# A new approach to the formulation of scalar flux closure

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## 1. Motivation and objectives

The solution of fluid dynamics equations for a turbulent flow requires the modeling of turbulence statistics if the averaged form of the equations are used. This is usually the case except in direct numerical solution methods which are limited to low Reynolds numbers. The major effort of the researchers in this field is to develop closure models that improve the accuracy of turbulent flow predictions. However, it is understood that the more accurate the models are, the more complex they will be. The second order closure models seemed to provide a compromise between complexity and accuracy. In this class of models the exact equations for Reynolds stresses and scalar fluxes are derived and the unknown terms are modeled in terms of the other known parameters.

The modeling of Reynolds stress and scalar flux transport equations is done separately, although the same approaches are used in most cases. It must be mentioned that the area of scalar transport has received less attention than momentum transport (Reynolds stress). Therefore, turbulence models for scalar fluxes are rather less well developed than models for Reynolds stresses. This may be in part because prediction of the mean flow and Reynolds stress is often a prerequisite to prediction of convective scalar transport. But, conversely, because of this intimate coupling between momentum and scalar flux, models of scalar transport may provide constraints on the momentum model.

This report shows that if a stochastic differential equation (Langevin equation) for velocity fluctuation vector is known, it is possible to derive the equations for scalar flux transport. Durbin and Speziale (1994) showed that the second moment of this stochastic differential equation gives an equation for the evolution of Reynolds stress tensor. Similarly, the stochastic equation will give an equation for scalar flux. Therefore, a coupling between these two is present. The basis for the present work is that there should be Langevin equations that can produce acceptable models for both the Reynolds stress tensor and the scalar flux vector. Having found this basic Langevin equation, the amount of work needed to model the second order closure problems is reduced; using the well developed models for Reynolds stress equations, it will be possible to derive corresponding models for scalar flux equation.

## 2. Accomplishments

### *2.1 Langevin equation and scalar flux closure*

The simplest Langevin equation for a random velocity vector is

$$du_i = -\frac{c_1}{2T}u_i dt + \sqrt{c_0\epsilon}\, dW_i(t), \tag{1}$$

where $u_i$ is the velocity fluctuation vector, $t$ is the independent variable time, $T$ is the turbulent time scale $(k/\epsilon)$ where $k$ is the turbulent kinetic energy per unit mass and $\epsilon$ is the rate of dissipation of $k$, and $W_i(t)$ is the Wiener stochastic process (Arnolds, 1974). $c_1$ and $c_0$ are constants which are determined later. It was shown by Durbin and Speziale (1994) that the second moment of this equation,

$$\frac{d\overline{u_iu_j}}{dt} = -\frac{c_1}{T}\overline{u_iu_j} + c_0\epsilon\delta_{ij}, \tag{2}$$

is an equation for the evolution of Reynolds stresses in the absence of mean velocity gradient provided that $c_1 = 2$ and $c_0 = 2/3$.

In homogeneous turbulent flow the position of a fluid particle is determined by the following equation.

$$\frac{dX_i}{dt} = u_i + X_jU_{i,j} \tag{3}$$

Here, $X_i$ is the Lagrangian position vector of the particle and $U_i$ is the velocity of the fluid particle, which is at position $X_i$ at time $t$; $U_{i,j}$ is constant in homogeneous turbulence. The dispersion tensor $K_{ij}$ is defined as

$$K_{ij} = \overline{u_iX_j}. \tag{4}$$

It can be shown that if the molecular diffusion of the scalar contaminant $\Theta$ is neglected (high Peclet number), the turbulent scalar flux is related to the dispersion tensor by

$$\overline{u_i\theta} = -K_{ij}\Theta_{,j}. \tag{5}$$

Therefore, if a transport equation for $K_{ij}$ is known, the equation for the transport of scalar contaminant can be derived using Eq. 5.

The transport equation for $K_{ij}$ is simply obtained by substituting Eqs. 1 and 3 in

$$\begin{aligned} d(u_iX_j) &= (u_i + du_i)(X_j + dX_j) - u_iX_j \\ &= u_idX_j + X_jdu_i + du_idX_j, \end{aligned} \tag{6}$$

and averaging. This is the same method used by Durbin and Speziale (1994) to derive the transport equation for Reynolds stresses. The result is:

$$\frac{dK_{ij}}{dt} = \overline{u_iu_j} - \frac{c_1}{2T}K_{ij}. \tag{7}$$

Note that the mean velocity gradient and therefore the second term of Eq. 3 is zero for the case considered here. The coefficient of the second term of Eq. 7 ($c_1/2$) does not agree with the empirical values which are about $2c_1$ where $c_1 = 1.8$ (Launder, 1978). Therefore, Eq. 1 can not be used as a base Langevin equation for both Reynolds stress and scalar flux closure models. However, a modified form of this equation given as

$$du_i = -\frac{c_M}{T}u_idt + \sqrt{(2c_M - 1)\epsilon}p_{ik}d\mathcal{W}'_{t_k} + \sqrt{c_0\epsilon}d\mathcal{W}_{t_i} \tag{8}$$

provides a consistent Langevin equation for both momentum and scalar flux transport. In Eq. 8 $p_{ij}$ is the generalized square root of $b_{ij}$ defined by $p_{ij}^2 - \frac{1}{3}p_{kk}^2\delta_{ij} = b_{ij}$ and $c_0 = \frac{2}{3}\left[2c_M - 1 - (c_M - \frac{c_1}{2})p_{kk}^2\right]$. Note that $\mathcal{W}_t$ and $\mathcal{W}_t'$ are independent Wiener processes and $\overline{d\mathcal{W}_t d\mathcal{W}_t'} = 0$. It can be shown that the second moment of Eq. 8 is Eq. 2 and the evolution equation for $K_{ij}$ is

$$\frac{dK_{ij}}{dt} = -\frac{c_M}{T}K_{ij} + \overline{u_i u_j} \tag{9}$$

The scalar gradient evolves by $d(\Theta_{,j})/dt = -U_{k,j}\Theta_k$ (which is zero in this case but not in general). Hence the transport equation of the scalar flux, $\overline{u_i\theta}$, is simply obtained by taking $d/dt$ of Eq. 5, substituting Eq. 9 for $dK_{ij}/dt$, and using the above mentioned evolution equation for $\Theta_{,j}$. The final result is

$$\frac{d\overline{u_i\theta}}{dt} = -\overline{u_i u_j}\Theta_{,j} - \frac{c_M}{T}\overline{u_i\theta}. \tag{10}$$

This is the equation for the transport of scalar flux in the absence of mean velocity gradient. The first and second terms are the production by mean scalar gradient and the slow part of the pressure-scalar gradient correlation respectively.

The importance of this method is that there is no need to develop a separate closure model for the equation of scalar transport if there is already a closure model for the transport of Reynolds stresses. It was shown (Durbin and Speziale, 1994) that for any Reynolds stress closure model there is a Langevin equation, the second moment of which is that model equation. Having this Langevin equation, it is possible to derive a transport equation for the scalar flux by the method outlined above.

### *2.2 Results*

The general linear model for the evolution of Reynolds stress tensor is

$$\begin{aligned}\frac{d\overline{u_i u_j}}{dt} = &-\frac{c_1}{T}(\overline{u_i u_j} - \frac{2}{3}k\delta_{ij}) - c_2(P_{ij} - \frac{2}{3}P\delta_{ij}) - c_3(D_{ij} - \frac{2}{3}P\delta_{ij}) \\ &- c_s k S_{ij} + P_{ij} - \frac{2}{3}\epsilon\delta_{ij}\end{aligned} \tag{11}$$

where

$$P_{ij} = -\overline{u_i u_k}U_{j,k} - \overline{u_j u_k}U_{i,k},$$
$$D_{ij} = -\overline{u_i u_k}U_{k,j} - \overline{u_j u_k}U_{k,i},$$
$$P = \frac{1}{2}P_{ii}.$$

A special case of this model is the IP model where $c_3 = C_s = 0$. It can be shown that the second moment of Langevin equation

$$du_i = -\frac{c_M}{T}u_i dt + \sqrt{(2c_M - c_1)\epsilon}\, p_{ik} d\mathcal{W}_{t_k}' + (c_2 - 1)u_k\partial_k U_i dt + \sqrt{c_0\epsilon}\, d\mathcal{W}_{t_i} \tag{12}$$

is the special case of Eq. 11 corresponding to the IP model, provided that

$$c_0 = \frac{2}{3}\left[2c_M - 1 - c_2\frac{P}{\epsilon} - (c_M - \frac{c_1}{2})p_{kk}^2\right].$$

Following the procedure mentioned in Section 2, it can be shown that the evolution equation for $K_{ij}$ is

$$\frac{dK_{ij}}{dt} = \overline{u_i u_j} - \frac{c_M}{T}K_{ij} + K_{ik}U_{j,k} + (c_2 - 1)K_{kj}U_{i,k}. \tag{13}$$

Note that $K_{ij}$ is not a symmetric tensor. The scalar flux equation is

$$\frac{d\overline{u_i\theta}}{dt} = -\frac{c_M}{T}\overline{u_i\theta} - \overline{u_i u_j}\Theta_{,j} + (c_2 - 1)\overline{u_k\theta}U_{i,k}. \tag{14}$$

The significance of this result is that the coefficients of the scalar flux model are not independent of those in the Reynolds stress equations (Eq. 11).

The dimensionless dispersion tensor is defined as

$$D_{ij} = \frac{\epsilon}{k^2}K_{ij}.$$

An evolution equation for $D_{ij}$ can be obtained. However, in equilibrium, the rate of change of $D_{ij}$ is zero. Therefore, the following algebraic equation is obtained.

$$\frac{D_{ij}}{g_k} = \tau_{ij} + D_{ik}(S^*_{kj} - \omega^*_{kj}) + (c_2 - 1)(S^*_{ik} + \omega^*_{ik})D_{kj} \tag{15}$$

where $\tau_{ij} = \overline{u_i u_j}/k$, $S^*_{ij} = TS_{ij}$, $\omega^*_{ij} = T\omega_{ij}$ and

$$g_k = \left[c_M + c_{\epsilon 2} - c_{\epsilon 1}\frac{P}{\epsilon} + 2\frac{P}{\epsilon} - 2\right]^{-1}.$$

In a two-dimensional uniform shear flow:

$$S_{ij} = \frac{1}{2}\begin{pmatrix} 0 & S \\ S & 0 \end{pmatrix} \quad \text{and} \quad \omega_{\mathrm{ij}} = \frac{1}{2}\begin{pmatrix} 0 & S \\ -S & 0 \end{pmatrix}$$

It can be shown that in this case

$$\begin{aligned} D_{11} &= g_k\left[\tau_{11} + c_2 g_k S^*\tau_{12} - 2(1 - c_2)(g_k S^*)^2\tau_{22}\right], \\ D_{12} &= g_k\left[\tau_{12} + (c_2 - 1)g_k S^*\tau_{22}\right], \\ D_{21} &= g_k\left[\tau_{12} + g_k S^*\tau_{22}\right], \\ D_{22} &= g_k\tau_{22}. \end{aligned} \tag{14}$$

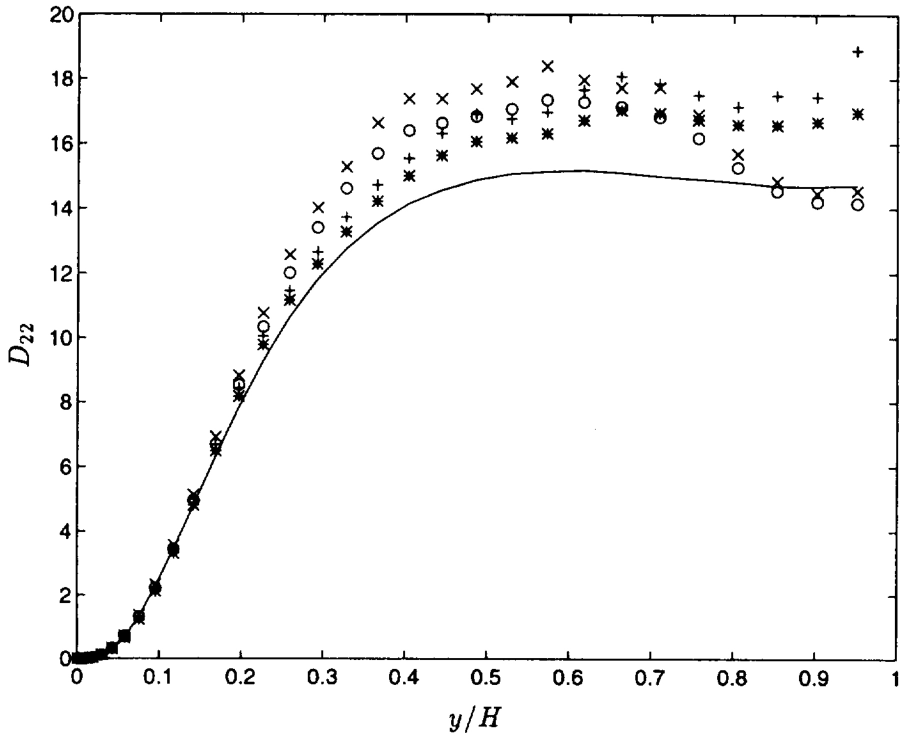


FIGURE 1. Eddy diffusivity profiles according to the IP model; ——— , model prediction; $*$, DNS(HS) Pr=0.71; $+$, DNS(HS) Pr=2.0; $\circ$, DNS(HW) Pr=0.71; $\times$, DNS(HW) Pr=2.0.

Evaluation of $D_{22}$ with $c_M = 3.4$ is compared to the numerical data of Kim and Moin (1989) in Fig. 1. The DNS data are for heat source (HS) and heated wall (HW) cases. With $c_M = 3.4$ the value calculated for $D_{12}$ is not in good agreement with the numerical data; a value close to 0.85 gives more reasonable results. However, this value of $c_M$ is preferred in order to predict the transverse scalar flux, $\overline{v\theta}$, as accurate as possible. This component of scalar flux has the main contribution in channel flow and boundary layer heat transfer.

The same calculations were done for the general linear model and the results are

$$\begin{aligned}
D_{11} &= \frac{g_k}{\Delta}\left[\tau_{11} + (\frac{2}{\Delta} + c_2 - 2)g_k S^* \tau_{12} - 2(1-c_2)\frac{(g_k S^*)^2}{\Delta}\tau_{22}\right],\\
D_{12} &= \frac{g_k}{\Delta}\left[\tau_{12} - (1-c_2)g_k S^* \tau_{22}\right],\\
D_{21} &= \frac{g_k}{\Delta}\left[\tau_{12} + c_3 g_k S^* \tau_{11} + (\frac{2}{\Delta} - 1)g_k S^* \tau_{22} + 2c_3\frac{(g_k S^*)^2}{\Delta}\tau_{12}\right],\\
D_{22} &= \frac{g_k}{\Delta}\left[\tau_{22} + c_3 g_k S^* \tau_{12}\right],
\end{aligned} \tag{15}$$

where $\Delta = 1 + (1-c_2)c_3(g_k S^*)^2$ and $g_k = \left[c_M + (2-c_{\epsilon 1})\frac{P}{\epsilon} + c_{\epsilon 2} - 2\right]^{-1}$. The expression for $D_{22}$ given by Eq. 15 shows that for high enough values of $S^*$ there is a possibility for $D_{22}$ to become negative if $c_3$ is not equal to zero; for the channel flow case this happens in the near wall region. The negative value of $D_{22}$ does not have any physical interpretation and is not supported by DNS data of Kim and Moin (1989). However, a non-zero value of $c_3$ is necessary to predict different values for $b_{22}$ and $b_{33}$ in homogeneous shear flow.

## 4. Future work

The main purpose of this research is to obtain a consistent way of deriving both Reynolds stress tensor and scalar flux vector closures from same Langevin equation for velocity fluctuation vector. The following main problems must be resolved before this goal is achieved:

1. The coefficient of the slow term ($c_M$) in the evolution equation of different components of scalar flux must be different in order to get a good agreement with experimental or DNS data for all the components of scalar flux. Therefore, a simple constant value does not seem to solve the problem.
2. As mentioned at the end of Section 3 a non-zero value of $c_3$ is necessary to differentiate the values of $b_{22}$ and $b_{33}$ in a homogeneous shear flow. On the other hand, a non-zero value of this constant causes the model to predict negative values of $D_{22}$ for high enough $S^*$ which seems unreasonable.

The solution of these two problems is the main focus of this research.

## REFERENCES

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