PASSIVE SCALAR FLUX MODELLING FOR CFD

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ABSTRACT

Modelling of passive scalar transport in turbulent flows is considered, with the scope of testing an additional simplification of the explicit algebraic model (EASFM), recently proposed by Wikström, Wallin and Johansson (Phys. Fluids, 2000). Here the possibility to use a constant value for the turbulent scalar to dynamical time-scale ratio is examined, with the aim of avoiding two additional transport equations needed in the original model. The simplified EASFM is calibrated against homogeneous shear flow and turbulent channel flow. A model was added for considering the neglected diffusion terms in regions with low turbulence production. The resulting model was found to be able to predict all of the scalar flux components well, even though the scalar to dynamical time-scale ratio needed in the model, was assumed to be equal to a constant.

INTRODUCTION

The characteristic feature of passive scalars is that its concentration, Θ, is influenced by the turbulent motion, but does not itself influence the velocity field. The scalar can for example be temperature, or concentration of some pollutant. The passive scalar flux, $\overline{u_i\theta}$, is commonly modelled through a gradient diffusion assumption, or eddy-diffusivity model (EDM)

$$\overline{u_i\theta} = -\frac{\nu_t}{Pr_t}\frac{\partial\Theta}{\partial x_i}, \qquad (1)$$

where Pr_t is the turbulent Prandtl number.

Unfortunately, the eddy-diffusivity model is not able to predict realistic values of all components of $\overline{u_i\theta}$, since it predicts the scalar flux to be aligned with the mean scalar gradient, which in most cases is a bad approximation. In, e.g., shear layers the streamvise flux is actually larger than the flux in the gradient direction. However, in thin shear layers this effect is of minor importance for the mean scalar field.

Recently a new fully explicit algebraic scalar flux model was published by Wikström et al. (2000). They formed an algebraic relation for the passive scalar flux, $\overline{u_i\theta}$, in terms of mean flow quantities by applying an equilibrium condition in the transport equations for the normalized passive scalar flux. This is a reasonable assumption in many flows if the velocity and scalar gradients are large. With a special choice in the model of the pressure scalar-gradient correlation and molecular destruction, an attractive simplification of the general explicit model was obtained by Wikström et al. The model is valid also for three-dimensional mean flows and relates the scalar flux vector to the Reynolds stresses, $\overline{u_iu_j}$, the mean flow gradient, $\partial U_i/\partial x_j$, the mean scalar gradient, $\partial\Theta/\partial x_i$, and the time scale ratio, r

$$r = \frac{K_\theta/\varepsilon_\theta}{K/\varepsilon}. \qquad (2)$$

The resulting model reads,

$$\overline{u_i\theta} = -(1 - c_{\theta 4}) B_{ij}\overline{u_j u_k}\frac{K}{\varepsilon}\frac{\partial\Theta}{\partial x_k}, \qquad (3)$$

where the tensor B_{ij} is an explicit function of the mean flow gradient normalized by the turbulence time scale ($\tau = K/\varepsilon$), the production to dissipation ratio, $\mathcal{P}_K/\varepsilon$, and the time scale ratio, r. The model was evaluated with promising results by Wikström et al. for homogeneous shear flow with imposed mean scalar gradients in three different directions, turbulent channel flow, and a flow field downstream of a heated cylinder.

The model proposed by Wikström et al. also needs two additional transport equations for the half scalar variance, $K_\theta \equiv \overline{\theta^2}/2$ and its dissipation rate, ε_θ, in order to determine the time scale ratio, r. The modelling of the K_θ and ε_θ equations was not addressed by Wikström et al. (2000), but considered by Johansson & Wikström (1999).

In this study we will examine a simplified approach with the assumption of an algebraic relation for the time-scale ratio, r, with the aim of avoiding the additional transport equations, and also for developing a complete model including near-wall treatment. Investigations show that the time-scale ratio, r, to some extent is approximately constant in different flow cases, so the first attempt will be to set r equal to a constant. The resulting model is validated in some simple flow cases.

DESCRIPTION OF THE ALGEBRAIC MODEL FOR SCALAR TRANSPORT

The scalar flux vector, $\overline{u_i\theta}$, appearing in the Reynolds averaged transport equation for the mean scalar originates from the averaging of the nonlinear advection term and needs to be modelled. The transport equation for the scalar-flux vector can formally be derived and can alternatively be replaced by a transport equation for the normalized scalar flux $\xi_i \equiv \overline{u_i\theta}/\sqrt{KK_\theta}$. This reads

$$\begin{gathered}\frac{D\xi_i}{Dt} - \mathcal{D}_i^{(\xi)} = \\ -\frac{1}{2}\xi_i\left(\frac{\mathcal{P}_\theta - \varepsilon_\theta}{K_\theta} + \frac{\mathcal{P}_K - \varepsilon}{K}\right) + \frac{\mathcal{P}_{\theta i} + \Pi_{\theta i} - \varepsilon_{\theta i}}{\sqrt{KK_\theta}},\end{gathered} \qquad (4)$$

where,

$$\begin{gathered}\mathcal{P}_\theta = -\overline{u_i\theta}\frac{\partial\Theta}{\partial x_i}, \quad \mathcal{P}_K = -\overline{u_i u_j}\frac{\partial U_i}{\partial x_j}, \\ \mathcal{P}_{\theta i} = -\overline{u_i u_j}\frac{\partial\Theta}{\partial x_j} - \overline{u_j\theta}\frac{\partial U_i}{\partial x_j}.\end{gathered} \qquad (5)$$

are the production terms in the K, K_θ and $\overline{u_i\theta}$ equations, respectively. The term $\mathcal{D}_i^{(\xi)}$, is the molecular and turbulent diffusion of ξ_i.

In order to close the system of equations for the normalized scalar flux, models for the pressure scalar-gradient correlation, $\Pi_{\theta i}$ and the destruction rate tensor, $\varepsilon_{\theta i}$, and transport equations for K_θ and ε_θ are needed. Moreover, it is necessary to model the Reynolds stresses $\overline{u_i u_j}$ in an appropriate way where all components are accounted for. Hence, standard eddy-viscosity models are not adequate for this purpose.

The equilibrium assumption

In nearly homogeneous steady flow, advection and diffusion of the non-dimensional scalar flux may be neglected, see Wikström et al. (2000). If the driving forces, the velocity and scalar gradients, are large this assumption is fair, but in regions where production terms on the right hand side of (4) are small, the equilibrium assumption may be incorrect. One example of that is in the center of a turbulent channel flow, where the magnitudes of the gradients are small. This is a known problem also for algebraic Reynolds stress models based on a similar approach, where the advection and diffusion of the Reynolds stress anisotropy are neglected.

The equilibrium assumption implies that the left hand side of (4) is neglected, resulting in an algebraic implicit relation (the *r.h.s.* of eq. (4) = 0).

Modelling $\Pi_{\theta i} - \varepsilon_{\theta i}$

The pressure scalar-gradient correlation, $\Pi_{\theta i}$, and the destruction rate tensor, $\varepsilon_{\theta i}$, in (4) contain higher-order correlations, which are unknown and must therefore be modelled. A general model that covers most published suggestions may be written as,

$$\begin{gathered}\Pi_{\theta i} - \varepsilon_{\theta i} = -\left(c_{\theta 1} + c_{\theta 5}\frac{K}{\varepsilon K_\theta}\overline{u_k\theta}\frac{\partial\Theta}{x_k}\right)\frac{\varepsilon}{K}\overline{u_i\theta} \\ + c_{\theta 2}\overline{u_j\theta}\frac{\partial U_i}{\partial x_j} + c_{\theta 3}\overline{u_j\theta}\frac{\partial U_j}{\partial x_i} + c_{\theta 4}\overline{u_i u_j}\frac{\partial\Theta}{\partial x_j},\end{gathered} \qquad (6)$$

see Wikström et al. (2000). This model is nonlinear in the term multiplied by $c_{\theta 5}$, but by choosing $c_{\theta 5} = 1/2$ in (6), the non-linear term will automatically eliminate the corresponding non-linearity caused by the $\xi_i\mathcal{P}_\theta$ - term in (4). In addition, the $c_{\theta 1}$ coefficient was suggested by Wikström et al. (2000), to be a function of the time-scale ratio, r (see table 1).

model	$c_{\theta 1}$	$c_{\theta 2}$	$c_{\theta 3}$	$c_{\theta 4}$	$c_{\theta 5}$
WWJ	$1.6\frac{r+1}{r}$	0	0	0	0.5
HWWJ^a	4.51	−0.25	0	0.04	0.5
HWWJ^d	4.51	−0.47	0.020	0.08	0.5
HWWJ^f	4.51	−0.50	−0.012	0.02	0.5

Table 1: The different combinations of the parameter values in the model of $\Pi_{\theta i} - \varepsilon_{\theta i}$ given by (6).

The explicit algebraic solution

The implicit algebraic relation resulting from the equilibrium assumption and with the general model for $\Pi_{\theta i} - \varepsilon_{\theta i}$ (6) may be solved resulting in a fully explicit relation for $\overline{u_i\theta}$, see Wikström et al. (2000). The specific choice of $c_{\theta 5} = 1/2$ in (6) reduces the complexity of the solution given by (3), and yields

$$\mathbf{B} = \frac{(G^2-\frac{1}{2}Q_1)\mathbf{I}-G(c_S\mathbf{S}+c_\Omega\mathbf{\Omega})+(c_S\mathbf{S}+c_\Omega\mathbf{\Omega})^2}{G^3-\frac{1}{2}GQ_1+\frac{1}{2}Q_2}. \tag{7}$$

The normalized mean strain and rotation rate tensors are defined as $S_{ij} \equiv (\tau/2)(U_{i,j} + U_{j,i})$ and $\Omega_{ij} \equiv (\tau/2)(U_{i,j} - U_{j,i})$. $\mathbf{I}$ is the identity matrix. Moreover, $c_S = 1 - c_{\theta 2} - c_{\theta 3}$ and $c_\Omega = 1 - c_{\theta 2} + c_{\theta 3}$. $Q_1 \equiv c_S^2 \mathrm{tr}\{\mathbf{S}^2\} + c_\Omega^2 \mathrm{tr}\{\mathbf{\Omega}^2\}$ and $Q_2 \equiv (2/3)c_S^3 \mathrm{tr}\{\mathbf{S}^3\} + 2c_S c_\Omega^2 \mathrm{tr}\{\mathbf{S}\mathbf{\Omega}^2\}$ where tr{} denotes the trace. Finally

$$G = \frac{1}{2}\left(2c_{\theta 1} - 1 - \frac{1}{r} + \frac{\mathcal{P}_K}{\varepsilon}\right). \tag{8}$$

We see that the time-scale ratio, r, only enters in the expression for G in (8) together with the $c_{\theta 1}$ coefficient. The effect of the variation of r in different flow regions may, thus, be replaced by a constant r and a variation of $c_{\theta 1}$. In this study we will study the possibility of choosing both r and $c_{\theta 1}$ as constants. Seven sets of constants (a-g) were tested by Högström (2000) of which three are further studied here, labeled (HWWJ^{a,d,f}).

When the time-scale ratio, r, is defined according to (2), and the model coefficients $c_{\theta 2}$-$c_{\theta 4}$ are set to zero, this model is referred to as the (WWJ) model.

CALIBRATION OF THE ALGEBRAIC MODEL AGAINST GENERIC CASES

The first attempt will be to set r to a constant, calibrated for different cases studied. Using DNS data as input to turbulence models reveals how accurate the models are, and can therefore be used for calibration of the model constants.

In table 1, a comparison between the model constants tested in the different flow cases can be seen. The value of the $c_{\theta 1}$ parameter for the (HWWJ) model is equivalent to the (WWJ) model with $r = 0.55$. Also other values for the $c_{\theta 1}$ coefficient has been tested and it has been shown by Högström (2000) that different sets of these parameters can give almost identical results in the flow cases studied below.

	$\frac{d\Theta}{dx}$	$\frac{d\Theta}{dy}$	$\frac{d\Theta}{dz}$	K_θ	r
Case 1	2.5	0	0	0.417	0.536
Case 2	0	2.5	0	0.080	0.618
Case 3	0	0	2.5	0.123	0.501

a_{11}	a_{12}	a_{22}	$\frac{dU}{dy}$	K	ε
0.455	−0.317	−0.340	28.284	10.741	54.494

Table 2: Homogeneous shear flow with mean scalar gradients in each of the three orthogonal directions. DNS data of Rogers et al. (1986), case C128U at $St = 12$.

Homogeneous shear flow

In this study, data have been used from direct numerical simulation (DNS), of homogeneous shear flow with mean scalar gradients in three orthogonal directions made by Rogers et al. (1986). Data from the simulation can be seen in table 2.

In table 3, the predicted scalar fluxes using the different models can be seen. Model (HWWJ^a) was chosen in order to minimize the overall deviation from DNS in all cases. Model (HWWJ^d) predicts the $\overline{v\theta}$ component best in case 2, while model (HWWJ^f) predicts the $\overline{u\theta}$ best in case 1. However, there are no significal differences between the (HWWJ) models and the original (WWJ) model, so for this case the assumption of a constant $r = 0.55$ can be defended.

The eddy-diffusivity approach (EDM) might be expected to work only for the flux component in the same direction as the mean scalar and velocity gradients. This is the case for the $\overline{v\theta}$ flux component in thin shear layers or for Case 2 so it is not expected that the eddy-diffusivity approach can give realistic values for the other cases and flux components. Surprisingly, EDM cannot even give good prediction of the $\overline{v\theta}$ flux component for Case 2.

	Case 1		Case 2		Case 3
	$\overline{u\theta}$	$\overline{v\theta}$	$\overline{u\theta}$	$\overline{v\theta}$	$\overline{w\theta}$
DNS data	−2.41	0.45	0.94	−0.36	−0.67
WWJ	−2.05	0.42	1.13	−0.46	−0.70
HWWJ^a	−2.14	0.40	1.13	−0.42	−0.70
HWWJ^d	−2.05	0.33	1.14	−0.37	−0.67
HWWJ^f	−2.41	0.45	1.35	−0.45	−0.72
EDM	−0.54	0	0	−0.54	−0.54

Table 3: Homogeneous shear flow with mean scalar gradients in each of the three orthogonal directions. The predictions of scalar fluxes for the models (WWJ) and (HWWJ), compared to DNS data of Rogers et al. (1986), case C128U at $St = 12$. The fluxes predicted with an eddy-diffusivity model (EDM) with $Pr_t = 0.89$ and $C_\mu = 0.09$ is also shown.

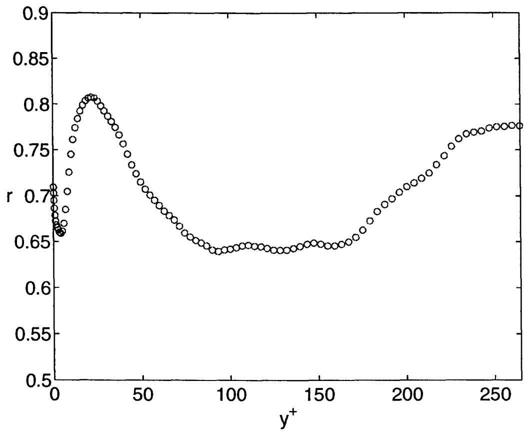

Figure 1: The time-scale ratio, r according equation (2) with DNS data for turbulent channel flow.

Turbulent channel flow

A DNS of a turbulent channel flow with a passive scalar and a Prandtl number of 0.71, was generated by Wikström (1998). The Reynolds number based on the centerline mean velocity and the channel half-width, δ, was 5000, and the Reynolds number based on the wall friction velocity, u_τ, and the channel half-width was 265.

The time-scale ratio r, is approximately constant in the log-region but significally higher near the wall and in the center of the channel, see figure 1. The choice $r = 0.55$ seems to be rather low in this case, but one needs to remember that it is the combination of r and $c_{\theta 1}$ that enters into the model through the G expression (8).

The models (HWWJ^{a,d,f}) and (WWJ) are presented in figure 2 where the scalar flux quantities are normalized with

$$\frac{\nu}{Pr}\left(\frac{\partial \Theta}{\partial y}\right)_{wall}. \tag{9}$$

We can see that model (HWWJ^a) predicts the scalar fluxes somewhere in the middle, compared to the other models. Model (HWWJ^f) predicts $\overline{u\theta}$ best, but over-predicts $\overline{v\theta}$ near the wall, and the opposite is true for model (HWWJ^d). There is a clear tendency that all models over-predict $\overline{v\theta}$ in the channel center.

The influence of the different model coefficients was studied by Högström (2000). It was found that $c_{\theta 3}$ has a strong influence in the region $0 < y^+ < 50$ for both components. For example, by choosing a small negative $c_{\theta 3}$, $\overline{u\theta}$ increases towards the DNS data, but simultaneously the overshooting for $\overline{v\theta}$ near the wall increases. The curves will also become steeper at the wall when $c_{\theta 3}$ is negative. When using

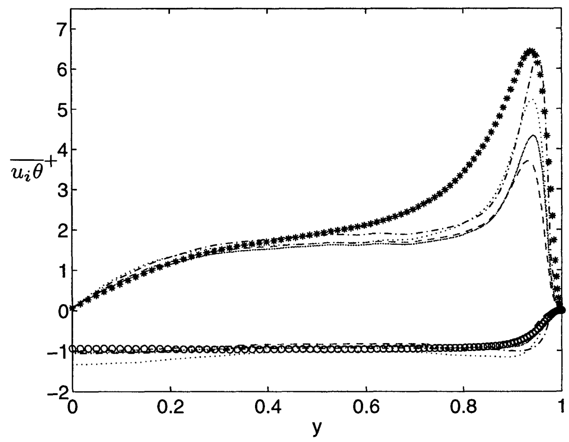

Figure 2: Comparison of model (WWJ) and (HWWJ) models with $r = 0.55$ in turbulent channel flow. $\cdots$, (WWJ); —, (HWWJ^a); - - -, (HWWJ^d); - · -, (HWWJ^f); $*$, $-\overline{u\theta}^+$ from DNS; $\circ$, $\overline{v\theta}^+$ from DNS.

$c_{\theta 3}$ in the model, $c_{\theta 2}$ will also influence the $\overline{v\theta}$ component. For small $c_{\theta 3}$ this influence is quite small though. All these effects can be seen in figure 2. The behaviour of the $\overline{v\theta}$ flux component will influence the level in the log-layer when doing fully coupled computations of the channel flow, as will be seen later.

In all these computations, near wall corrections of the turbulent time scale K/ε, have been made in accordance with Durbin's (1993), suggested time-scale, $\tau \equiv \max(K/\varepsilon, 6.0\sqrt{\nu/\varepsilon})$, in order to have the correct near-wall asymptotic behaviour for the flux. By introducing near-wall damping functions for the $c_{\theta 2}$ and $c_{\theta 4}$ coefficients a better matching of the near wall fluxes may be obtained (see Högström (2000) for details). The near-wall damping functions are, however, rather ad hoc and cannot be expected to be of general validity and are, thus, excluded from this study.

CHANNEL FLOW COMPUTATIONS

By the extensive use of computer algebra software, a turbulence model tester was constructed. The same principal was also used by Grégoire (2000). This way of solving complex systems of differential equations dramatically decreases the time consumed in the process of going from idea to solution. Moreover, it gives a nice overview of all equations and model constants needed to close the system, and errors usually introduced by human mistakes are minimized.

The numerical method is second order in space also on stretched grids, demonstrated by computations on grids with different resolutions. During all computations below, a

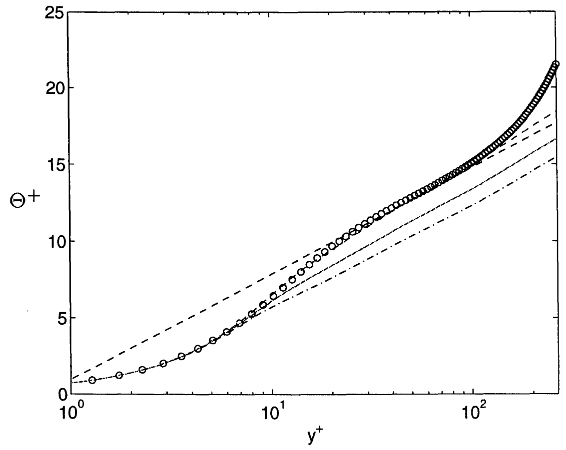

Figure 3: EASFM based on the low Reynolds number EARSM and the $K-\omega$ model. Comparison of the (HWWJ) models with the mean scalar log-law, for turbulent channel flow. Computed $\Theta^+ - \Theta^+_{wall}$ using —, (HWWJ^a); - - -, (HWWJ^d); -·-·-, (HWWJ^f) compared to - - -, (log-law) and o, (DNS).

stretched grid with 100 grid points and a stretch factor of 1.04 was chosen.

The scalar flux model contains the Reynolds stress tensor and accurate modelling of all components of that is needed, which excludes all eddy-viscosity models. A reasonable level of modelling that mathes the modelling level for the scalar flux is explicit algebraic Reynolds stress models (EARSM). For the channel flow computations we have chosen the EARSM proposed by Wallin & Johansson (2000) solved together with the Wilcox (1994) low-Reynolds number $K-\omega$ model, which gives correct behaviour for all Reynolds stress components in the near-wall region. The diffusion term correction in the EARSM was also used (see Wallin & Johansson 2000). These equations were solved together with the proposed (HWWJ) models.

Figure 3 shows the result from these computations showing the normalized mean scalar compared to the DNS data and the log-law. That figure clearly shows that the different (HWWJ) models gives different levels in the log-layer. That is mainly because of the differences in the near-wall region between the models, shown in figure 2. Among these models, the model (HWWJ^d) gives the best results. Consistently with figure 3 the model (HWWJ^d) gives the best prediction of Θ_τ, see table 4.

There is, however, a significant deviation in the channel center between the computations and the DNS data. That difference is caused by the overpredicted $\overline{v\theta}$ flux component, also seen in figure 2. The over-predicted effective eddy diffusivity leads to a reduced gradient

Model	u_τ	Θ_τ
DNS data	0.033	0.046
HWWJ^a	0.033	0.060
HWWJ^d	0.033	0.054
HWWJ^f	0.033	0.064
HWWJ^d+DM	0.033	0.047
EDM	0.033	0.051

Table 4: EASFM based on EARSM and the $K-\omega$ model. Comparison of wall gradient values, in terms of u_τ and $\Theta_\tau \equiv (\nu/Pru_\tau)(\partial\Theta/\partial y)_\mathrm{w}$ for the (HWWJ) models, the eddy-diffusivity model (EDM), and DNS data.

locally around the channel center and as a consequence an over-predicted wall gradient, see table 4. The reason for that is that the equilibrium assumption is a bad approximation in that region, where the production terms are small.

One possibility to overcome the problem in the channel center is to model the neglected diffusion $\mathcal{D}_i^{(\xi)}$ of ξ_i in (4). Such a model (analogous to that for the EARSM) where $\mathcal{D}_i^{(\xi)}$ is modelled in the direction of ξ_i could read $\mathcal{D}_i^{(\xi)} = C_{D\theta}(\mathcal{D}^{(K)}/K)\xi_i$ and can easily be incorporated into the explicit formulation by modifying the expression for G in (8)

$$G = \tfrac{1}{2}\left(2c_{\theta 1} - 1 - \tfrac{1}{r} + \tfrac{\mathcal{P}_K}{\varepsilon}\right) + C_{D\theta}\max\left(1 - \tfrac{\mathcal{P}_K}{\varepsilon}, 0\right). \tag{10}$$

The max function is introduced for avoiding any influence of the model where $\mathcal{P}_K > \varepsilon$. The model (HWWJ^d+DM) was tested and with $C_{D\theta} = 8.0$ a good fit of Θ_τ to the DNS data was obtained, see table 4.

In figure 4, the (HWWJ^d) model with and without diffusion model (DM) is compared and one can see that the behaviour in the channel center is much improved with the diffusion model. This is even more clear by looking at the mean scalar profile without the near-wall scaling, in figure 5. The error in the channel center contaminates the complete field for the model without diffusion correction.

Computational results using the eddy-diffusivity model (EDM) (1) is also shown in these figures (4 and 5). The level in the log region is somewhat underpredicted in figure 4, which is a matter of calibration of the near-wall modelling. Othervise, EDM compares rather well with DNS data, which is to be expected since this modelling approach is calibrated from boundary layer flows. When predicting $\overline{v\theta}$ with the gradient diffusion assumption, the eddy viscosity ν_t was defined according to the $k-\omega$ model, and the turbulent Prandtl number, Pr_t, was set to a constant, equal to 0.89. The Reynolds stress $\overline{uv}$, was