# Influence of timescale ratio on scalar flux relaxation: modelling Sirivat & Warhaft's homogeneous passive scalar fluctuations

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(Received 18 January 1985 and in revised form 18 July 1985)

A second-order modelling technique is used to investigate the behaviour of homogeneous scalar turbulence. Special attention is paid to the influence of timescale ratio on scalar flux relaxation. We develop a model for the scalar flux equation in a homogeneous turbulence and consider both a scalar field without mean-scalar gradients and one with constant mean-scalar gradients based on Sirivat & Warhaft (1981) experiments. Good agreement with experiment in all the cases is obtained.

## 1. Introduction

In this paper we study a homogeneous passive scalar field in a decaying, homogeneous turbulence without mean velocity using a second-order modelling technique. We consider both a scalar field without mean-scalar gradients and one with constant mean-scalar gradients based on Sirivat & Warhaft's (1981) experiments.

Newman, Launder & Lumley (1981) studied these two fundamental flows. Their paper presented a model for the scalar dissipation equation  $\epsilon_{\theta} = \kappa \langle \theta_{,j} \theta_{,j} \rangle$  and pointed out the importance of considering varying the timescale ratio,  $r \equiv (q^2/\epsilon)/(\langle \theta^2 \rangle/\epsilon_{\theta})$ , from flow to flow. The main contribution of this paper lies in the provision of a model for the return to isotropy in the scalar flux equation. This model is also strongly dependent on the timescale ratio. Sirivat & Warhaft's experiments provide data for various timescale ratios and therefore are very useful for testing various closure models.

We calculate three flows without mean-temperature gradients and seven flows with constant mean-temperature gradients. The good agreement with experiment gives us confidence that our model can provide a basis for models describing more complex scalar flows.

## 2. A model for the scalar flux equation in homogeneous turbulence

#### Preliminaries

The exact transport equations describing the evolution of the intensity of scalar fluctuations in a homogeneous turbulent flow without mean velocity and buoyancy may be written as (Lumley 1978)

$$\langle \theta^2 \rangle_{,i} + 2 \langle \theta u_i \rangle \Theta_{,i} + \langle \theta^2 u_i \rangle_{,i} = -2\epsilon_{\theta}, \qquad (2.1)$$

$$\langle u_i u_j \rangle_{,t} = -\epsilon \beta b_{ij} - \frac{2}{3} \epsilon \delta_{ij}, \qquad (2.2)$$

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$$\langle \theta u_i \rangle_{,t} + \langle u_i u_j \rangle \Theta_{,j} + \langle \theta u_i u_j \rangle_{,j} = \frac{\phi_{ij}^{\theta} \langle \theta u_j \rangle \epsilon}{q^2}, \qquad (2.3)$$

$$\epsilon_{\theta,i} + \left\langle \epsilon_{\theta} \, u_i \right\rangle_{,i} = \frac{-\psi^{\theta} \epsilon_{\theta}^2}{\langle \theta^2 \rangle}, \tag{2.4}$$

$$\epsilon_{,t} = \frac{-\psi\epsilon^2}{q^2},\tag{2.5}$$

where  $\Theta$  is the mean-scalar distribution,  $\langle \rangle$  stands for averaging,  $\epsilon_{\theta} = \kappa \langle \theta_{,j} \theta_{,j} \rangle$  the dissipation rate of  $\frac{1}{2}\langle \theta^2 \rangle$ ,  $\epsilon = \nu \langle u_{i,j} u_{i,j} \rangle$  the dissipation rate of  $\frac{1}{2}q^2$ ,  $q^2 = \langle u_i u_i \rangle$ and  $b_{ij} = \langle u_i u_j \rangle / q^2 - \frac{1}{3} \delta_{ij}$ . To close (2.1)-(2.5) we need expressions for third-order moments  $\langle \theta^2 u_i \rangle$ ,  $\langle \theta u_i u_j \rangle$ ,  $\langle \epsilon_{\theta} u_i \rangle$  and for  $\beta$ ,  $\phi_{ij}^{\theta}$ ,  $\psi^{\theta}$  and  $\psi$ . All the models except for  $\phi_{ij}^{\theta}$  are discussed in detail by Lumley (1978). Here we concentrate on  $\phi_{ij}^{\theta}$ , which is responsible for return to isotropy in the scalar flux equations. We can show that  $\phi_{ij}^{\theta} = 0$   $(i \neq j)$  and assume  $\phi_{ij}^{\theta}$  is an isotropic tensor; then  $\phi_{ij}^{\theta} \langle \theta u_j \rangle$  may be written as  $\phi^{\theta} \langle \theta u_i \rangle$ , as most workers do. A number of workers choose different constant values of  $\phi^{\theta}$  in their particular flows. For example Zeman & Lumley (1979) chose  $\phi^{\theta} = 7.5$ and Newman et al. (1981) chose  $\phi^{\theta} = 6.6$ . In general,  $\phi^{\theta}$  should not be a constant. Based on realizability, Lumley (1978) obtained a complicated tensor expression for  $\phi_{ii}^{\theta}$  which included the effects of timescale ratio, anisotropy, Reynolds number and correlation coefficient of  $\theta$  and  $u_i$ . In this paper we develop a simpler (and more convincing) form for  $\phi^{\theta}$ , also based on realizability. We find that  $\phi^{\theta}$  also includes the effects of all quantities mentioned above. While the inclusion of the timescale ratio in Lumley (1978) was a formal deduction, here it is in addition a necessity made evident by the data.

## 2.1. Model for $\phi^{\theta}$

In a homogeneous flow without mean velocity and mean-scalar gradients, the equations for scalar flux, variance and Reynolds stress are

$$\langle \theta u_i \rangle_{,t} = \frac{-\phi^{\theta} \langle \theta u_i \rangle \epsilon}{q^2},$$
 (2.6)

$$\left\langle \theta^2 \right\rangle_{,\,t} = -2\epsilon_\theta,\tag{2.7}$$

$$\langle u_i u_j \rangle_{,t} = -\epsilon \beta b_{ij} - \frac{2}{3} \epsilon \delta_{ij}.$$
 (2.8)

Let us introduce a scalar F:

$$F = 1 + 27III + 9II, (2.9)$$

where II = 
$$-\frac{1}{2}b_{ij}b_{ij}$$
, III =  $\frac{1}{3}b_{ij}b_{jk}b_{ki}$ ,  $b_{ij} = R_{ij} - \frac{1}{3}\delta_{ij}$ ,  $R_{ij} = \frac{\langle u_i u_j \rangle}{q^2}$ .

Expression (2.9) is nine times the invariant expression introduced in Lumley (1978), where the factor of nine is introduced for numerical convenience.

The normalized Reynolds-stress tensor has the following properties:

$$R_{ij} = R_{ji}, \quad R_{ii} = 1,$$
 (2.10)

and the eigenvalues of  $R_{ij}$  are non-negative.

Using (2.10), F can be written as

$$F = 9R_{ii}^3 - \frac{27}{2}R_{ii}^2 + \frac{9}{2},\tag{2.11}$$

$$R_{ii}^2 = R_{ij} R_{ij}, \quad R_{ii}^3 = R_{ij} R_{jk} R_{ki}.$$

where

We can show that

$$0 \leqslant F \leqslant 1. \tag{2.12}$$

In fact, it is straightforward to show that F is 27 times the product of the three eigenvalues of  $R_{ij}$  (the third principal invariant of  $R_{ij}$ ), so that it will vanish if and only if one (or more) of these vanishes. An eigenvalue vanishes if, in non-principal axes, a component vanishes or Schwarz's inequality becomes an equality.

Using (2.8) and  $q_{t}^2 = -2\epsilon$ , we obtain

$$F_{,t} = -\frac{(\beta - 2) (9III + 2II) \epsilon}{q^2}.$$
 (2.13)

To satisfy realizability, and guarantee that F remain non-negative, we require that  $F_{t}$  vanish as F vanishes, i.e.

$$F_{t} \to 0 \quad \text{as } F \to 0.$$
 (2.14)

This is necessary, but not sufficient, to guarantee that  $F \ge 0$ ; we should say something about higher derivatives. Since turbulence will remain two-dimensional until disturbed, we expect that

$$F_{t} = F_{t} = \dots \to 0 \quad \text{as } F \to 0.$$

Since 9III + 2II vanishes only if the turbulence is one-dimensional or isotropic, we assume

$$\beta = 2 + GF, \tag{2.15}$$

where G is a function of invariants and other parameters. More general forms are possible, but do not appear to be necessary. This is the minimum sufficient to assure (2.14), and is consistent with the form given by Lumley (1978). Comparing with Lumley's form, G should be

$$G = \frac{1}{9} \exp\left[-D/R_{L}^{\frac{1}{2}}\right] (72/R_{L}^{\frac{1}{2}} + A \ln\left[1 + B(-\Pi + C\Pi I)\right]), \qquad (2.16)$$

where

$$A = 80.1, B = 62.4, C = 2.3, D = 7.77.$$

Similarly to the above procedure, we introduce a normalized tensor  $D_{ij}$ ,

$$D_{ij} = \frac{\langle \theta^2 \rangle \langle u_i \, u_j \rangle - \langle \theta u_i \rangle \langle \theta u_j \rangle}{\langle \theta^2 \rangle q^2 - \langle \theta u_p \rangle \langle \theta u_p \rangle}, \qquad (2.17)$$

which has the same properties as  $R_{ii}$ , i.e.

$$D_{ij} = D_{ji}, \quad D_{ii} = 1,$$
 (2.18)

and the eigenvalues of  $D_{ij}$  are non-negative (see Lumley 1978). If we introduce a scalar  $F_D$ ,

$$F_D = 9D_{ii}^3 - \frac{27}{2}D_{ii}^2 + \frac{9}{2}, \tag{2.19}$$

we shall be able to show that

$$0 \leqslant F_D \leqslant 1. \tag{2.20}$$

In fact, in the principal axes of  $D_{ii}$ 

$$F_D = 27D_{11}D_{22}D_{33}, \quad D_{11} + D_{22} + D_{33} = 1, \tag{2.21}$$

which follows from (2.19). Thus,  $F_D$  is proportional to the third invariant of  $D_{ij}$ . Similarly to F, non-negative  $F_D$  will give a realizability condition that  $F_{D,t}$  must vanish as  $F_D$  vanishes, i.e.

$$F_{D,t} \to 0 \quad \text{as } F_D \to 0.$$
 (2.22)

In addition, Lumley (1983) shows that  $F_D$  will not stay at the state of  $F_D = 0$  when  $F_D$  vanishes, unlike F. So we must also require

$$F_{D.tt} > 0 \quad \text{as } F_D \to 0. \tag{2.23}$$

This can be only satisfied if  $F_{D,t} \propto F_D^{\frac{1}{2}}$  as  $F_D \rightarrow 0$ . The conditions (2.22) and (2.23) will guide us to find a form for  $\phi^{\theta}$ . We have from (2.19)

$$F_{D,t} = 27(D_{ij,t} D_{jk} D_{ki} - D_{ij,t} D_{ij}).$$
(2.24)

Using (2.6)–(2.8), we can write

$$D_{ij,t} = \frac{\langle \theta^2 \rangle \epsilon}{d_{pp}} \Big\{ b_{ij} (2\phi^{\theta} - 2r - \beta) + \frac{\delta_{ij}}{3 - D_{ij}} (2\phi^{\theta} - 2r - 2) \Big\},$$
(2.25)

where  $d_{pp} = \langle \theta^2 \rangle \langle u_p u_p \rangle - \langle \theta u_p \rangle \langle \theta u_p \rangle$ ,  $r = (q^2/\epsilon) \epsilon_{\theta} / \langle \theta^2 \rangle$ . Substituting (2.25) into (2.24) gives

$$\begin{split} F_{D,t} &= 27 \left( \frac{\langle \theta^2 \rangle \epsilon}{d_{pp}} \right) \{ (D_{ij} \, b_{jk} \, D_{ki} - b_{ij} \, D_{ij} + \frac{4}{3} D_{ii}^2 - D_{ii}^3 - \frac{1}{3}) (2 \phi^\theta - 2 - \beta) \\ &+ [\frac{4}{3} D_{ii}^2 - D_{ii}^3 - \frac{1}{3}] \, (\beta - 2) \}. \end{split}$$
(2.26)

If we use (2.19) to express  $D_{ii}^3$  in terms of  $F_D$  and  $D_{ii}^2$ , and require that the part not proportional to  $F_D$  vanish proportional to  $F_D^4$ , we obtain

$$\phi^{\theta} = \frac{1}{2}\beta + r - \frac{\frac{1}{2}(\beta - 2)\left[(1 - D_{ii}^{2})/6\right]}{D_{ij}b_{jk}D_{ki} - b_{ij}D_{ij} + (1 - D_{ii}^{2})/6} + HF_{D}^{\frac{1}{2}}.$$
(2.27)

*H* is an undetermined function of the timescale ratio *r*, invariants of  $D_{ij}$  etc. This is the form of  $\phi^{\theta}$  we are looking for, which will ensure that (2.22) and (2.23) are satisfied. As before, more complex forms of the final term in (2.27) are possible, but do not appear to be necessary. In the case of isotropic turbulence ( $b_{ij} \equiv 0$ ), the form of  $\phi^{\theta}$  (2.27) becomes

$$\phi^{\theta} = 1 + r + H(F_D)^{\frac{1}{2}}.$$
(2.28)

The function H has to be determined by experiments. We find that good agreement with Sirivat & Warhaft's (1981) experiments (for different mean-temperature gradients and different timescale ratios) is obtained by taking  $H = 1.1r^2$ .

### 3. Flows with and without constant mean-temperature gradients

The equations for a homogeneous isotropic turbulence with constant meantemperature gradient are

$$\langle \theta^2 \rangle_{,t} + 2 \langle \theta w \rangle \frac{\partial \Theta}{\partial x_3} = -2\epsilon_{\theta},$$
 (3.1)

$$q_{,t}^2 = -2\epsilon, \tag{3.2}$$

$$\langle \theta w \rangle_{,t} + \langle w^2 \rangle \frac{\partial \Theta}{\partial x_3} = \frac{-\phi^{\theta} \langle \theta w \rangle \epsilon}{q^2},$$
 (3.3)

$$\epsilon_{\theta,t} = \frac{-\psi^{\theta}\epsilon_{\theta}^{2}}{\langle \theta^{2} \rangle}, \qquad (3.4)$$

$$\epsilon_{,t} = \frac{-\psi\epsilon^2}{q^2}.$$
(3.5)

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∂ <b>∂</b> /∂x (°C/m)	$\left<  heta^2 \right>_{exp} \ (^{\circ}\mathrm{C}^2)$	$-\langle \theta w \rangle_{exp}$ (°C m/s)	$^{\epsilon_{ heta exp}}(^{\circ}C^{2}/s)$	$\langle  heta^2  angle_{ m cal} \ (^{ m o}{ m C}^2)$	$-\langle \theta w \rangle_{cal}$ (°C m/s)	$\overset{\epsilon_{ heta_{\mathrm{Cal}}}}{(^{\mathrm{o}}\mathrm{C}^{2}/\mathrm{s})}$
10.3	0.01280	0.01101	0.09346	0.01280	0.01101	0.08500
3.68	0.001 705	0.003981	0.011 20	0.001 705	0.003918	0.0105
4.48	0.002287	0.003978	0.01492	0.002287	0.003978	0.01592
$\langle \theta^2 \rangle_{exp}, \langle \theta w \rangle_{exp}$	$\epsilon_{\theta}, \epsilon_{\theta} \exp - \exp [- \exp (1 - \exp (1 + e)))}))))))))))))))))))))))))))))))))$	perimental	results at	x/M=40,	$\left< \theta^2 \right>_{\rm cal}, \left< \theta u \right>$	$\langle v \rangle_{cal}, \epsilon_{\theta  cal} - initial$

TABLE 1. Initial conditions at x/M = 40 for U = 3.4 m/s

∂ <b>∂</b> /∂x (°C/m)	$\left< rac{ heta^2}{ m (^oC^2)}  ight>_{ m exp}$	−⟨θw⟩ <sub>exp</sub> (°C m/s)	${\rm e}_{\theta_{\rm exp}}({\rm °C}^{2}/{\rm s})$	$egin{array}{l} \langle  heta^2  angle_{ m cal} \ (^{ m o}{ m C}^2) \end{array}$	$-\langle \theta w \rangle_{cal}$ (°C m/s)	${\rm \stackrel{{\scriptstyle \epsilon_{{_{{ { m CBl}}}}}}{(^{\rm o}{ m C}^2/{ m s})}}$				
1.81	0.0004471	0.0009456	0.001 240	0.0004471	0.0009456	0.001 300				
8.1	0.009059	0.005551	0.02428	0.009059	0.004551	0.02500				
$2.24^{+}$	0.0009240	0.0009336	0.002091	0.0009240	0.0009336	0.001 580				
1.78	0.0004955	0.0006401	0.001515	0.0004955	0.0006401	0.00185				
† Values given at $x/M = 80$ . Notation as in table 1.										

TABLE 2. Initial conditions at x/M = 40 for U = 6.3 m/s

Initial conditions for  $\langle \theta^2 \rangle$ ,  $q^2$ ,  $\langle \theta w \rangle$ ,  $\epsilon_{\theta}$  and  $\epsilon$  (tables 1 and 2) are given by Sirivat & Warhaft's (1981) experiments for different mean-temperature gradients  $\partial \Theta / \partial x_3$ .  $\langle \theta w \rangle$  (in the  $x_3$ -direction) is the only non-zero component of the heat flux.

The models for  $\phi^{\theta}$ ,  $\psi^{\theta}$  and  $\psi$  are

$$\begin{split} & \phi^{\theta} = 1 + r + 1.1 r^2 F_D^{\frac{1}{2}}, \quad F_D = \frac{1 - \rho^2}{(1 - \rho^2/3)^3}, \quad \rho^2 = \frac{\langle \theta w \rangle^2}{\langle \theta^2 \rangle \langle w^2 \rangle}, \\ & \psi^{\theta} = 2 - \frac{2 - \psi_{00}}{r} + 2.05 \langle \theta w \rangle \left(\frac{\partial \Theta}{\partial x_3}\right) \Big/ \epsilon_{\theta}, \quad \psi_{00} = \frac{14}{5} + 0.98 \exp\left[-2.83 R_L^{\frac{1}{2}}\right] \\ & \psi = \psi_{00}. \end{split}$$

To normalize (3.1)-(3.5), we define

$$\begin{split} \Theta' &= \frac{\Theta}{T_{,}}, \quad \left\langle \theta^2 \right\rangle' = \frac{\left\langle \theta^2 \right\rangle}{T^2}, \quad t' = \frac{t}{l_0/u_0}, \quad x'_3 = \frac{x_3}{l_0}, \\ q^{2'} &= \frac{q^2}{3u_0^2}, \quad \epsilon'_\theta = \frac{\epsilon_\theta}{T^2 u_0/l_0}, \quad \epsilon' = \frac{\epsilon}{u_0^3/l_0}, \\ \left\langle w^2 \right\rangle' &= \frac{\left\langle w^2 \right\rangle}{u_0^2} = q^{2'}, \quad \left\langle \theta w \right\rangle' = \frac{\left\langle \theta w \right\rangle}{T u_0}, \end{split}$$

where  $u_0$ ,  $l_0$  and T are the turbulent fluctuating velocity, length and temperature scales at the first measuring position.

The equations become

$$\begin{split} \langle \theta^2 \rangle_{,t}' + 2 \langle \theta w \rangle' \frac{\partial \Theta'}{\partial x_3'} &= -2\epsilon_{\theta}', \\ q_{,t}^{2'} &= -\frac{2}{3}\epsilon', \\ \langle \theta w \rangle_{,t}' + q^{2'} \frac{\partial \Theta'}{\partial x_3'} &= -\frac{1}{3} \phi^{\theta} \langle \theta w \rangle' \frac{\epsilon'}{q^{2'}}, \end{split}$$

$$\begin{split} \epsilon_{\theta,t}^{'} &= -\psi^{\theta} \frac{\epsilon_{\theta}^{2'}}{\langle \theta^{2} \rangle^{'}}, \\ \epsilon_{t,t}^{'} &= \frac{1}{3} \psi \frac{\epsilon^{'2}}{q^{2'}}, \end{split}$$

The values of  $u_0$ ,  $l_0$  are determined from data at the first position x/M = 40 where M is mesh size of the grid and x is downstream distance from the grid. Sirivat & Warhaft's (1981) data give the following relations:

$$\frac{\langle w^2 \rangle}{U^2} = E \left( \frac{x}{M} \right)^a, \quad l = \frac{\langle w^2 \rangle^{\frac{3}{2}}}{\epsilon}, \quad \epsilon = -\frac{3}{2} \frac{\mathrm{d} \langle w^2 \rangle}{\mathrm{d} t}, \quad t = \frac{x}{U}$$

where E = 0.0468, a = -1.24 for the case of U = 3.4 m/s (mean velocity) and E = 0.0622, a = -1.29 for the case of U = 6.3 m/s, the mesh size M = 0.025 m; we can calculate  $\langle w^2 \rangle$  and l at x/M = 640 and choose  $u_0 = \langle w^2 \rangle^{\frac{1}{2}}$ ,  $l_0 = l$  at x/M = 40. In our calculations we chose  $T = (\theta^2)^{\frac{1}{2}}$  at x/M = 40, and the values of  $u_0$  and  $l_0$  are respectively 0.074701 m/s and 0.011071 m for the case of U = 3.4 m/s, and 0.145515 m/s and 0.011937 m for U = 6.3 m/s.

We carried out calculations for flows with different mean-temperature gradients  $\partial \Theta/\partial x_3$ . Three flows without mean-temperature gradients  $\partial \Theta/\partial x_3 = \alpha = 0$ , but with different timescale ratios were calculated. The calculations shown on figure 1 are in very good agreement with experiments. To see the influence of the timescale ratio on the calculations, we also plot the results with  $r \equiv 1$  in figure 1. Obviously, in the second and third plots the calculations with fixed r = 1 (dashed lines) deviate from experiment. This is because r = 1 underestimates the temperature dissipation rate  $e_{\theta}$ , and hence causes the temperature intensity  $\langle \theta^2 \rangle$  to decay too slowly.

We also carried out calculations for seven flows with different constant meantemperature gradients  $(\partial \Theta / \partial x_3 = \alpha \neq 0)$ . The normalized temperature intensity  $\langle \theta^2 \rangle'$ , heat flux  $\langle \theta w \rangle'$ , temperature dissipation rate  $\epsilon'_{\theta}$ , and timescale ratio r are shown in figures 2–10. The dashed lines (which correspond to  $r \equiv 1$ ) in the figures show the influence of the timescale ratio on the calculations. In figure 11, we show the influence of the form of  $\phi^{\theta}$  on the calculations. If we choose  $\phi^{\theta}$  to have a constant value of 4.8, the calculations in several cases (for example  $\alpha = 1.81$  °C/m) could fit the experimental data reasonably well but in other cases (say  $\alpha = 1.78$  °C/m) the calculations will fail (see figure 11). In figure 11 the calculations of heat flux  $\langle \theta w \rangle'$  (with model  $\phi^{\theta} = 4.8$ ) apparently deviate from experiments. Therefore there is no universal constant value of  $\phi^{\theta}$  for all flows: from a physical point of view, the return to isotropy  $(\phi^{\theta} \langle \theta u_i \rangle \epsilon/q^2)$ in the heat-flux equation should depend on the production mechanisms of the velocity and temperature fields. The timescale ratio r, as Newman *et al.* (1981) pointed out, depends on these production mechanisms and changes among flows with differing influences of the production mechanisms. Therefore  $\phi^{\theta}$  must depend on the timescale ratio and must change its value from flow to flow. The form  $\phi^{\theta} = 1 + r + H(r) F_{A}^{\frac{1}{2}}$ ((2.28)) with  $H = 1.1r^2$  works very well in all the cases we have, as shown in figures 2-10.

## 4. Conclusion

We have presented a model for the passive scalar flux equation. We have demonstrated two aspects of the influence of the timescale ratio on scalar flux relaxation. First, we must use the equation for  $\epsilon_{\theta}$  to calculate the real value of the







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FIGURE 11. Comparing normalized heat flux with different forms for  $\phi^{\theta}$  in the heat-flux equation.

timescale ratio r rather than estimating  $\epsilon_{\theta}$  directly through explicit specification of a constant value for the timescale ratio  $r = (q^2/\epsilon)/(\langle \theta^2 \rangle/\epsilon_{\theta})$  (most of the dashed lines in the figures deviate from experiment). Secondly, the  $\phi^{\theta}$  in the scalar flux equation must not be a universal constant and the form of  $\phi^{\theta}$  should include the effect of the timescale ratio. The results of our calculations compared with Sirivat & Warhaft (1981) show that our model can correctly estimate the behaviour of homogeneous scalar turbulence and could provide a basis for models describing more complex scalar flows.

This work was supported in part by the US Office of Naval Research under the following programs: Physical Oceanography (Code 422PO), Power (Code 473); in part by the US National Science Foundation under grant no. ATM 79-22006; and in part by the US Air Force Geophysics Laboratory.

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