is usually assumed as a constant around 0.8 for turbulent shear flows in engineering calculation. However, model of constant turbulent Prandtl number is questionable in consideration of the different transportation regimes of scalar turbulence at various molecular Prandtl number (Tennekes and Lumley, 1972). For instance, at greater molecular Prandtl number (Pr>1) scalar turbulence is transported by inertial-convection in the inertial subrange; whereas there is inertial-diffussion transportation in the inertial subrange at very small molecular Prandtl numbers (Pr<<1)

In large eddy simulation of turbulence, the subgrid Prandtl number Pr_t is also utilized for evaluation of the turbulent subgrid flux of scalar when an eddy viscosity type model is used for the subgrid Reynolds stress. The subgrid Prandtl number was investigated by Moin et al (1991) in an uniform shear flow at Pr=0.2, 0.7 and 2.0. They found that subgrid Prandtl numbers were approximately around 0.8. However, their results showed some regular variation of subgrid Prandtl number with molecular Prandtl number; for instance, the subgrid Prandtl number took minimum around Pr=0.7 (see Figure 5 of their paper).

In this paper we investigate the turbulent scalar flux in both homogeneous and inhomogeneous turbulence at different molecular Prandtl numbers. Two testing cases are studied, namely statistically stationary isotropic turbulence with uniform mean scalar gradient and turbulent channel flow with constant scalar at the wall. The results show evident variation of turbulent Prandtl number with molecular Prandtl number.

2. THE GOVERNING EQUATIONS AND NUMERICAL METHODS

The governing equations for the stationary isotropic turbulence with constant mean scalar gradient can be written as

$$\frac{\partial u_i}{\partial x_i}=0 \tag{1}$$

$$\frac{\partial u_i}{\partial t}+u_j\frac{\partial u_i}{\partial x_j}=-\frac{1}{\rho}\frac{\partial p}{\partial x_i}+\nu\frac{\partial^2 u_i}{\partial x_j \partial x_j}+f_i \tag{2}$$

$$\frac{\partial \theta}{\partial t}+u_j\frac{\partial \theta}{\partial x_j}=\kappa\frac{\partial^2 \theta}{\partial x_j \partial x_j}-u_3 G \tag{3}$$

in which u_i is velocity fluctuations and f_i is the random force imposed at lower wave numbers; θ is the scalar fluctuation and G is the mean scalar gradient in x_3 direction, thus $-u_3 G$ is the source term for scalar turbulence. Coefficients ν and κ are molecular viscosity and diffusivity respectively, and $\nu/\kappa = Pr$ is defined as molecular Prandtl number.

Since both flow turbulence and scalar turbulence are homogenous in this case we can pose periodic conditions in three spatial directions and spectrum method is the best choice for numerical computation. The initial velocity spectrum is constructed by the method proposed by Rogallo (1981) and the random forcing term is imposed in the low wave numbers as proposed by Overholt and Pope (1998). The grid resolution is 256^3 and Taylor-scale Reynolds number equals to 50; the molecular Prandtl numbers range from 0.1 to 3.0.

In the turbulent channel flow, which is driven by longitudinal pressure gradient, the governing equation can be written as

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{4}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{5}$$

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \kappa \frac{\partial^2 \theta}{\partial x_j \partial x_j} \tag{6}$$

in which θ is the instantaneous quantity of scalar turbulence, i.e. its mean plus fluctuation. The flow Reynolds number is 2666, based on the bulk velocity and half width of the channel and molecular Prandtl number ranges from 0.3 to 1.2. The grid number is assigned as 128□129□128 in longitudinal, normal and spanwise direction respectively. Constant scalar values are posed at the channel walls with $\theta = -1$ at $y = -1$ and $\theta = 1$ at $y = 1$. Both flow and scalar field are homogeneous in longitudinal and spanwise directions, hence the periodical condition is posed and Fourier decomposition is used in these directions. In the normal direction flow variables are decomposed by Chebyshev polynomials. The equation is solved numerically by pseudo-spectrum method. The details of the numerical scheme can be found elsewhere (Xu et al 1996)

3. RESULTS AND DISCUSSIONS

3.1 Reynolds averaged Prandtl number

Figure 1 shows the variation of Reynolds averaged Prandtl number, which is defined as $Pr_T = \nu_T/\kappa_T$, with molecular Prandtl number in stationary isotropic turbulence. The eddy viscosity ν_T is calculated by k-ε model, i.e. $\nu_T = C_\mu k^2/\varepsilon$ with C_μ=0.09, and eddy diffusivity is determined by $\kappa_T = -\langle u_3\theta\rangle / G$. The relationship between Pr_T and Pr can be best fitted by a linearly reciprocal function $Pr_T = A + B/Pr$ with A=0.332 and B=0.0077 at Re_λ=50.

Figure 2 presents Reynolds average Prandtl number in the outer layer of the turbulent channel flow, i.e. Y^+>30, in which $\nu_T = -\langle u'v'\rangle / (\partial U/\partial y)$ and $\kappa_T = -\langle v'\theta'\rangle / (\partial\langle\theta\rangle/\partial y)$. The variation of Pr_T is also best fitted by a linear reciprocal function $Pr_T = A + B/Pr$ as given in Figure 2 (a). Note that the Taylor-scale Reynolds number is varied in the channel flow and we can consider the both A and B as functions of Taylor-scale Reynolds number, which is calculated by $Re_\lambda = \sqrt{2K/3}\sqrt{10\nu K/\varepsilon}/\nu$ with K, ε equaling to turbulent kinetic energy and dissipation. The variation of coefficients A and B with Taylor-scale Reynolds number is shown in Figure 2 (b). The turbulent flow in the outer layer of the channel can be regarded as fully developed, hence we may conclude that the linear reciprocal relationship between Reynolds average Prandtl number and molecular Prandtl number is a common rule in fully developed turbulence.

The linear reciprocal relationship indicates that the eddy diffusivity is smaller at low molecular Prandtl number or the scalar flux is smaller at lower molecular Prandtl number. It can be well understood if we look at the spectrum of scalar flux $E_{w\theta}(k)$, shown in Figure 3 (a) for isotropic turbulence. The narrower band of spectrum at smaller molecular Prandtl number indicates that the diffusion is stronger in the transportation. The total scalar flux can be calculated by the integration of $E_{w\theta}(k)$ in spectral space, i.e. $h = \int E_{w\theta}(k)dk$. The eddy diffusivity is proportional to the flux and turbulent Prandtl number is inverse proportion to the flux. The reciprocal of the scalar flux, scaled on the mean gradient G, grid mesh Δ and root mean square of velocity fluctuation w_{rms}, is denoted by H, which is proportional to turbulent Prandtl number. Figure 3 (b) shows that H is also a linear reciprocal function of molecular Prandtl number. In summary, the spectral analysis interprets the linear reciprocal relationship between Pr_T and Pr. Similar analysis can be made for turbulent channel flow in which one dimensional spectrum of scalar flux is used since the flow is inhomogeneous in normal direction. Figure 4 (a) is the scalar flux calculated from the one dimensional spectra at different Y^+ and molecular Prandtl numbers. Figure 4 (b) shows relationship between H and molecular Prandtl number in some location of outer layer in the channel. The results confirm the linear reciprocal relationship between turbulent Prandtl number and molecular Prandtl number.

3.2 Subgrid Prandtl number

The subgrid Prandtl number is defined by $Pr_t = \nu_t/\kappa_t$, in which ν_t is subgrid eddy viscosity and κ_t is subgrid eddy diffusivity. If we use dynamic procedure, proposed by Germano and Piomelli (1991), for gradient transportation model of Smagorinsky type, the subgrid eddy viscosity and diffusivity can be expressed as $\nu_t = C\Delta_1^2|S|$ and $\kappa_t = D\Delta_1^2|S|$. The coefficients C and D are determined as follows

$$C = -L_{ij}M_{ij} / 2\Delta_1^4 M_{ij}M_{ij} \tag{7}$$

$$D = -L_j M_j / \Delta_1^4 M_j M_j \tag{8}$$

in which $M_{ij}=\alpha^2|S|S_{ij}-|S|S_{ij}$, $M_j=\alpha^2|S|R_j-|S|R_j$ and $L_{ij}=\left(\overline{\hat{u}_i\hat{u}_j}-\overline{\hat{u}_i}\,\overline{\hat{u}_j}\right)-\delta_{ij}\left(\overline{\hat{u}_k\hat{u}_k}-\overline{\hat{u}_k}\,\overline{\hat{u}_k}\right)/3$, $L_j=\left(\hat{u}_i\theta-\hat{u}_i\theta\right)$, $|\hat{S}|=\left(2\hat{S}_{ij}\hat{S}_{ij}\right)^{1/2}$; $\hat{S}_{ij}$ is the filtered strain rate and $\hat{R}_j$ is filtered gradient of scalar.

The upper hat ^ is the first filtering with length Δ and upper bar denotes the second filtering with length $\alpha\Delta$, in which α=2 is adopted in computation. In terms of the dynamic coefficients C and D the turbulent Prandtl number can be expressed simply as

$$Pr_t=\nu/\kappa=\langle C\rangle/\langle D\rangle \qquad (9)$$

The results of subgrid Prandtl number for isotropic case are presented in Figure 5 and for turbulent channel flow in Figure 6. While Reynolds averaged Prandtl number is a linearly reciprocal function of molecular Prandtl number, the subgrid Prandtl number takes a minimum around Pr~1.0.

The behavior of subgrid Prandtl number can be well interpreted in terms of the transportation of scalar flux from resolved part to unresolved part. In spectral space the governing equation of scalar turbulence and its filtered form can be written as follows

$$\left(\partial/\partial t+2\kappa k^2\right)E_\theta(k)=T_\theta(k)+A\theta^* w \qquad (10)$$

$$\left[\partial/\partial t+2(\kappa+\kappa_t)k^2\right]E_\theta^<(k)=T_\theta^<(k)+A\theta^{*<}w^< \qquad (11)$$

in which $T_\theta(k)$ is the transfer spectrum for scalar flux and $T_\theta^<(k)$ is the counterpart of $T_\theta(k)$ for resolved turbulence; and the subgrid Prandtl number is defined as

$$2\nu_t k^2 E_\theta^<(k)/Pr_t=-\left(T_\theta(k)-T_\theta^<(k)\right)=-T_\theta^>(k) \qquad (12)$$

The transfer spectrum of scalar flux and its resolved part are computed by the following equations

$$T_\theta(k)=Im\left[\theta^*(k)k_j\int u_j(\bar{p})\theta(k-\bar{p})d\bar{p}\right] \qquad (13)$$

$$T_\theta^<(k)=T_\theta(k)\ for\ |k|,|\bar{p}|,|k-\bar{p}|<k_c;\quad =0,\ otherwise \qquad (14)$$

in which k_c is the cutoff wave number. $T_\theta^>(k)$ is then computed simply by the subtraction of $T_\theta^<(k)$ from $T_\theta(k)$ and it is shown in Figure 7.

The cutoff wave number is 64. The negative value of transfer spectrum indicates import of scalar flux from resolved scale turbulence into subgrid scalar turbulence. The import is larger at greater Prandtl number. To estimate the total transfer of scalar flux from the resolved scale to subgrid scale turbulence of passive scalar, we calculate the integration of $T_\theta^>(k)$, i.e.

$$\Pi_\theta^>=\int T_\theta^>(k)dk \qquad (15)$$

$\Pi_\theta^>(k)$ can be regarded as the production of subgrid scalar flux and is shown in Figure 8. It clearly shows a maximum of $\Pi_\theta^>(k)$ around Pr=1.0 (less than 1) and thus there should be a minimum of Pr_t according to equation (12). This is the explanation why the subgrid Prandtl number takes a minimun around Pr=1.0

In the turbulent channel flow the transportation of turbulent flux between resolved and unresolved scalar turbulence can be computed in physical space as follows

$$\frac{1}{2}\frac{\partial\langle\theta'\rangle^2}{\partial t}=\frac{1}{2}\kappa\frac{\partial^2\langle\theta'^2\rangle}{\partial x_j\partial x_j}-\kappa\left\langle\frac{\partial\theta'}{\partial x_j}\frac{\partial\theta'}{\partial x_j}\right\rangle-\left\langle\theta'\frac{\partial\left(u_j\theta-\overline{u_j\theta}\right)}{\partial x_j}\right\rangle \qquad (16)$$

The last term of equation (16) represents the transportation of turbulent scalar energy from resolved to unresolved part and it should be proportional to the subgrid eddy diffusivity. That is

$$Tr=-\left\langle\theta'\partial\left(u_j\theta-\overline{u_j\theta}\right)/\partial x_j\right\rangle\propto\kappa_t \qquad (17)$$

The result of Tr verse molecular Prandtl number is plotted in Figure 9, in which a maximum of transportation appears around Pr~1, equivalently subgrid Prandtl number takes a minimum around Pr~1.

4. CONCLUDING REMRKS

Both Reynolds averaged Prandtl number and subgrid Prandtl number are varying with the molecular Prandtl number in fully developed turbulence. Constant turbulent Prandtl number, either in RANS or LES, can be accepted for large molecular Prandtl numbers, e.g. Pr>1. However great variation of turbulent Prandtl number occurs at small molecular Prandtl number, in particular Pr<<1. The reason for that is attributed to the transfer mechanism of the scalar flux between large- and small-scale of scalar turbulence.

We should emphasize that the variation property we have found in paper is only valid in the fully developed turbulence. In the near-wall region the relationship between turbulent Prandtl number and molecular Prandtl number is different from that in the outer region and behaves complicatedly as shown in Figure 10 for the subgrid Prandtl number in the near-wall region of the turbulent channel flow. The Taylor scale Reynolds number is very low in near-wall region and the turbulence is highly anisotropic with quasi-ordered motion. The near-wall behavior of scalar turbulence need to be further investigated

ACKNOWLEDGEMENT

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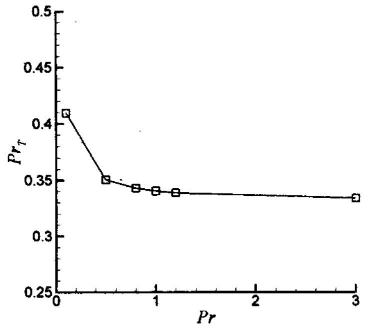
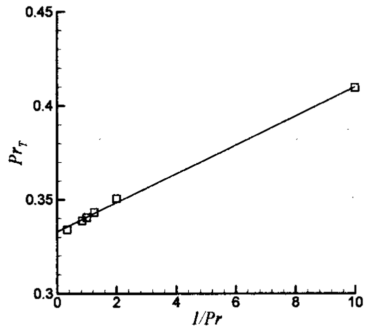
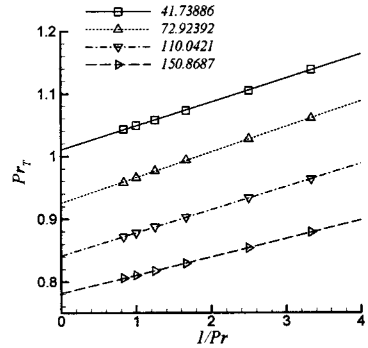


(a) Pr_T verse Pr

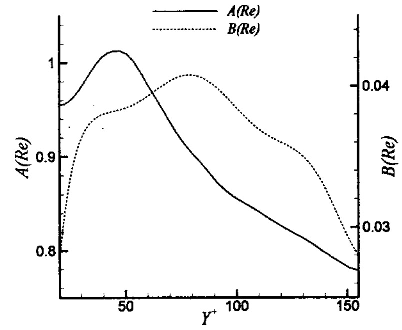


(b) Best fitted curve, Pr_T verse $1/Pr$

Figure 1 Turbulent Prandtl number verse molecular Prandtl number, in isotropic turbulence Re_λ=50

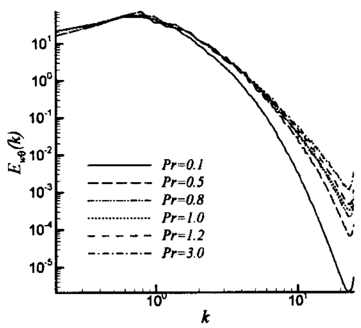


(a) Best fitted curve, Pr_T verse $1/Pr$

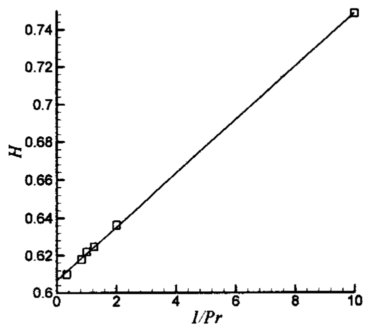


(b) Coefficients A and B

Figure 2 Turbulent Prandtl number verse molecular Prandtl number in turbulent channel flow with Re=2666

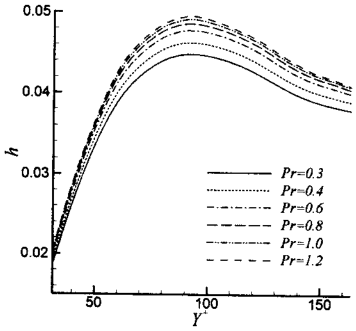


(a) Spectrum of scalar flux

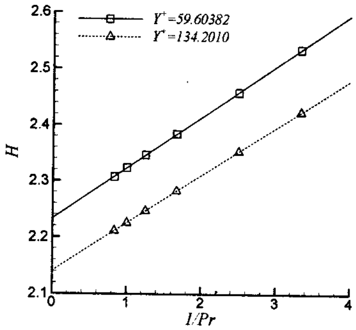


(b) Integration of spectrum of (a)

Figure 3 Spectrum analysis in isotropic turbulence



(a) The variation of scalar flux, calculated by one-dimensional spectrum



(b) *H* verse *Pr*

Figure 4 Interpretation of linear reciprocal relationship between Pr_T and *Pr* by spectrum analysis in channel flow

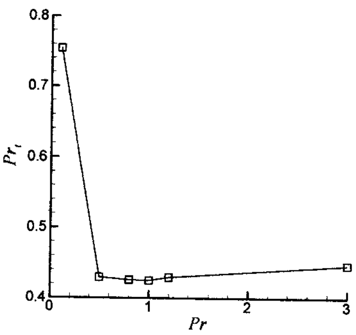


Figure 5 Subgrid Prandtl number Pr_t verse *Pr* in isotropic turbulence

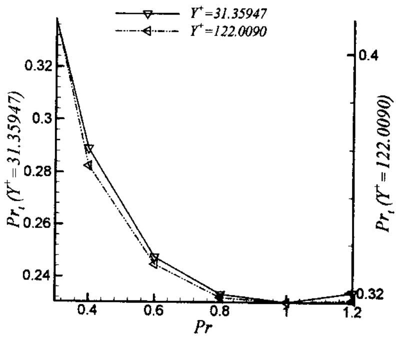


Figure 6 Subgrid Prandtl number Pr_t verse *Pr* In the outer layer of a turbulent channel flow

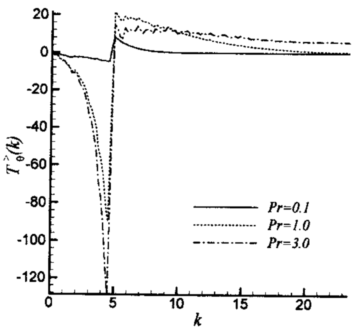


Figure 7 The transfer spectrum of scalar flux for isotropic turbulence with constant mean scalar gradient at Re_λ=50

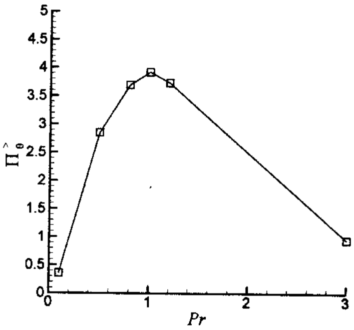


Figure 8 Production of subgrid scalar flux for isotropic turbulence with constant mean scalar gradient at Re_λ=50

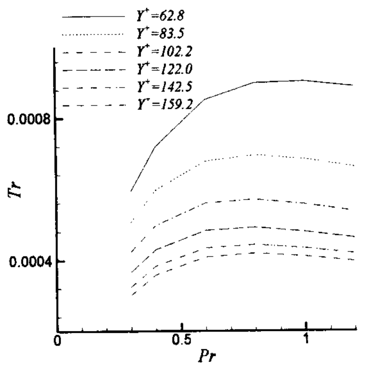


Figure 9 Transportation of scalar flux between resolved and unresolved turbulence in turbulent channel flow

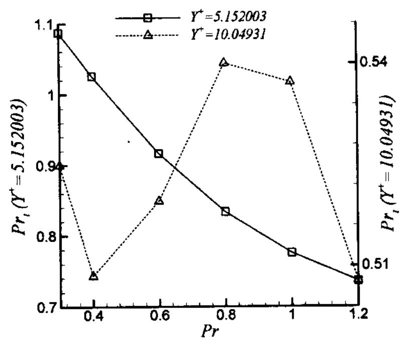


Figure 10 The subgrid turbulent Prandtl number in the near wall region of a turbulent channel flow