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Statistical modelling of passive-scalar diffusion in turbulent shear flows

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Modelling of turbulent passive-scalar diffusion is studied using the statistical results from a two-scale direct-interaction approximation. In this model, the mean scalar, the scalar variance and the dissipation rate of scalar variance constitute fundamental diffusion quantities. The turbulent scalar flux is written in the form of an anisotropic eddy-diffusivity representation. This representation, paving the way for explaining anisotropic heat transport, is tested against typical experimental data. The present model equation for the dissipation rate of scalar variance also gives a theoretical justification for the existing equations that are adopted in the second-order models.

1. Introduction

In the study of scalar diffusion (for instance, temperature diffusion) in turbulent shear flows, numerical simulation based on some kind of turbulence model is becoming quite useful with the rapid progress of computers. Among various levels of models, those of eddy diffusivity as well as eddy viscosity, represented by the k–ϵ model, are most popularly used, mainly owing to the simplicity of model. In almost all eddy-diffusivity models, the turbulent scalar flux is modelled using the concept of isotropic eddy diffusivity. A drawback of such models is that they cannot predict the anisotropy of turbulent scalar flux that arises from the mean velocity gradient. Moreover, the dependence of the turbulent Prandtl number on the molecular Prandtl number cannot be explained by most of those models.

In order to overcome such difficulties, second-order models have been developed, where no modelling of Reynolds stress and scalar flux is done. A representative model for passive-scalar diffusion is that of Newman, Launder & Lumley (1981). This model was extended by Elghobashi & Launder (1983) to apply to the thermal mixing layer. Various models for scalar diffusion are reviewed extensively by Rodi (1980). One major complexity of the second-order models is that third-order correlations concerning the velocity and scalar as well as the scalar-pressure-gradient correlation should be modelled using second-order quantities. Such modelling inevitably introduces uncertainties that are not encountered in simple eddy-viscosity and eddy-diffusivity models.

A big obstable common to k–ϵ and second-order modelling is that there has been no theoretical justification of the model equation for the dissipation rate of scalar variance using two-point closure theories such as the direct-interaction approximation (DIA). This situation not only makes the mathematical base of scalar-diffusion models uncertain, but it also becomes a big obstacle when some additional effects such as buoyancy are incorporated into existing models. Therefore, it is important to study the statistical modelling of turbulent scalar diffusion by using two-point closure theories. In particular, the recent progress in large-eddy and full simulations is increasing the importance of such statistical modelling, for model constants can be determined using those simulations once the form of model is suggested by two-point closure theories.

The statistical study of turbulent flows with mean velocity and temperature gradients by two-point closure theories was initiated by Kraichnan using DIA (Kraichnan 1959, 1964). In the case of a velocity gradient, this pioneering work was extended by Leslie (1973) using two coordinate systems, the centroid and difference coordinates. The author then combined DIA with a scale-parameter expansion method from perturbation methods to formulate a two-scale DIA (TSDIA). Using TSDIA, an anisotropic eddy-viscosity representation for the Reynolds stress was derived leading to the possibility of explaining the anisotropy of turbulent intensities within the framework of k–ϵ modelling (Yoshizawa 1984*b*). This representation has been applied to channel and duct flows, and its usefulness has been confirmed (Nisizima & Yoshizawa 1987; Speziale 1987). A theoretical justification was also given to model equations for the dissipation rate of turbulent kinetic energy that are used in both the k–ϵ and the second-order models (Yoshizawa 1987).

In this paper, we make use of the results from TSDIA to overcome some deficiencies of eddy-diffusivity models in scalar turbulent diffusion. Namely, we derive a coupled system of model equations for the mean scalar, the scalar variance and the dissipation rate of scalar variance, into which an anisotropic eddy-diffusivity representation for the turbulent scalar flux is incorporated. Some of the present results are shown to give a theoretical justification to existing model equations that have been applied with some success to real simulations. Also, the anisotropic eddy-diffusivity representation is tested directly using experimental data of Tavoularis & Corrsin (1981, 1985), and its usefulness is confirmed.

2. Ensemble-mean form of the fundamental equations

We denote the ensemble mean of the velocity and passive scalar by $\boldsymbol{U}$ and Θ, and their fluctuations by $\boldsymbol{u}'$ and θ'. Then, the equation for Θ is

$$\frac{\mathrm{D}\Theta}{\mathrm{D}t} \equiv \left(\frac{\partial}{\partial t}+U^a\frac{\partial}{\partial x^a}\right)\Theta = \frac{\partial}{\partial x^a}\left(H^a+\kappa\frac{\partial\Theta}{\partial x^a}\right), \tag{1}$$

where κ is the molecular scalar diffusivity, $\boldsymbol{H}$ is the turbulent scalar flux defined by

$$\boldsymbol{H} = -\langle\theta'\boldsymbol{u}'\rangle, \tag{2}$$

($\langle\ \rangle$ denotes the ensemble mean), and the summation convention is adopted for repeated superscripts.

The scalar variance characterizing the intensity of scalar fluctuation, which is given by

$$k_\theta = \langle\theta'^2\rangle, \tag{3}$$

satisfies

$$\frac{\mathrm{D}k_\theta}{\mathrm{D}t} = P_\theta-\epsilon_\theta+D_{k_\theta}. \tag{4}$$

Here, the production term P_θ, the dissipation term ϵ_θ (dissipation rate of scalar variance), and the diffusion term D_{k_θ} are respectively defined as

$$P_\theta = 2H^a \frac{\partial \Theta}{\partial x^a}, \tag{5}$$

$$\epsilon_\theta = 2\kappa \left\langle \left(\frac{\partial \theta'}{\partial x^a} \right)^2 \right\rangle, \tag{6}$$

$$D_{k_\theta} = -\frac{\partial}{\partial x^a} \langle \theta'^2 u'^a \rangle + \kappa \frac{\partial^2 k_\theta}{\partial x^a \partial x^a}. \tag{7}$$

In the present passive-scalar diffusion the counterparts for the velocity field are given by

$$\frac{\mathrm{D}U^\alpha}{\mathrm{D}t} = -\frac{\partial \hat{P}}{\partial x^\alpha} + \frac{\partial}{\partial x^a}\left(R^{\alpha a} + \nu \frac{\partial U^\alpha}{\partial x^a} \right), \tag{8}$$

$$\frac{\mathrm{D}k}{\mathrm{D}t} = P - \epsilon + D_k, \tag{9}$$

with the solenoidal condition

$$\frac{\partial U^a}{\partial x^a} = 0. \tag{10}$$

In (8), $\hat{P}$ is the mean pressure divided by fluid density, ν is the kinematic viscosity, and the Reynolds stress $R^{\alpha\beta}$ is defined by

$$R^{\alpha\beta} = -\langle u'^\alpha u'^\beta \rangle. \tag{11}$$

In (9), the turbulent kinetic energy k, the production term P, the dissipation term ϵ and the diffusion term D_k are written as

$$k = \tfrac{1}{2}\langle (u'^a)^2 \rangle, \tag{12}$$

$$P = R^{ab} \frac{\partial U^b}{\partial x^a}, \tag{13}$$

$$\epsilon = \nu \left\langle \left(\frac{\partial u'^b}{\partial x^a} \right)^2 \right\rangle, \tag{14}$$

$$D_k = -\frac{\partial}{\partial x^a} (\tfrac{1}{2}\langle u'^a u'^b u'^b \rangle + \langle p' u'^a \rangle + \nu \frac{\partial^2 k}{\partial x^a \partial x^a} \tag{15}$$

(p' is the fluctuation of the pressure).

3. Statistical modelling

3.1. *Statistical results from TSDIA*

A two-scale direct-interaction approximation (TSDIA) has already been applied to the investigation of an anisotropic eddy-diffusivity representation for the turbulent scalar flux and to the calculation of other important quantities (Yoshizawa 1984*a*, 1985*b*). For the modelling of scalar diffusion that follows, let us summarize the results obtained previously. A brief summary of the theoretical framework of TSDIA is given in the Appendix.

The scalar variance k_θ of (3) can be written as

$$k_\theta = a_{k_\theta}\epsilon_\theta\epsilon^{-\frac{1}{3}}l_\theta^{\frac{2}{3}} - a_{k_\theta\epsilon_\theta}\epsilon^{-\frac{2}{3}}l_\theta^{\frac{4}{3}}\frac{\mathrm{D}\epsilon_\theta}{\mathrm{D}t} + a_{k_\theta\epsilon}\epsilon_\theta\epsilon^{-\frac{5}{3}}l_\theta^{\frac{4}{3}}\frac{\mathrm{D}\epsilon}{\mathrm{D}t} - a_{k_\theta l_\theta}\epsilon_\theta\epsilon^{-\frac{2}{3}}l_\theta^{\frac{1}{3}}\frac{\mathrm{D}l_\theta}{\mathrm{D}t}, \tag{16}$$

using the characteristic length l_θ in scalar diffusion, where numerical factors are estimated as

$$a_{k_\theta} \approx 0.365, \quad a_{k_\theta\epsilon_\theta} \approx 0.0493, \quad a_{k_\theta\epsilon} \approx 0.0227, \quad k_{k_\theta l_\theta} \approx 0.194. \tag{17}$$

Roughly speaking, l_θ means the largest spatial scale of scalar fluctuations, and is similar to the concept of integral scale used frequently (for its more detailed definition, see the Appendix). We should point out that the first term in (16) comes from the zeroth-order analysis in the scale expansion of TSDIA, whereas the remaining three come from the first-order analysis.

The turbulent scalar flux $\boldsymbol{H}$ is given by

$$H^\alpha = \kappa_\mathrm{e}\frac{\partial\Theta}{\partial x^\alpha} + \kappa_{\mathrm{eA}}^{\alpha a}\frac{\partial\Theta}{\partial x^a}. \tag{18}$$

Here, the first term gives the familiar isotropic eddy-diffusivity representation, and κ_e is written as

$$\kappa_\mathrm{e} = a_\kappa l_\theta^{\frac{4}{3}}\epsilon^{\frac{1}{3}}, \tag{19}$$

where

$$a_\kappa \approx 0.0597. \tag{20}$$

The second term represents the anisotropic scalar diffusion generated by shear flows, and the anisotropic eddy diffusivity $\kappa_{\mathrm{eA}}^{\alpha\beta}$ is expressed as

$$\kappa_{\mathrm{eA}}^{\alpha\beta} = -l_\theta^2\left[a_{\kappa\mathrm{A}}\left(\frac{\partial U^\alpha}{\partial x^\beta}+\frac{\partial U^\beta}{\partial x^\alpha}\right)+a'_{\kappa\mathrm{A}}\left(\frac{\partial U^\alpha}{\partial x^\beta}-\frac{\partial U^\beta}{\partial x^\alpha}\right)\right], \tag{21}$$

where

$$a_{\kappa\mathrm{A}} \approx 8.92\times10^{-3}, \quad a'_{\kappa\mathrm{A}} \approx 0. \tag{22}$$

In TSDIA, we have approached vanishing $a'_{\kappa\mathrm{A}}$, which means that $\kappa^{\alpha\beta}$ is a symmetric tensor. As will be discussed later, the experiment by Tavoularis & Corrsin (1985) shows that it is not symmetric, although its asymmetry is not so strong; so, we shall retain the antisymmetric part in (21) to use in constructing a more accurate model relation for $\kappa_{\mathrm{eA}}^{\alpha\beta}$.

Noticing that the first and the remaining three terms in (16) are of the zeroth and the first orders in the TSDIA scale expansion, respectively, we solve (16) with respect to l_θ to obtain

$$l_\theta = C_{l_\theta}k_\theta^{\frac{3}{2}}\epsilon_\theta^{-\frac{3}{2}}\epsilon^{\frac{1}{2}} + C_{l_\theta k_\theta}k_\theta^{\frac{3}{2}}\epsilon_\theta^{-\frac{5}{2}}\epsilon^{\frac{1}{2}}\frac{\mathrm{D}k_\theta}{\mathrm{D}t} - C_{l_\theta\epsilon_\theta}k_\theta^{\frac{5}{2}}\epsilon_\theta^{-\frac{7}{2}}\epsilon^{\frac{1}{2}}\frac{\mathrm{D}\epsilon_\theta}{\mathrm{D}t} + C_{l_\theta\epsilon}k_\theta^{\frac{5}{2}}\epsilon_\theta^{-\frac{5}{2}}\epsilon^{-\frac{1}{2}}\frac{\mathrm{D}\epsilon}{\mathrm{D}t}, \tag{23}$$

where

$$C_{l_\theta} \approx 4.53, \quad C_{l_\theta k_\theta} \approx 14.8, \quad C_{l_\theta\epsilon_\theta} \approx 12.4, \quad C_{l_\theta\epsilon} \approx 3.80. \tag{24}$$

This relation will play a key role in the modelling of scalar diffusion based on k_θ and ϵ_θ that follows.

3.2. *Modelling of the ϵ_θ equation*

In turbulent scalar diffusion, l_θ, k_θ and ϵ_θ are very important quantities as the bulk properties of the diffusion process. In the model, we can choose any two of them since these three quantities are equivalent through (16) or (23). In other words, one model based on k_θ and ϵ_θ should be transferable with another model based on, for instance, k_θ and l_θ. This principle of the transferability of models requires an algebraic relationship among l_θ, k_θ and ϵ_θ. So we impose

$$l_\theta = C_{l_\theta} k_\theta^{\frac{3}{2}} \epsilon_\theta^{-\frac{3}{2}} \epsilon^{\frac{1}{2}} \tag{25}$$

by retaining only the first term in (23). As a result, we have

$$\frac{\mathrm{D}\epsilon_\theta}{\mathrm{D}t} = \lambda_{\epsilon_\theta k_\theta} \frac{\epsilon_\theta}{k_\theta} \frac{\mathrm{D}k_\theta}{\mathrm{D}t} + \lambda_{\epsilon_\theta \epsilon} \frac{\epsilon_\theta}{\epsilon} \frac{\mathrm{D}\epsilon}{\mathrm{D}t}, \tag{26}$$

where

$$\lambda_{\epsilon_\theta k_\theta} = C_{l_\theta k_\theta} / C_{l_\theta \epsilon_\theta} \approx 1.20, \tag{27}$$

$$\lambda_{\epsilon_\theta \epsilon} = C_{l_\theta \epsilon} / C_{l_\theta \epsilon_\theta} \approx 0.306. \tag{28}$$

Equation (26) shows that a model equation for ϵ_θ can be constructed from the model equations for k_θ and ϵ, with the aid of a differential transformation. The above method has already been applied to the velocity field, and a model equation very similar to the ϵ-equation in the k–ϵ and the second-order models has been obtained (Yoshizawa 1987). Thus, we have

$$\frac{\mathrm{D}\epsilon}{\mathrm{D}t} = C_{\epsilon 1} \frac{\epsilon}{k} P - C_{\epsilon 2} \frac{\epsilon^2}{k} + D_\epsilon, \tag{29}$$

where

$$C_{\epsilon 1} \approx 1.7, \quad C_{\epsilon 2} \approx 1.7, \tag{30}$$

and the remaining term D_ϵ is mainly related to the diffusion effect, and will be referred to later. In the familiar k–ϵ and second-order models, $C_{\epsilon 1}$ and $C_{\epsilon 2}$ are optimized as

$$C_{\epsilon 1} \approx 1.45, \quad C_{\epsilon 2} \approx 1.9 \tag{31}$$

(Bradshaw, Cebeci & Whitelaw 1981), which are close to (30).

We combine (26) with (4) for k_θ and (29) for ϵ. Then, we obtain

$$\frac{\mathrm{D}\epsilon_\theta}{\mathrm{D}t} = C_{\epsilon_\theta 1} \frac{\epsilon_\theta}{k_\theta} P_\theta + C_{\epsilon_\theta 2} \frac{\epsilon_\theta}{k} P - C_{\epsilon_\theta 3} \frac{\epsilon_\theta^2}{k_\theta} - C_{\epsilon_\theta 4} \frac{\epsilon_\theta \epsilon}{k} + D_{\epsilon_\theta}, \tag{32}$$

where D_{ϵ_θ} is given by

$$D_{\epsilon_\theta} = \lambda_{\epsilon_\theta k_\theta} \frac{\epsilon_\theta}{k_\theta} D_{k_\theta} + \lambda_{\epsilon_\theta \epsilon} \frac{\epsilon_\theta}{\epsilon} D_\epsilon. \tag{33}$$

Numerical factors are estimated as

$$C_{\epsilon_\theta 1} = C_{\epsilon_\theta 3} \approx 1.20, \quad C_{\epsilon_\theta 2} = C_{\epsilon_\theta 4} \approx 0.520, \tag{34}$$

using the theoretically estimated values (27), (28) and (30).

3.3. *Anisotropic eddy diffusivity*

Using (25), the isotropic and anisotropic eddy diffusivities of (19) and (21) are expressed as

$$\kappa_{\mathrm{e}} = C_{\kappa} k_{\theta}^{2} \epsilon_{\theta}^{-2} \epsilon, \tag{35}$$

$$\kappa_{\mathrm{eA}}^{\alpha\beta} = -k_{\theta}^{3} \epsilon_{\theta}^{-3} \epsilon \left[C_{\kappa\mathrm{A}} \left(\frac{\partial U^{\alpha}}{\partial x^{\beta}} + \frac{\partial U^{\beta}}{\partial x^{\alpha}} \right) + C'_{\kappa\mathrm{A}} \left(\frac{\partial U^{\alpha}}{\partial x^{\beta}} - \frac{\partial U^{\beta}}{\partial x^{\alpha}} \right) \right], \tag{36}$$

respectively, where $C_{\kappa} \approx 0.446,\ C_{\kappa\mathrm{A}} \approx 0.183,\quad C'_{\kappa\mathrm{A}} \approx 0.$ (37)

Corresponding to (18) with (35) and (36), the anisotropic eddy-viscosity representation for the Reynolds stress is given by

$$R^{\alpha\beta} = -\tfrac{2}{3} k \delta^{\alpha\beta} + \nu_{\mathrm{e}} \left(\frac{\partial U^{\alpha}}{\partial x^{\beta}} + \frac{\partial U^{\beta}}{\partial x^{\alpha}} \right) + \tau^{\alpha\beta} \tag{38}$$

(Yoshizawa 1984*b*), where $\delta^{\alpha\beta}$ is the Kronecker delta symbol, the eddy viscosity ν_{e} is written as

$$\nu_{\mathrm{e}} = C_{\nu} k^{2} \epsilon^{-1}, \tag{39}$$

with

$$C_{\nu} \approx 0.078, \tag{40}$$

and $\tau^{\alpha\beta}$ represents the anisotropic effect generated by the mean velocity gradient.

From (35) and (39), the turbulent Prandtl number Pr_{t} is

$$Pr_{\mathrm{t}} \equiv \nu_{\mathrm{e}}/\kappa_{\mathrm{e}} = (C_{\nu}/C_{\kappa})\, r^{2}. \tag{41}$$

Here, r is the ratio of the velocity dissipation timescale to the scalar one, which is defined by

$$r = \left(\frac{k}{\epsilon}\right) \Big/ \left(\frac{k_{\theta}}{\epsilon_{\theta}}\right). \tag{42}$$

As will be discussed later, r is an important quantity leading to the space and time variation of Pr_{t}.

3.4. *Summary of the anisotropic $k_{\theta}-\epsilon_{\theta}$ model*

Summarizing the results obtained above, we reach the following system of equations for passive-scalar diffusion:

(*a*) (1) for the mean scalar Θ;

(*b*) (18) for the scalar flux $\boldsymbol{H}$ with (35) (isotropic eddy diffusivity) and (36) (anisotropic eddy diffusivity);

(*c*) (4) for k_{θ} with $D_{k_{\theta}}$ modelled appropriately;

(*d*) (32) for ϵ_{θ} with $D_{\epsilon_{\theta}}$ modelled appropriately.

Here, we should mention the reliability of the present system and the model constants in it. This system is founded on TSDIA and its additional simplification (see the Appendix), and is not free from the inherent limitations arising from them. Therefore, the results should be regarded as indicative only. In particular, the model constants should be viewed as an approximation when optimizing them in actual simulation. As will be shown later, however, some of these results give a mathematical justification to the empirical relations that have already been confirmed as working well.

4. Discussion

4.1. *Turbulent Prandtl number*

In models of the k–ϵ type, the isotropic eddy diffusivity κ_e is often modelled as

$$\kappa_e = C'_\kappa k^2 \epsilon^{-1}, \tag{43}$$

corresponding to the isotropic eddy viscosity ν_e. Expression (43) can be derived if l_θ in (19) is made equal to the velocity counterpart that is given by

$$l = C_l k^{\frac{3}{2}} \epsilon^{-1}, \tag{44}$$

where C_l is estimated as

$$C_l \approx 1.84 \tag{45}$$

from TSDIA (Yoshizawa 1984*b*). C'_κ in (43) is now

$$C'_\kappa \approx 0.135 \tag{46}$$

(Yoshizawa 1984*a*), which should be compared with the value 0.1 adopted usually.

In relation to (43), we should point out the following facts. One is the decoupling of (1) from (4) since κ_e is expressed in terms of k and ϵ only. The reliability of this decoupling is rather questionable since the scalar flux $\boldsymbol{H}$ depends on scalar fluctuations whose intensity is determined by (4). Another is the independence of the turbulent Prandtl number Pr_t of the molecular Prandtl number $Pr\,(\equiv \nu/\kappa)$. In reality, from (39) and (43) we have

$$Pr_t = C_\nu / C'_\kappa, \tag{47}$$

which is constant so long as some sort of dependence of C'_κ on Pr is not assumed. Experiments show, however, the considerable dependence of Pr_t on Pr.

The above two points stem solely from the approximation

$$l_\theta \approx l. \tag{48}$$

In the present paper, from (25), (42) and (44) we have

$$l/l_\theta = A r^{\frac{3}{2}}, \tag{49}$$

where

$$A = C_l / C_{l_\theta} \approx 0.506. \tag{50}$$

In the experiment on grid turbulence by Warhaft & Lumley (1978), r varies between 0.67 and 2.38, and depends on the ratio of the initial lengthscales of velocity and temperature. This dependence was also examined by Durbin (1982) using a Lagrangian statistical model of particle dispersion (Durbin 1980; Stanpountzis *et al.* 1986). These results suggest that (48) is valid only in a very limited situation.

From (49), we have

$$r = C_r (l/l_\theta)^{\frac{2}{3}} \tag{51}$$

with

$$C_r \approx 1.57. \tag{52}$$

Herring *et al.* (1982) used some two-point closure theories such as DIA to investigate the dependence of r on the ratio of velocity and temperature integral scales L_v and L_θ. These two integral scales are a little different from our l and l_θ in definition, but the two pairs (l, l_θ) and (L_v, L_θ) are very similar in that they give a measure of the lengthscales around which the spectra of kinetic energy and scalar variance have their peaks. For large Reynolds numbers, Herring *et al.* found

$$r = 1.63 (L_v / L_\theta)^{\frac{2}{3}}. \tag{53}$$

The coincidence between (53) and (51) with (52) is remarkable even after making allowances for the difference in the definition of the lengthscales. In turbulent flows with mean fields, l and l_θ are closely associated with the state of those fields. So, r is considered to change in space and time.

In order to eliminate the above difficulty concerning Pr_t within the framework of eddy-diffusivity modelling, Nagano & Kim (1987) proposed

$$\kappa_e = C''_\kappa(k^2/\epsilon)\, r^{-\frac{1}{2}} \tag{54}$$

(C''_κ ($=0.156$) is a model constant), which should be compared with our counterpart

$$\kappa_e = C_\kappa(k^2/\epsilon)\, r^{-2}. \tag{55}$$

Nagano & Kim used (54) to examine the heat transfer in wall turbulent flows, and showed that (54) is capable of explaining the measured dependence of Pr_t on Pr. The model (54) is not always justified from the statistical viewpoint, as can be seen from (55). However, Nagano & Kim's work is interesting as an attempt to incorporate the r-dependence into κ_e.

4.2. *The ϵ_θ equation*

A model equation for ϵ_θ plays an important role in both the k_θ–ϵ_θ eddy-diffusivity and second-order models. Let us compare the present ϵ_θ equation with the counterpart that has been developed by Newman *et al.* (1981) and by Elghoboshi & Launder (1983) using the second-order modelling. In the latter two works, the second P-related term in (32), which represents the effect from the velocity production term, is not taken into account. Newman *et al.* optimized the model constants as

$$C_{\epsilon_\theta 1} \approx 1.0, \quad C_{\epsilon_\theta 3} \approx 1.01, \quad C_{\epsilon_\theta 4} \approx 0.88, \tag{56}$$

using our definition for ϵ_θ and P_θ. Elghobashi & Launder proposed

$$C_{\epsilon_\theta 1} \approx 0.9, \quad C_{\epsilon_\theta 3} \approx 1.1, \quad C_{\epsilon_\theta 4} \approx 0.80. \tag{57}$$

It is noteworthy that (34) obtained from a purely statistical method is close to (56) and (57). Moreover, Nagano & Kim (1987) proposed inclusion of the second P-related term in (32), and optimized $C_{\epsilon_\theta 2}$ as

$$C_{\epsilon_\theta 2} \approx 0.72, \tag{58}$$

as well as (57). Equation (58) is also close to the present value 0.52 in (34). From these results, it may be concluded that a theoretical justification has been given by a two-point closure theory to the model ϵ_θ equation that has been successfully used in the eddy-diffusivity and second-order models. In particular, the above comparison shows the reason why the optimized values $C_{\epsilon_\theta 1}$ and $C_{\epsilon_\theta 3}$ or $C_{\epsilon_\theta 2}$ and $C_{\epsilon_\theta 4}$ are close to each other.

The present derivation of the model ϵ_θ equation is not merely interesting in that an empirically constructed model equation can be justified using a closure theory. It also gives a clear guiding principle for incorporating effects such as those of buoyancy and MHD, the terms for which were difficult to forsee from the existing ϵ_θ equation. The principle may be summarized as follows:

(*a*) we first calculate k_θ with such effects, as in (16);

(*b*) we insert it into an expression for l_θ such as (23);

(*c*) from the transferability principle, we require an algebraic relation such as (25), which leads to a model ϵ_θ equation with the additional effects incorporated.

For instance, let us consider that the buoyancy effect adds the Boussinesq term

$\boldsymbol{A}\Theta$ into the right-hand side of (8), where $\boldsymbol{A} = -\gamma \boldsymbol{g}$ in terms of the thermal expansion coefficient γ and the gravitational acceleration vector $\boldsymbol{g}$. Then, TSDIA suggests that a term proportional to

$$\boldsymbol{A}\cdot\nabla\theta \tag{59}$$

should be added to the existing ϵ_θ equation.

In order to model the remaining diffusion-like term D_{ϵ_θ} in (32), we need to model D_ϵ and D_{k_θ}, as is seen from (33). In the previous derivation of the model ϵ-equation, it was shown (Yoshizawa 1987) that D_ϵ can be modelled, in the most general form, as

$$D_\epsilon = \frac{\partial}{\partial x^a}\left(C_{\epsilon\epsilon}\frac{k^2}{\epsilon}\frac{\partial \epsilon}{\partial x^a}\right) + \frac{\partial}{\partial x^a}\left(C_{\epsilon k}\,k\frac{\partial k}{\partial x^a}\right) + C'_{\epsilon 1}\left(\frac{\partial k}{\partial x^a}\right)^2 + C'_{\epsilon 2}\frac{k}{\epsilon}\frac{\partial k}{\partial x^a}\frac{\partial \epsilon}{\partial x^a} + C'_{\epsilon 3}\frac{k^2}{\epsilon^2}\left(\frac{\partial \epsilon}{\partial x^a}\right)^2, \tag{60}$$

using the following model relation for D_k:

$$D_k = \frac{\partial}{\partial x^a}\left(C_{kk}\frac{k^2}{\epsilon}\frac{\partial k}{\partial x^a}\right) + \frac{\partial}{\partial x^a}\left(C_{k\epsilon}\frac{k^3}{\epsilon^2}\frac{\partial \epsilon}{\partial x^a}\right). \tag{61}$$

Here, $C_{\epsilon\epsilon}, C_{\epsilon k}, \ldots, C_{k\epsilon}$ are model constants. In the usual model, only the first terms in (60) and (61) are retained. The second term in (61), expressing the diffusion effect from ϵ, was first pointed out by Leslie (1973), and then by Yoshizawa (1982). The importance of the second terms in (60) and (61) or the cross-diffusion terms has been clarified by Takemitsu (1987), who applied the k–ϵ model including such effects to channel flows. As a result, it was shown that the local minimum of ν_e on the centreline, which cannot be predicted by the usual k–ϵ model, can be simulated accurately.

Regarding the modelling of D_{k_θ}, TSDIA gives (Yoshizawa 1984*a*)

$$\langle \theta'^2 u'^a \rangle = -a_{k_\theta\epsilon}\,\epsilon_\theta\,\epsilon^{-1} l_\theta^2 \frac{\partial \epsilon}{\partial x^a} - a_{k_\theta l_\theta}\,\epsilon_\theta\, l_\theta \frac{\partial l_\theta}{\partial x^a} - a_{k_\theta\epsilon_\theta}\, l_\theta^2 \frac{\partial \epsilon_\theta}{\partial x^a}, \tag{62}$$

where the numerical factors are

$$a_{k_\theta\epsilon} \approx 1.77\times 10^{-3}, \quad a_{k_\theta l_\theta} \approx 0.0814, \; a_{k_\theta l_\theta} \approx 0.0106. \tag{63}$$

From (25) and (62), D_{k_θ} of (7) is modelled as

$$D_{k_\theta} = \frac{\partial}{\partial x^a}\left(C_{k_\theta k_\theta} k_\theta^2 \epsilon_\theta^{-2}\epsilon \frac{\partial k_\theta}{\partial x^a}\right) - \frac{\partial}{\partial x^a}\left(C_{k_\theta\epsilon_\theta} k_\theta^3 \epsilon_\theta^{-3}\epsilon \frac{\partial \epsilon_\theta}{\partial x^a}\right) + \frac{\partial}{\partial x^a}\left(C_{k_\theta\epsilon} k_\theta^3 \epsilon_\theta^{-2}\frac{\partial \epsilon}{\partial x^a}\right), \tag{64}$$

where

$$C_{k_\theta k_\theta} \approx 2.51, \quad C_{k_\theta\epsilon_\theta} \approx 2.29, \quad C_{k_\theta\epsilon} \approx 0.872, \tag{65}$$

and the κ-related term has been neglected. In the usual model, only the first term of (64) is retained. For the temperature transport in channel flows, however, the third of the three terms exerts the greatest influence (S. Nisizima, private communication). This fact can be easily understood from the situation where ϵ becomes very large near the wall since ϵ is proportional to y^{-1} (y is the distance from the wall) in the logarithmic-velocity region.

We substitute (60) and (64) into (33) to obtain D_{ϵ_θ}, which includes the diffusion and cross-diffusion terms

$$\left.\begin{aligned}
&\frac{\partial}{\partial x^a}\left(k_\theta \epsilon_\theta^{-1}\epsilon \frac{\partial k_\theta}{\partial x^a}\right), \quad \frac{\partial}{\partial x^a}\left(k_\theta^2 \epsilon_\theta^{-2}\epsilon \frac{\partial \epsilon_\theta}{\partial x^a}\right), \quad \frac{\partial}{\partial x^a}\left(k_\theta^2 \epsilon_\theta^{-1}\frac{\partial \epsilon}{\partial x^a}\right), \\
&\frac{\partial}{\partial x^a}\left(k^2 \epsilon_\theta \epsilon^{-2}\frac{\partial \epsilon}{\partial x^a}\right), \quad \frac{\partial}{\partial x^a}\left(k \epsilon_\theta \epsilon^{-1}\frac{\partial k}{\partial x^a}\right).
\end{aligned}\right\} \tag{66}$$

Quantity	$x/h = 7.5$	$x/h = 9.5$	$x/h = 11$	Units
dU/dy	46.8	46.8	46.8	s^{-1}
$d\Theta/dy$	9.5	9.5	9.5	°C m^{-1}
k	0.268	0.358	0.444	$m^2\ s^{-2}$
ϵ	1.94	2.65	3.42	$m^2\ s^{-3}$
k_θ	0.0119	0.0134	0.0156	°C^2
ϵ_θ	0.25	0.30	0.35	°$C^2\ s^{-1}$
$\langle\theta'u'\rangle$	0.0306	0.0400	0.051	°C ms^{-1}
$\langle\theta'v'\rangle$	−0.0145	−0.0184	−0.023	°C ms^{-1}

TABLE 1. Data by Tavoularis & Corrsin (1981)

Besides (66), however, D_{ϵ_θ} contains terms that cannot be classified using the familiar concepts of production, dissipation and diffusion, for instance terms such as

$$k_\theta \epsilon_\theta^{-2} \epsilon \frac{\partial k_\theta}{\partial x^a} \frac{\partial \epsilon_\theta}{\partial x^a}. \tag{67}$$

This situation was also encountered in the diffusion term D_ϵ in the ϵ-equation, (60). At the present stage, it is not clear which terms are indispensable in (66), (67), etc. This point is left for future work based on the practical application of the present model.

4.3. *Anisotropic eddy-diffusivity representation*

In the present k_θ–ϵ_θ model, the anisotropic eddy-diffusivity representation (18) with (35) and (36) plays a key role. So, let us test this model representation by using experimental data from a relatively simple flow situation. This kind of test of model relation has also been performed by Leslie (1980) for the modelling of the pressure–strain correlation.

Temperature transport in turbulent flows with a constant mean temperature gradient has been examined experimentally in detail by Tavoularis & Corrsin (1981, 1985). There, special attention was paid to the anisotropic temperature transport arising from the constant mean velocity gradient. The anisotropic part $\kappa_{eA}^{\alpha\beta}$ of our eddy diffusivity, which is given by (36), is closely related to the mean velocity gradient. Further, the Reynolds number R_λ based on the Taylor microscale in Tavoularis & Corrsin's data is about 200–270. So it is relevant to compare their data with the present result based on the concept of fully developed turbulence.

In this subsection, the mean and fluctuating velocity components in the x-, y- and z-directions are denoted by (U, V, W) and (u', v', w'), respectively. In Tavoularis & Corrsin's experiments, the mean velocity and temperature are given as

$$\frac{dU}{dy} = \text{constant}, \frac{d\Theta}{dy} \text{ or } \frac{d\Theta}{dz} = \text{constant}, \quad V = W = 0. \tag{68}$$

They measured various important turbulence properties at three points downstream of the shear generator and heating system of square-duct type (the side of the square duct is denoted by h).

Tavoularis & Corrsin's (1981) data are summarised in table 1 in our notation. Here, we should briefly discuss ϵ_θ (our ϵ_θ is twice the scalar dissipation rate of Tavoularis & Corrsin). Accurate measurement of ϵ_θ is very difficult in general. Tavoularis & Corrsin measured it by two methods: the budget equation of k_θ; and a direct

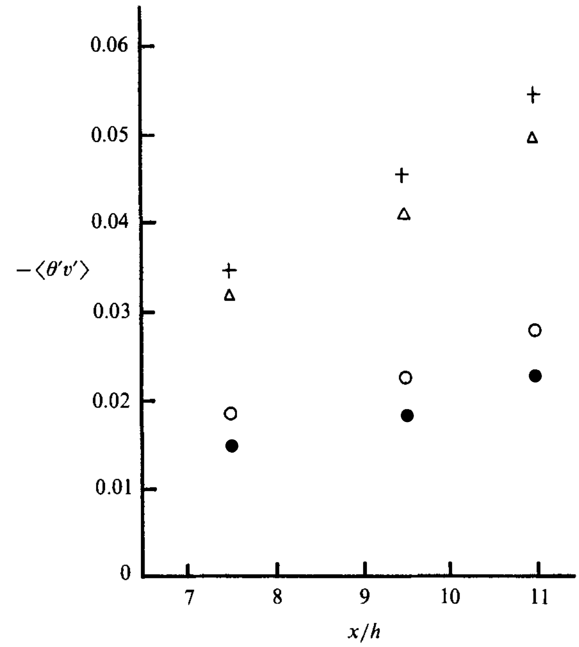

FIGURE 1. $-\langle\theta' v'\rangle$: ●, Tavoularis & Corrsin (1981); ○, present model (70); +, Nagano & Kim's (1987) model (54); △, standard model (43).

measurement using temperature derivatives. The values for ϵ_θ thus found do not coincide. In table 1, we have adopted the value obtained by the former method because, in the direct measurement of ϵ_θ, small fluctuations must be resolved more accurately than with the method based on the budget equation, and so ϵ_θ from the direct measurement tends to become smaller than ϵ_θ by the budget equation. The author considers that the latter is more reliable. Moreover, ϵ in table 1 was measured from the budget equation for k. So, making allowances for the self-consistency concerning the measurement of the dissipation rates of k and k_θ we adopted ϵ_θ from the budget equation.

In the flow configuration (68), our representation (18) with (35) and (36) gives

$$\langle\theta' u'\rangle = (C_{\kappa \mathrm{A}} + C'_{\kappa \mathrm{A}}) \frac{k_\theta^3}{\epsilon_\theta^3} \epsilon \frac{\mathrm{d}U}{\mathrm{d}y} \frac{\mathrm{d}\Theta}{\mathrm{d}y}, \tag{69}$$

$$\langle\theta' v'\rangle = -C_\kappa \frac{k_\theta^2}{\epsilon_\theta^2} \epsilon \frac{\mathrm{d}\Theta}{\mathrm{d}y}. \tag{70}$$

Of these two expressions, (70) corresponds to isotropic eddy transport, whereas (69) is the anisotropic eddy transport given rise to by the mean velocity gradient.

Let us first compare (70) with the experimental results by Tavoularis & Corrsin (1981). The comparison is shown in figure 1. In the figure, we have included the results that are obtained by the familiar representation (43) with $C'_\kappa \approx 0.1$ and by Nagano & Kim's (1987) model (54) with $C''_\kappa \approx 0.158$. Our results are fairly good. It is rather surprising that the popularly used representation (43) gives values that are too large.

Next, we proceed to the anisotropic heat transport part about which the isotropic eddy-diffusivity representation for $\boldsymbol{H}$ can say nothing. The comparison is given in

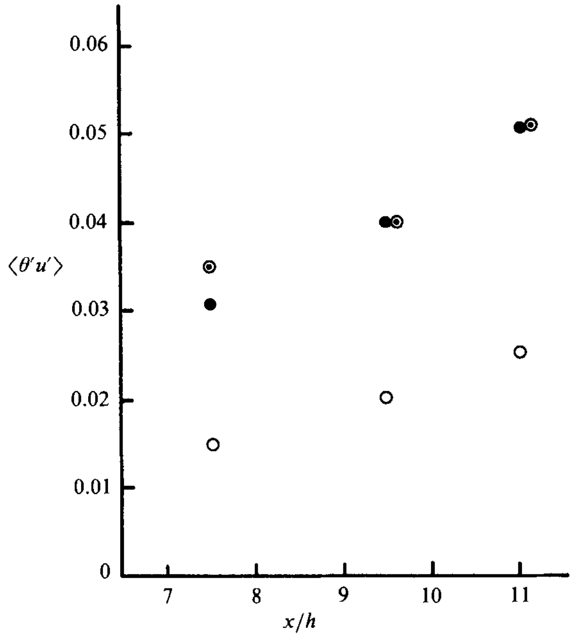

FIGURE 2. $\langle\theta'u'\rangle$: ●, Tavoularis & Corrsin (1981); ○, present model (69) with $C'_{\kappa A} \approx 0$; ⊙, present improved model (69) with (72).

figure 2. The present model (69) with $C'_{\kappa A} \approx 0$ does predict positive anisotropic heat flux. Its magnitude is, however, half the experimental value. The cause of this discrepancy is inferred as follows. First, the model constant $C_{\kappa A}$ in (37) is estimated using the inertial-range simplification, and is not free from the numerical inaccuracy arising from it. Second, our anisotropic eddy-diffusivity tensor $\kappa^{\alpha\beta}_{eA}$ is symmetric since $C'_{\kappa A} \approx 0$. Tavoularis & Corrsin (1985) carried out a quasi-Lagrangian analysis based on their experimental data to suggest that $\kappa^{\alpha\beta}_{eA}$ is not symmetric.

To correct this inadequacy, let us retain both $C_{\kappa A}$ and $C'_{\kappa A}$ to construct a more reliable model for $\kappa^{\alpha\beta}_{eA}$. To estimate those constants, we make use of $\langle\theta'u'\rangle$ at $x/h = 11$ in figure 2 and Tavoularis & Corrsin's estimate of the asymmetry of $\kappa^{\alpha\beta}_{eA}$ at $x/h = 11$. From those data, we have

$$C_{\kappa A}+C'_{\kappa A} \approx 0.37, \quad \frac{C_{\kappa A}-C'_{\kappa A}}{C_{\kappa A}+C'_{\kappa A}} \approx 0.55, \tag{71}$$

which lead to

$$C_{\kappa A} \approx 0.29, C'_{\kappa A} \approx 0.08. \tag{72}$$

It is noteworthy that $C'_{\kappa A}$ in the antisymmetric part is about one-quarter of $C_{\kappa A}$ in the symmetric part. Using (72), we calculate $\langle\theta'u'\rangle$ at $x/h = 7.5$ and 9.5. These results are also included in figure 2. The agreement with the data is satisfactory. Therefore, it can be expected that the present anisotropic representation, particularly the improved version with (72), is useful in the actual simulation of heat transfer.

Finally, we refer to the counter-gradient diffusion effect. This effect is often seen in combustion phenomena, and comes from the situation where the zeros of the turbulent heat flux and the mean temperature gradient do not coincide with each other. In such a situation, the buoyancy force often plays a key role, and some buoyancy-related terms should be added to the present representation (18) for $\boldsymbol{H}$. For instance, under the Boussinesq approximation TSDIA suggests that the terms proportional to

$$A,\ (A\cdot\nabla)\,U,\ \nabla(A\cdot U) \tag{73}$$

should be included in H, where A is a parameter used in (59). The study of counter-diffusion effects based on such an improvement is left for future work.

5. Conclusion

In this paper, we have derived a turbulence model for the diffusion of a passive scalar in a deductive manner. The major results can be summarized as follows.

(*a*) A model for the isotropic eddy diffusivity that accounts for the dependence of turbulent Prandtl number on molecular Prandtl number was obtained.

(*b*) A model for the anisotropic eddy diffusivity was obtained, which is related to mean velocity gradient and can explain anisotropic heat transport observed experimentally.

(*c*) A theoretical justification was given to the model equation for the dissipation rate of scalar variance that is very important in both the existing eddy-diffusivity and second-order models. This justification paves the way for incorporating additional effects such as buoyancy and MHD effects in a systematical manner.

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Appendix. A brief summary of TSDIA

TSDIA was originally formulated for the calculation of the Reynolds stress $R^{\alpha\beta}$ and other important properties such as the triple velocity correlation in turbulent flows with mean velocity gradient (Yoshizawa 1984*b*, 1985*a*). This formalism has been extended to MHD turbulent flows closely associated with controlled fusion physics (Yoshizawa 1985*c*, 1988).

TSDIA may be summarized as the following five key steps.

(*a*) A small-scale parameter δ that disappears automatically in the final stage of analysis is introduced, using which two space and time scales are defined as

$$\xi\ (=x), \quad X\ (=\delta x); \quad \tau\ (=t), \quad T\ (=\delta t). \tag{A 1}$$

Here, (ξ,τ) express the rapid space and time variation of fluctuations, whereas (X,T) express the slow variation of mean fields. Using (A 1), a quantity f with mean F and fluctuation f' is written as

$$f = F(X;T)+f'(\xi,X;\tau,T), \tag{A 2}$$

where f, F and f' denote (u,θ,p), $(U,\Theta,\hat{P})$ and (u',θ',p'), respectively.

(*b*) The fluctuation f' is written in the Fourier representation of the rapid space variable ξ:

$$f'(\xi,X;\tau,T) = \int f''(k,X;\tau,T)\exp\left[-\mathrm{i}k\cdot(\xi-U\tau)\right]\mathrm{d}k. \tag{A 3}$$

(*c*) f'' is expanded using the scale parameter δ as

$$f''(k,X;\tau,T) = \sum_{n=0}^{\infty}\delta^n f''_n(k,X;\tau,T). \tag{A 4}$$

Consequently, f''_n $(n \geq 1)$ can be expressed in terms of f''_0, the response functions associated with f''_0, and the mean-field gradients. The equation for the lowest-order field f''_0 does not depend on the mean field directly, but the dependence of f''_0 on the mean field is retained through $\boldsymbol{X}$ and T. This lowest-order field is called the basic field.

(*d*) Using (A 4), various bulk properties such as $R^{\alpha\beta}$ and $\boldsymbol{H}$ can be calculated with the aid of DIA (Kraichnan 1959, 1964). At the present time, the basic field is regarded as isotropic with the inhomogeneity through $\boldsymbol{X}$.

(*e*) Expressions obtained for $R^{\alpha\beta}$, etc. are very complicated as they are since they are written in terms of two-time velocity covariance, the response functions, etc. of the basic field. So, we perform a simplification based on the inertial-range concept: the scalar and velocity covariances, and the response functions are approximated by their inertial-range form. For instance, the low-wavenumber part of the scalar basic field is estimated by extending the lower limit of the inertial-range spectrum to a characteristic wavenumber k_M. The present characteristic scalar length l_θ in (16) or (23) is related to k_M as

$$k_M = 2\pi/l_\theta. \tag{A 5}$$

As can be seen from (18) for $\boldsymbol{H}$ and (38) for $R^{\alpha\beta}$, the results from TSDIA have the following prominent properties. In the zeroth-order analysis with respect to the scale parameter δ, the results are not related directly to mean-field gradients, as in the first term of (38). In the first-order analysis, the terms including the first derivatives of mean field appear. Moreover, in the second-order analysis the results associated with the products of the first derivatives of the mean field or the second derivatives are obtained, which lead to the anisotropic eddy-viscosity and eddy-diffusivity terms in $R^{\alpha\beta}$ and $\boldsymbol{H}$.

From these properties we may conclude that TSDIA is a systematic method for performing the derivative expansion with respect to mean field. In this sense, TSDIA is very similar to Leslie's (1973) pioneering work on turbulence with a mean velocity gradient. In that work, the two-coordinate system based on the centroid and difference coordinates is introduced at the start of the analysis. This coordinate system, however, is not always appropriate to the direct treatment of a fluctuating field as in steps (*a–d*) (for a more detailed discussion, see Yoshizawa 1985*b*), but it becomes useful in the analysis of correlation functions in combination with the spherical harmonics expansion method.

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