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A PRIORI TEST OF SGS MODELS IN COMPRESSIBLE TURBULENCE

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ABSTRACT

An *a priori* study of subgrid-scale models for the unclosed terms in the energy equation is carried out using the flow field obtained from the direct simulation of homogeneous isotropic turbulence. Scale-similar models involve multiple filtering operations to identify the smallest resolved scales and have been shown to be the most active in the interaction with the unresolved subgrid scales (SGS). In the present study these models are found to give more accurate prediction of the SGS stresses and heat fluxes than eddy-viscosity and eddy-diffusivity models, as well as improve prediction of the SGS turbulent diffusion, SGS viscous dissipation, and SGS viscous diffusion.

1 Introduction

Large-eddy simulation (LES) is a technique intermediate between the direct simulation (DNS) of turbulent flows and the solution of the Reynolds-averaged equations. In LES the contribution of the large, energy-carrying structures to momentum and energy transfer is computed accurately, and only the effect of the smallest scales of turbulence is modeled. Since the small scales tend to be more homogeneous and universal, and less affected by the boundary conditions than the large ones, there is hope that their models can be simpler and require fewer adjustments when applied to different flows than similar models for the Reynolds-averaged Navier-Stokes equations.

While a substantial amount of research has been carried out into the modeling aspects and requirements for incompressible flows, the applications of large-eddy simulation to compressible flows have been significantly fewer. One of the reasons for the comparatively small number of calculations of compressible flows is undoubtedly the additional complexity introduced by the need to solve an energy equation, which introduces extra unclosed terms. In addition to the subgrid scale stresses that must be modeled in incompressible flows as well, several other unclosed terms appear in the filtered equations for compressible flows. Furthermore, the form of the unclosed terms depends on the form of the energy equation chosen (internal or total energy, total energy of the resolved field or enthalpy).

Early applications of LES to compressible flows used a transport equation for the internal energy per unit mass, ε (Moin *et al.* 1991, El-Hady *et al.* 1994) or for the enthalpy per unit mass, h (Speziale *et al.* 1988, Erlebacher *et al.* 1992). In these equations, the SGS heat flux was modeled in a manner similar to that used for the SGS stresses, and the remaining terms (the SGS pressure-dilatation Π_{dil}, and the SGS contribution to the viscous dissipation, ε_v) were neglected.

Vreman *et al.* (1995b) performed *a priori* tests using DNS data obtained from the calculation of a mixing layer at Mach numbers in the range 0.2–0.6 to establish the validity of these assumptions. They found that the SGS pressure-dilatation and SGS viscous dissipation are of the same order as the divergence of the SGS heat flux Q_j, and that modeling ε_v improves the results, especially at moderate or high Mach numbers.

Vreman *et al.* (1995a,1995b) proposed the use of a transport equation for the total energy of the filtered field, rather than either the enthalpy or the internal energy equations; the same unclosed terms that appear in this equation are also present in the internal energy and enthalpy equations. This equation was also used by

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Normand and Lesieur (1992), who neglected both Π_{dil} and ε_v.

Very few calculations have been carried out using the transport equation for the total energy, despite the desirable feature that it is a conserved quantity, and that all the SGS terms in this equation can be cast in conservative form. This equation has a completely different set of unclosed terms, whose modeling is not very advanced yet. Knight *et al.* (1998) performed the LES of isotropic homogeneous turbulence on unstructured grids and compared the results obtained with the Smagorinsky (1963) model with those obtained when the energy dissipation was provided only by the dissipation inherent in the numerical algorithm. They modeled the SGS heat flux and an SGS turbulent diffusion term, and neglected the SGS viscous diffusion.

In this paper, the flow field from a DNS of homogeneous isotropic turbulence is used to compute the terms in the energy equations, and evaluate possible models for their parameterization. The work will be focused mainly in the total energy equation, both because of the lack of previous studies of the terms that appear in it, and because of the desirability of solving a transport equation for a conserved quantity.

In the following section, the governing equations are presented, the terms that require closure are defined, and the DNS database used for the *a priori* tests is described. In Sections 3 and 4 several models for the unclosed terms are presented and tested. Finally, some conclusions are drawn in Section 5.

2 Problem formulation

2.1 Governing equations

To separate the large from the small scales, LES is based on the definition of a filtering operation: a filtered (or resolved, or large-scale) variable, denoted by an overbar, is defined as (Leonard 1974)

$$\overline{f}(\mathbf{x}) = \int_D f(\mathbf{x}')G(\mathbf{x},\mathbf{x}';\overline{\Delta})d\mathbf{x}', \tag{1}$$

where D is the entire domain and G is the filter function, and $\overline{\Delta}$ is the filter width, *i.e.*, the wavelength of the smallest scale retained by the filtering operation. The filter function determines the size and structure of the small scales.

In compressible flows, it is convenient to use Favre-filtering (Favre 1965a, 1965b) to avoid the introduction of subgrid-scale terms in the equation of conservation of mass. A Favre-filtered variable is defined as:

$$\tilde{f} = \overline{\rho f}/\overline{\rho}. \tag{2}$$

To obtain the equations governing the motion of the resolved eddies, the Favre-filtering operation must be applied to the equations of conservation of mass, momentum and energy. In compressible flows, in addition to the mass and momentum equations, one can choose between solving an equation for the internal energy, enthalpy or total energy. The filtered equations of motion, then, can be put in the form:

$$\frac{\partial\overline{\rho}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\right) = 0, \tag{3}$$

$$\frac{\partial\overline{\rho}\,\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_i\widetilde{u}_j + \overline{p} - \widetilde{\sigma}_{ji}\right) = -\frac{\partial\tau_{ji}}{\partial x_j} \tag{4}$$

$$\frac{\partial(\overline{\rho}\,\widetilde{\varepsilon})}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{u}_j\widetilde{\varepsilon}\right) + \frac{\partial\widetilde{q}_j}{\partial x_j} + \overline{p}\widetilde{S}_{kk} - \widetilde{\sigma}_{ji}\widetilde{S}_{ij} = -C_v\frac{\partial Q_j}{\partial x_j} - \Pi_{dil} + \varepsilon_v, \tag{5}$$

$$\frac{\partial(\overline{\rho}\,\widetilde{h})}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{u}_j\widetilde{h}\right) + \frac{\partial\widetilde{q}_j}{\partial x_j} - \frac{\partial\overline{p}}{\partial t} - \widetilde{u}_j\frac{\partial\overline{p}}{\partial x_j} - \widetilde{\sigma}_{ji}\widetilde{S}_{ij} = -C_v\frac{\partial Q_j}{\partial x_j} - \Pi_{dil} + \varepsilon_v, \tag{6}$$

$$\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{E}) + \frac{\partial}{\partial x_j}\left[(\overline{\rho}\,\widetilde{E} + \overline{p})\widetilde{u}_j + \widetilde{q}_j - \widetilde{\sigma}_{ji}\widetilde{u}_j\right] = -\frac{\partial}{\partial x_j}\left(\gamma C_v Q_j + \frac{1}{2}J_j - D_j\right). \tag{7}$$

Here, u_j is the velocity in the j direction, ρ is the density, p the pressure and T the temperature, $\varepsilon = c_v T$ is the internal energy per unit mass, $h = \varepsilon + p/\rho$ is the enthalpy per unit mass, $E = \varepsilon + u_i u_i/2$ is the total energy per unit mass, and the diffusive fluxes are given by

$$\widetilde{\sigma}_{ij} = 2\widetilde{\mu}\widetilde{S}_{ij} - \frac{2}{3}\widetilde{\mu}\delta_{ij}\widetilde{S}_{kk}, \qquad \widetilde{q}_j = -\widetilde{k}\frac{\partial\widetilde{T}}{\partial x_j}, \tag{8}$$

where $\widetilde{\mu}$ is the molecular viscosity, and $\widetilde{k}$ is the thermal conductivity corresponding to the filtered temperature $\widetilde{T}$. The effect of the subgrid scales appears through the SGS stresses τ_{ij}, the SGS heat flux Q_j, the SGS pressure-dilatation Π_{dil}, the SGS contribution to the viscous dissipation, ε_v, the SGS turbulent diffusion $\partial J_j/\partial x_j$, and the SGS contribution to viscous diffusion, $\partial D_j/\partial x_j$; these quantities are defined as:

$$\tau_{ij} = \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right) \tag{9}$$

$$Q_j = \overline{\rho}\left(\widetilde{u_j T} - \widetilde{u}_j\widetilde{T}\right) \tag{10}$$

$$\Pi_{dil} = \overline{p S_{kk}} - \overline{p}\widetilde{S}_{kk} \tag{11}$$

$$\varepsilon_v = \overline{\sigma_{ji}S_{ij}} - \widetilde{\sigma}_{ji}\widetilde{S}_{ij} \tag{12}$$

$$J_j = \overline{\rho}\left(\widetilde{u_j u_k u_k} - \widetilde{u}_j\widetilde{u_k u_k}\right) \tag{13}$$

$$D_j = \overline{\sigma_{ji}u_i} - \widetilde{\sigma}_{ji}\widetilde{u}_j. \tag{14}$$

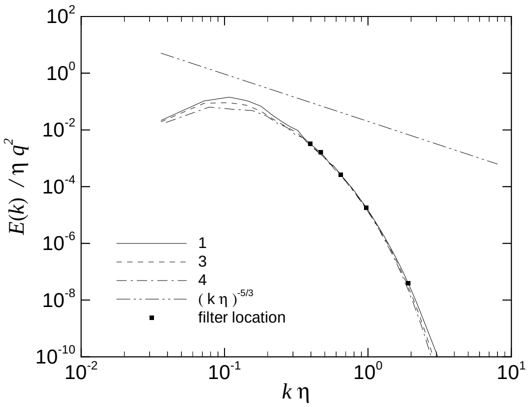

Figure 1. Energy spectra at $t/\tau_t = 1$, 3 and 4. The squares correspond to the filter-widths used in the *a priori* tests.

The equation of state has been used to express pressure-gradient and pressure-diffusion correlations in terms of Q_j and Π_{dil}. It is also assumed here that

$$\overline{\mu(T)S_{ij}} \simeq \mu(\widetilde{T})\widetilde{S}_{ij}, \qquad (15)$$

and an equivalent equality involving the thermal conductivity applies. Vreman *et al.* (1995b) performed *a priori* tests using DNS data obtained from the calculation of a mixing layer at Mach numbers in the range 0.2–0.6, and concluded that neglecting the nonlinearities of the diffusion terms in the momentum and energy equations is acceptable.

2.2 A priori tests

One method to evaluate the performance of models for LES or RANS calculations is the *a priori* test, in which the velocity fields obtained from a direct simulation are filtered to yield the exact SGS terms, and the filtered quantities are used in a modeling *ansatz* to evaluate the accuracy of the parameterization. The database used in this study was obtained from the calculation of homogeneous isotropic turbulence decay.

The Navier-Stokes equations were integrated in time using a fourth-order order Runge-Kutta method. The spatial derivatives were computed using an eighth-order accurate central finite-difference scheme. The simulations were performed on grids with 256^3 points, so that a large range of scales is found in the energy spectrum. The computational domain is a periodic box with length 2π in each dimension. The fluctuating fields were initialized as in Martín and Candler (1996) and the DNS results were validated by comparison with the Martín and Candler (1996) simulations.

The calculation was performed at a Reynolds number $Re_\lambda = u'\lambda/\nu = 35$, where λ is the Taylor micro-scale and u' is the turbulence intensity, and at a turbulent Mach number $M_t = q/a = 0.52$, where $q^2 = u_i u_i$ and a is the speed of sound. Since the dilatational field is initially zero, the flow is allowed to evolve for one dimensionless time unit, $\tau_t = \lambda/u'$.

The subgrid scale quantities were then evaluated. The DNS fields were filtered using a top-hat filter

$$\overline{f}_i = \frac{1}{2n}\left(f_{i-\frac{n}{2}} + 2\Sigma_{i-\frac{n}{2}+1}^{i+\frac{n}{2}-1} f_i + f_{i+\frac{n}{2}}\right) \qquad (16)$$

with varying filter widths $\overline{\Delta} = n\Delta$, where Δ is the grid size and $n = 2$, 4, 6, 8 and 10. Figure 1 shows the energy spectrum including the location of the filter cutoffs. All the filter-widths tested lie in the decaying region of the spectrum. Most of the results will be shown for a filter-width $\overline{\Delta} = 8\Delta$, at the edge of the inertial range of the spectrum. With this filter width approximately 11% of the energy resides in the subgrid-scales, a value representative of actual LES. Two quantities are used to evaluate the accuracy of a model: the correlation coefficient of the modeled term with the exact one, defined as

$$C(f) = \frac{\langle f_{\rm model} f_{\rm DNS}\rangle}{rms(f_{\rm model})rms(f_{\rm DNS})}, \qquad (17)$$

and the L_2-norm of the modeled and exact terms.

3 Models for the momentum equation

The modeling of the SGS stresses has received comparatively more attention than any of the other unclosed terms in compressible flows. Yoshizawa (1986) proposed an eddy-viscosity model for weakly compressible turbulent flows using a multi-scale direct-interaction approximation method. The anisotropic part of the SGS stresses is parameterized using the Smagorinsky (1963) model, while the SGS energy τ_{kk} is modeled separately:

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = -C_s^2 2\overline{\Delta}^2\overline{\rho}|\widetilde{S}|\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\widetilde{S}_{kk}\right) = C_s^2\alpha_{ij} \qquad (18)$$

$$\tau_{kk} = C_I 2\overline{\rho}\overline{\Delta}^2|\widetilde{S}|^2 = C_I\alpha \qquad (19)$$

with $C_s = 0.16$ and $C_I = 0.09$.

Speziale *et al.* (1988) proposed the addition of a scale-similar part to the eddy-viscosity model of Yoshizawa. Scale-similar models are based on the assumption that the most active subgrid scales are those closer to the cutoff wavenumber, and that the scales with which they interact most are those right above the cutoff (Bardina *et al.*, 1980). The mixed model proposed by Speziale *et al.* (1988), and used by Erlebacher *et al.* (1992) and Zang *et* *al.* (1992) was given by

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = C_s\alpha_{ij} + A_{ij} - \frac{\delta_{ij}}{3}A_{kk} \tag{20}$$
$$\tau_{kk} = C_I\alpha + A_{kk}, \tag{21}$$

where $A_{ij} = \overline{\rho}\,(\widetilde{\widetilde{u}_i\widetilde{u}_j} - \widetilde{\widetilde{u}}_i\widetilde{\widetilde{u}}_j)$. Erlebacher *et al.* (1992) tested the constant coefficient model *a priori* and by comparing DNS and LES results of compressible isotropic turbulence and found good agreement in the dilatational statistics of the flow, as well as high correlation between the exact and the modeled stresses. Zang *et al.* (1992) compared the DNS and LES results of isotropic turbulence with various initial ratios of compressible to total kinetic energy. They obtained good agreement for the evolution of quantities such as compressible kinetic energy and fluctuations of the thermodynamic variables.

Moin *et al.*(1991) proposed a modification of the eddy-viscosity model (18–19) in which the two model coefficients were determined dynamically, rather than input *a priori*, using the identity (Germano 1992) $L_{ij} = T_{ij} - \widehat{\tau_{ij}}$, which relates the "resolved turbulent stresses",

$$L_{ij} = \left(\widehat{\overline{\rho u_i}\,\overline{\rho u_j}/\overline{\rho}}\right) - \widehat{\overline{\rho u_i}}\,\widehat{\overline{\rho u_j}}/\widehat{\overline{\rho}}\,, \tag{22}$$

the subgrid-scale stresses τ_{ij} and the subtest stresses $T_{ij} = \widehat{\overline{\rho}}\,\breve{\widetilde{u_i u_j}} - \widehat{\overline{\rho}}\,\breve{\widetilde{u}}_i\breve{\widetilde{u}}_j$, where $\breve{\widetilde{f}} = \widehat{\overline{\rho f}}/\widehat{\overline{\rho}}$, and the hat represents the application of the test filter $\widehat{G}$, of characteristic width $\widehat{\Delta} = 2\overline{\Delta}$. Moin *et al.* (1991) determined the model coefficients by substituting the models (18–19) into (22) and contracting with $\widetilde{S}_{ij}$; in this work the contraction proposed by Lilly (1992) to minimize the error in a least-squares sense will be used instead. Accordingly, the two model coefficients for the Dynamic Eddy-Viscosity model (denoted hereafter by the acronym DEV) will be given by

$$C = C_s^2 = \frac{\langle L_{ij}M_{ij}\rangle}{\langle M_{kl}M_{kl}\rangle} - \frac{1}{3}\frac{\langle L_{mm}M_{nn}\rangle}{\langle M_{kl}M_{kl}\rangle}, \qquad C_I = \frac{\langle L_{kk}\rangle}{\langle \beta - \widehat{\alpha}\rangle}, \tag{23}$$

where $\beta_{ij} = -2\widehat{\Delta}^2\widehat{\overline{\rho}}\,|\breve{\widetilde{S}}|(\breve{\widetilde{S}}_{ij} - \delta_{ij}\breve{\widetilde{S}}_{kk}/3)$, $M_{ij} = \beta_{ij} - \widehat{\alpha_{ij}}$, $\beta = 2\widehat{\Delta}^2\widehat{\overline{\rho}}\,|\breve{\widetilde{S}}|^2$, and the brackets $\langle\cdot\rangle$ denote averaging over the computational volume. Dynamic model adjustment can be also applied to the mixed model (20–21), to yield the Dynamic Mixed model (DMM)

$$C = \frac{\langle L_{ij}M_{ij}\rangle - \langle N_{ij}M_{ij}\rangle}{\langle M_{lk}M_{lk}\rangle} - \frac{1}{3}\frac{\langle L_{mm}M_{nn}\rangle + \langle N_{mm}M_{nn}\rangle}{\langle M_{lk}M_{lk}\rangle} \tag{24}$$
$$C_I = \frac{\langle L_{kk} - N_{kk}\rangle}{\langle \beta - \widehat{\alpha}\rangle}, \tag{25}$$

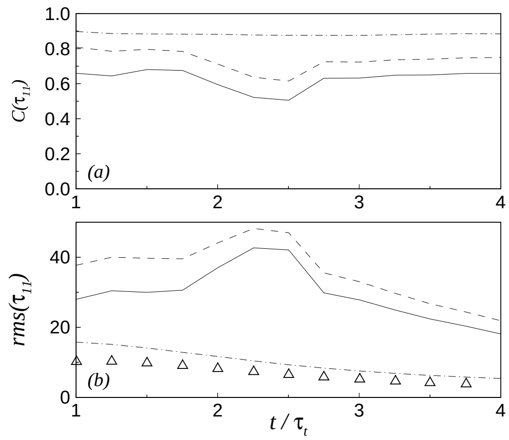

Figure 2. *A priori* comparison of the normal SGS stresses τ_{11}. ——— DEV; - - - DMM; —·— DMM-1; △ DNS. (a) Correlation coefficient; (b) *rms* fluctuations.

with $B_{ij} = \widehat{\overline{\rho}}\,(\breve{\widetilde{\widetilde{u}_i\widetilde{u}_j}} - \breve{\widetilde{\widetilde{u}}}_i\breve{\widetilde{\widetilde{u}}}_j)$, and $N_{ij} = B_{ij} - \widehat{A_{ij}}$. One advantage of mixed models is that they allow one to model the trace of the SGS stresses without requiring a separate term of the form (19). A one-coefficient dynamic mixed model (DMM-1) would be of the form

$$\tau_{ij} = C\alpha_{ij} + A_{ij}, \tag{26}$$

with

$$C = \frac{\langle L_{ij}M_{ij}\rangle - \langle N_{ij}M_{ij}\rangle}{\langle M_{lk}M_{lk}\rangle}. \tag{27}$$

Figures 2 and 3 compare the diagonal and off-diagonal components of the SGS stress tensor predicted by the various models. Consistent with the results of previous investigators eddy-viscosity models are not to be able to predict the *rms* of the SGS stresses very accurately. All models have high correlation with the DNS data, although, for the DEV model, that is due to the trace of τ_{kk}. The eddy-viscosity prediction of the off-diagonal terms (Fig. 3) has, in fact, a much lower correlation coefficient. In general, the one-coefficient mixed model (26–27) appears to be the most accurate among those tested. Its correlation with the exact SGS stresses is always greater than 0.8, and the prediction of the *rms* is consistently more accurate than that of the eddy-viscosity model (and is also more accurate than that obtained with the two-coefficient mixed model, in which the SGS energy is modeled separately).

The coefficient C_s remained nearly constant at a value of 0.15 throughout the calculation, consistent with the theoretical arguments (Yoshizawa 1986). The coefficient of the SGS energy, C_I,

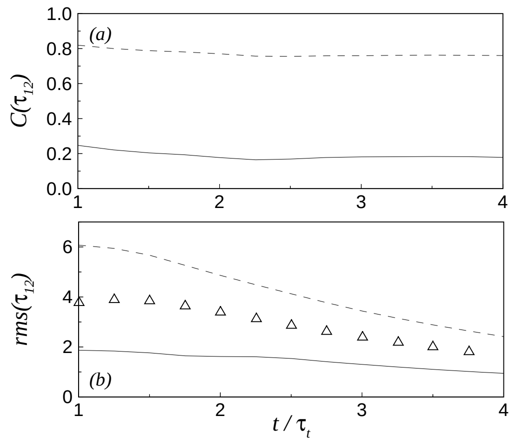

Figure 3. *A priori* comparison of the off-diagonal SGS stresses τ_{12}. ——— DEV; – – – DMM and DMM-1; △ DNS. (a) Correlation coefficient; (b) *rms* fluctuations.

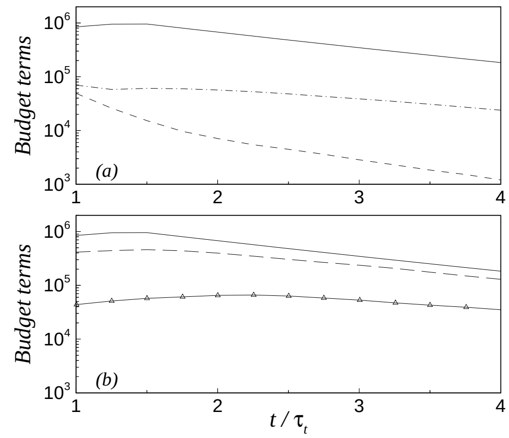

Figure 4. Comparison of unclosed terms in the energy equations. (a) Terms in the internal energy or enthalpy equations; (b) total energy equation. ——— Divergence of the SGS heat flux, $\partial Q_j/\partial x_j$; —·— SGS viscous dissipation ε_v; – – – pressure dilatation Π_{dil}; — — — SGS turbulent diffusion $\partial J_j/\partial x_j$; —△— SGS viscous diffusion $\partial D_j/\partial x_j$.

on the other hand, has a value three times higher than predicted by the theory, consistent with the results of Moin *et al.* (1991).

4 Models for the energy equations

A comparison of the magnitude of the unclosed terms in the three forms of the energy equation (5), (6) and (7) is shown in Fig. 4. Unlike in the mixing layer studied by Vreman *et al.* (1995b), in this flow the pressure dilatation Π_{dil} is negligible, and the viscous dissipation ε_v is less than one-tenth of the divergence of the SGS heat flux. Thus, the only term that requires modeling in the internal energy or enthalpy equations is Q_j. In the total energy equation, on the other hand, the SGS turbulent diffusion $\partial J_j/\partial x_j$ is significant. In the following, several models for the more significant terms will be examined.

The most important term to be closed (Fig. 4) is the divergence of the SGS heat flux (10). The simplest approach is to use an eddy-diffusivity model of the form:

$$Q_j = -\frac{\overline{\rho}\nu_T}{Pr_T}\frac{\partial \widetilde{T}}{\partial x_j} = -C\frac{\overline{\Delta}^2\overline{\rho}\,|\widetilde{S}|}{Pr_T}\frac{\partial \widetilde{T}}{\partial x_j}, \qquad (28)$$

where C is the eddy-viscosity coefficient in (23). The turbulent Prandtl number Pr_T can be fixed, or adjusted dynamically according to $Pr_T = C\langle T_k T_k\rangle/\langle K_j T_j\rangle$, where

$$K_j = \left(\widehat{\overline{\rho u_j}\,\overline{\rho T}/\overline{\rho}}\right) - \widehat{\overline{\rho u_j}}\,\widehat{\overline{\rho T}}/\widehat{\overline{\rho}}\,, \qquad (29)$$

$$T_j = -\widehat{\Delta}^2\widehat{\overline{\rho}}\,|\breve{S}|\frac{\partial \breve{\widetilde{T}}}{\partial x_j} + \widehat{\overline{\Delta}^2\overline{\rho}\,|\widetilde{S}|\frac{\partial \widetilde{T}}{\partial x_j}}. \qquad (30)$$

A mixed model of the form

$$Q_j = -C\frac{\overline{\Delta}^2\overline{\rho}\,|\widetilde{S}|}{Pr_T}\frac{\partial \widetilde{T}}{\partial x_j} + \left(\widetilde{\widetilde{u}_j\widetilde{T}} - \widetilde{\widetilde{u}}_j\widetilde{\widetilde{T}}\right) \qquad (31)$$

was proposed by Speziale *et al.* (1988). The model coefficient C is given by (24); Pr_T can again be assigned *a priori* or adjusted dynamically according to

$$Pr_T = C\frac{\langle T_k T_k\rangle}{\langle K_j T_j\rangle - \langle V_j T_j\rangle}, \qquad (32)$$

with

$$V_j = \widehat{\overline{\rho}}\left(\breve{\widetilde{\breve{\widetilde{u}}_j\breve{\widetilde{T}}}} - \breve{\widetilde{\breve{\widetilde{u}}}}_j\breve{\widetilde{\breve{\widetilde{T}}}}\right) - \overline{\rho}\left(\widehat{\widetilde{\widetilde{u}_j\widetilde{T}}} - \widetilde{\widetilde{u}}_j\widetilde{\widetilde{T}}\right). \qquad (33)$$

In Figure 5 the models described above are compared. The eddy-diffusivity models have poor correlation with the DNS data, as is the case with these types of model. The constant-Pr_T case (the value used was 0.7, following Zang *et al.* 1992) gives a very low value of the *rms* of the modeled Q_j. A lower value, $Pr_T = 0.4$, as used by Speziale *et al.* (1988) would, however, give *rms* fluctuations nearly identical to those predicted using the dynamic procedure. The mixed model gives the best correlation with the data (again around 0.8), but over-predicts the *rms*; at early times the mixed model gives results in better agreement with the data than the eddy-diffusivity one, but for $t/\tau_t > 3$ the latter gives

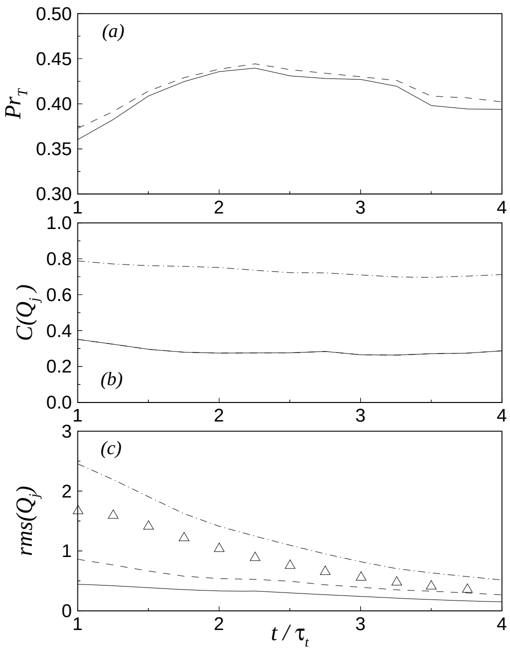

Figure 5. Coefficient, correlation and *rms* of the model for the SGS heat flux Q_j. (a) Turbulent Prandtl number, Pr_T; (b) correlation coefficient; (c) *rms*. ——— Eddy-diffusivity model, fixed Prandtl number; – – – eddy-diffusivity model, variable Prandtl number; —·— mixed model; △ DNS.

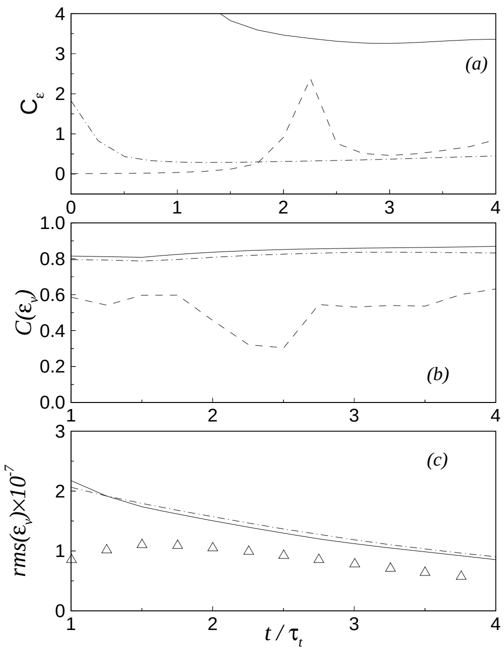

Figure 6. Coefficient, correlation and *rms* of the model for the viscous dissipation ε_v. (a) Model coefficient; (b) correlation coefficient; (c) *rms*. ——— Scale similar (34); – – – Dynamic (35); —·— Dynamic (36); △ DNS.

more accurate results. A limitation of this study is the fact that the filter width is already in the decaying region of the spectrum, a situation that has been shown to degrade the accuracy of the dynamic procedure (Meneveau and Lund 1997).

The other term that can be significant in the enthalpy or internal energy equations is the viscous dissipation ε_v. Vreman *et al.* (1995b) proposed three models for this term:

$$\varepsilon_v^{(1)} = C_{\varepsilon 1}\left(\widetilde{\tilde{\sigma}_{ji}\tilde{S}_{ij}} - \tilde{\tilde{\sigma}}_{ij}\tilde{\tilde{S}}_{ij}\right); \tag{34}$$

$$\varepsilon_v^{(2)} = C_{\varepsilon 2}\bar{\rho}\tilde{q}^3/\bar{\Delta}, \qquad \tilde{q}^2 \sim \bar{\Delta}^2|\tilde{S}|^2; \tag{35}$$

$$\varepsilon_v^{(3)} = C_{\varepsilon 3}\bar{\rho}\tilde{q}^3\bar{\Delta}, \qquad \tilde{q}^2 \sim \widetilde{\tilde{u}_k\tilde{u}_k} - \tilde{\tilde{u}}_k\tilde{\tilde{u}}_k. \tag{36}$$

The first is a scale-similar model; the second and third use dimensional analysis to represent the SGS dissipation as the ratio between the cube of the SGS velocity scale, $\tilde{q}$, and the length scale, and assign the velocity scale using either the Yoshizawa (1986) model (19) or the scale-similar model. For consistency, each of the last two models should be coupled with the corresponding model for τ_{kk}. Based on their DNS data, Vreman *et al.* (1995b) fixed the values of the coefficients that give the correct magnitude for this term and obtained: $C_{\varepsilon 1} = 8$, $C_{\varepsilon 2} = 1.6$ and $C_{\varepsilon 3} = 0.6$. Alternatively, the dynamic procedure can be used to give

$$\left\langle \widehat{\tilde{\sigma}_{ji}\tilde{S}_{ij}} - \widehat{\bar{\rho}\sigma_{ij}}\,\widehat{\bar{\rho}S_{ij}}/\hat{\bar{\rho}}^2 \right\rangle = \left\langle E_v^{(n)} - \widehat{\varepsilon_v^{(n)}} \right\rangle, \tag{37}$$

where

$$E_v^{(1)} = C_{\varepsilon 1}\left(\widetilde{\breve{\tilde{\sigma}}_{ji}\breve{\tilde{S}}_{ij}} - \breve{\tilde{\tilde{\sigma}}}_{ij}\breve{\tilde{\tilde{S}}}_{ij}\right); \tag{38}$$

$$E_v^{(2)} = C_{\varepsilon 2}\hat{\bar{\rho}}\,\breve{q}^3/\hat{\Delta}, \qquad \breve{q}^2 \sim \hat{\Delta}^2|\breve{S}|^2; \tag{39}$$

$$E_v^{(3)} = C_{\varepsilon 3}\hat{\bar{\rho}}\,\breve{q}^3/\hat{\Delta}, \qquad \breve{q}^2 \sim \widetilde{\breve{\tilde{u}}_i\breve{\tilde{u}}_j} - \breve{\tilde{\tilde{u}}}_i\breve{\tilde{\tilde{u}}}_j. \tag{40}$$

Model coefficients obtained from the dynamic procedure in this form (in which there is no contraction) can become ill-conditioned, since the two terms in the denominator may be approximately equal, giving spuriously high values of the denominator. This behavior was observed in model (34), in which acceptable results were obtained only if $C_{\varepsilon 1}$ was constrained to be positive, and model (35). The model given by (36), on the other hand, was well behaved.

Figure 6 compares the predictions of the three models. The values of the coefficients obtained from the present *a priori* test

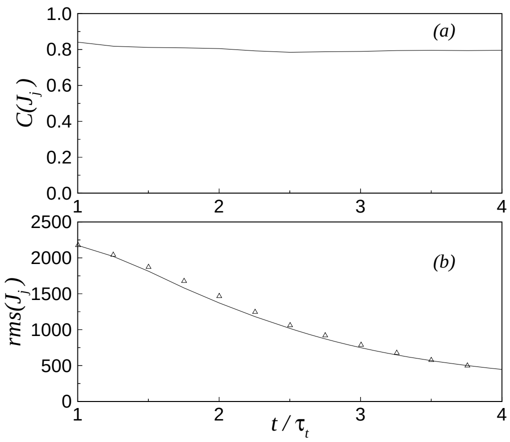

Figure 7. Correlation and *rms* of the model for the turbulent diffusion J_j. (a) correlation coefficient; (b) *rms*. ——— Knight *et al.* (1998) model; △ DNS.

are lower than those obtained in the mixing layer by Vreman *et al.* (1995b). The pure scale-similar model (34) and the model (36), which also uses scale similarity to supply the velocity scale, give the best correlation and nearly correct *rms* amplitudes. The *rms* predicted by the model (35) is two orders of magnitude larger than the others, and cannot be seen in the plot. In this flow the coefficients obtained from the mixing layer data would yield high values of the modeled *rms*, indicating some lack of universality for the modeling of this term.

The two terms in the total energy equation that require modeling are the SGS turbulent diffusion $\partial J_j/\partial x_j$ and the SGS viscous diffusion $\partial D_j/\partial x_j$. The only calculation that attempted to model the former was that by Knight *et al.* (1998). They argued that $\widetilde{u}_i \simeq \widetilde{\widetilde{u}}_i$ and proposed a model of the form

$$J_j \simeq \widetilde{u}_k \tau_{jk}. \tag{41}$$

This model is compared in Fig. 7 with the DNS data; τ_{jk} was obtained from the DMM-1 model (41). The model has a high correlation with the data (of order 0.8), and the *rms* also matches the data well. It should be noticed, however, that the model is built upon the prediction of the SGS stresses by DMM-1, which over-predicts the *rms* of the normal stresses by 30%, that of the off-diagonal ones by about 50%. It appears that the modeling assumption by itself might underestimate the diffusion, an error that is compensated by one of opposite sign in the SGS stress model. The high correlation, however, indicates that addition of a model coefficient, perhaps adjusted dynamically, may be beneficial.

The SGS viscous diffusion $\partial D_j/\partial x_j$ is the smallest of the terms in the total energy equation. It is 5% of the divergence of Q_j at $t/\tau_t = 1$, but increases to about 10% at the final time. No model for this term has been proposed in the literature to date.

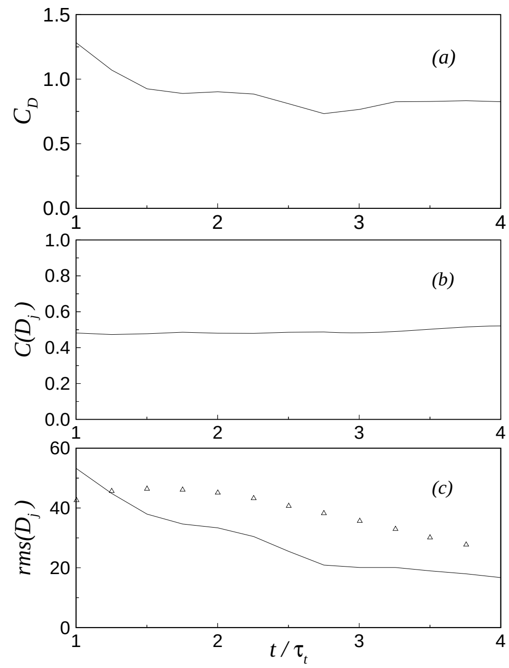

Figure 8. Coefficient, correlation and *rms* of the model for the viscous diffusion D_j. (a) Model coefficient; (b) correlation coefficient; (c) *rms*. ——— Scale-similar model; △ DNS.

One possibility is to parameterize it using a scale-similar model of the form

$$D_j = C_D(\widetilde{\widetilde{\sigma}_{ij}\widetilde{u}_i} - \widetilde{\widetilde{\sigma}}_{ij}\widetilde{\widetilde{u}}_i), \tag{42}$$

in which the coefficient can be obtained from

$$C_D = \frac{\left\langle \left[\frac{\widehat{\overline{\rho\sigma_{ij}}\,\overline{\rho u_i}}}{\overline{\rho}^2} - \frac{\widehat{\overline{\rho\sigma_{ij}}}\,\widehat{\overline{\rho u_i}}}{\widehat{\overline{\rho}}^2} \right] R_j \right\rangle}{\langle R_k R_k \rangle}, \tag{43}$$

where

$$R_l = \left(\breve{\widetilde{\widetilde{\sigma}}_{lk}\widetilde{\widetilde{u}}_k} - \breve{\widetilde{\widetilde{\sigma}}}_{lk}\breve{\widetilde{\widetilde{u}}}_k \right) - \left(\widehat{\widetilde{\widetilde{\sigma}}_{lk}\widetilde{u}_k} - \widehat{\widetilde{\widetilde{\sigma}}}_{lk}\widehat{\widetilde{u}}_k \right). \tag{44}$$

As can be seen from Fig. 8, however, this approach gives a fairly poor correlation, and fair agreement for the prediction of the *rms* intensities. This error may, however, be tolerable given the small contribution that this term gives to the energy budget.

5 Conclusions

Several mixed and eddy-viscosity models for the momentum and energy equations have been tested. The velocity, pressure, density and temperature fields obtained from the DNS of homogeneous isotropic turbulence at $Re_\lambda = 35$, $M_t = 0.52$ were filtered and the unclosed terms in the momentum, internal energy and total energy equations were computed.

In the momentum equation, mixed models were found to give better prediction, in terms of both correlation and *rms* amplitude, than the pure eddy-viscosity models. The dynamic adjustment of the model coefficient was beneficial, as already observed by Moin *et al.* (1991).

In the internal energy and enthalpy equations, in this flow, only the divergence of the SGS heat flux was significant; the SGS pressure dilatation Π_{dil} and viscous dissipation ε_v, which were significant in the mixing layer studied by Vreman *et al.* (1995b), were found to be negligible here. Once again, mixed dynamic models gave the most accurate results. In particular, the turbulent Prandtl number obtained dynamically was somewhat lower than the value of 0.7 often assigned *a priori*.

In the total energy equation two additional terms are present, one of which, the turbulent diffusion $\partial J_j/\partial x_j$ is significant. The model proposed by Knight *et al.* (1998), which parameterizes the turbulent diffusion in terms of the SGS stresses, correlates well with the actual SGS stresses, and predicts the correct *rms* amplitude. A mixed model for the SGS turbulent diffusion has also been proposed and tested, although this term is much smaller than the others.

Although the preliminary results obtained in this investigation are promising, and indicate that it is possible to model the terms in the energy equations, and in particular in the total energy one, accurately, further work is required to extend these results to cases in which the pressure-dilatation is significant, as well as to inhomogeneous flows. *A posteriori* testing of the models in actual calculations is also necessary for a complete evaluation of the model performance.

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