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ABSTRACT

A subgrid-scale model recently derived by Yoshizawa[1] for use in the large-eddy simulation of compressible turbulent flows is examined from a fundamental theoretical and computational standpoint. It is demonstrated that this model, which is only applicable to compressible turbulent flows in the limit of small density fluctuations, correlates somewhat poorly with the results of direct numerical simulations of compressible isotropic turbulence at low Mach numbers. An alternative model, based on Favre-filtered fields, is suggested which appears to reduce these limitations.

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In a recent article, Yoshizawa[1] developed sugrid-scale models for possible future use in the large-eddy simulation of compressible turbulent flows. These models were obtained by making use of a multiscale version of Kraichnan's DIA formalism.[2,3] While the study conducted by Yoshizawa is quite interesting, it will be pointed out in this work that the specific subgrid-scale stress model derived therein is limited to slightly compressible flows (i.e., to flows with small density fluctuations) and also correlates somewhat poorly with direct numerical simulations of isotropic compressible turbulence at low Mach numbers. This poor correlation arises from Yoshizawa's formulation of a Smagorinsky-type model which neglects entirely the effects of momentum exchanges between the small and large scales that are accounted for in the subgrid-scale Leonard and Cross stress terms. These inaccuracies can be reduced by a new subgrid-scale stress model that was recently derived by the authors.[4] The purpose of this work is to provide a comparison of these two alternative approaches. Subgrid-scale models are needed for the large-eddy simulation of compressible turbulence with important applications to high speed aerodynamic flows.

In the large-eddy simulation of compressible turbulent flows, any field quantity F in the flow domain D can be decomposed as follows

$$F = \overline{F} + F'' \tag{1}$$

where

$$\overline{F} = \int_D G(\underset{\sim}{x} - \underset{\sim}{z}, \Delta) F(\underset{\sim}{z}) d^3 z \tag{2}$$

is the filtered part and F'' is the subgrid scale part which accounts for the scales that are not resolved by the computational grid Δ. Yoshizawa[1] developed subgrid scale models (based on the filtering procedure (1)) by making use of Kraichnan's DIA formalism generalized to the compressible regime with a multiscale expansion. It was assumed therein that the length and time scales of the fluctuating fields were small compared with those of the mean fields. Such an assumption restricts the applicability of the models to flows with small density fluctuations (i.e., it is equivalent to making a small compressibility expansion). A Smagorinsky model for the subgrid scale stress was obtained to the first order when a state of isotropy was assumed for the zero-order solution. Comparable subgrid scale models of the gradient transport type were derived, to the first order, for the remaining subgrid scale correlations (e.g., the subgrid scale heat flux).

As an alternative to this approach, in line with the more traditional analyses of compressible turbulent flows, a Favre filter can be defined as follows:

$$\tilde{F} = \frac{\overline{\rho F}}{\bar{\rho}} \tag{3}$$

where ρ is the mass density. This gives rise to the alternative decomposition

$$F = \tilde{F} + F' \tag{4}$$

where F' is the subgrid scale part of F based on Favre filtering. The Favre filtered equations of motion for an ideal gas are given by[4]

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{v}_k) = 0 \tag{5}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{v}_k) + \frac{\partial}{\partial x_\ell}(\bar{\rho}\tilde{v}_k\tilde{v}_\ell) = -\frac{\partial \bar{p}}{\partial x_k} + \frac{\partial \bar{\sigma}_{k\ell}}{\partial x_\ell} + \frac{\partial \tau_{k\ell}}{\partial x_\ell} \tag{6}$$

$$C_p\left[\frac{\partial(\bar{\rho}\tilde{T})}{\partial t} + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{v}_k\tilde{T})\right] = \frac{\partial \bar{p}}{\partial t} + \overline{v_k \frac{\partial p}{\partial x_k}} + \bar{\Phi} + \frac{\partial}{\partial x_k}\left(\overline{\kappa \frac{\partial T}{\partial x_k}}\right) - \frac{\partial Q_k}{\partial x_k} \tag{7}$$

where v_k is the velocity vector, $p \equiv \rho RT$ is the thermodynamic pressure, T is the temperature, and R is the ideal gas constant. In (6) - (7),

$$\sigma_{k\ell} = -\frac{2}{3}\mu \underset{\sim}{\nabla}\cdot\underset{\sim}{v}\,\delta_{k\ell} + \mu\left(\frac{\partial v_k}{\partial x_\ell} + \frac{\partial v_\ell}{\partial x_k}\right) \tag{8}$$

$$\tau_{k\ell} = -\bar{\rho}(\widetilde{\tilde{v}_k\tilde{v}_\ell} - \tilde{v}_k\tilde{v}_\ell + \widetilde{v'_k\tilde{v}_\ell} + \widetilde{\tilde{v}_k v'_\ell} + \widetilde{v'_k v'_\ell}) \tag{9}$$

$$\Phi = -\frac{2}{3}\mu(\underset{\sim}{\nabla}\cdot\underset{\sim}{v})^2 + \mu\left(\frac{\partial v_k}{\partial x_\ell} + \frac{\partial v_\ell}{\partial x_k}\right)\frac{\partial v_\ell}{\partial x_k} \tag{10}$$

$$Q_k = C_p\bar{\rho}(\widetilde{\tilde{v}_k\tilde{T}} - \tilde{v}_k\tilde{T} + \widetilde{v'_k\tilde{T}} + \widetilde{\tilde{v}_k T'} + \widetilde{v'_k T'}) \tag{11}$$

are the molecular stress tensor, the subgrid scale stress tensor, the viscous dissipation, and the subgrid scale heat flux, respectively, whereas μ is the dynamic viscosity and κ is the thermal conductivity.

In order to achieve closure of the equations of motion (5) - (7), subgrid scale models for $\tau_{k\ell}$ and Q_k must be provided. We recently proposed the following models[4]

$$\tau_{k\ell} = -\bar{\rho}(\widetilde{\tilde{v}_k\tilde{v}_\ell} - \tilde{\tilde{v}}_k\tilde{\tilde{v}}_\ell) + 2C_R\bar{\rho}\Delta^2 II_{\tilde{s}}^{1/2}(\tilde{S}_{k\ell} - \frac{1}{3}\tilde{S}_{mm}\delta_{k\ell}) - \frac{2}{3}C_I\bar{\rho}\Delta^2 II_{\tilde{s}}\delta_{k\ell} \tag{12}$$

$$Q_k = C_p\bar{\rho}[(\widetilde{\tilde{v}_k\tilde{T}} - \tilde{\tilde{v}}_k\tilde{\tilde{T}}) - \frac{C_R}{Pr_T}\Delta^2 II_{\tilde{s}}^{1/2}\frac{\partial\tilde{T}}{\partial x_k}] \tag{13}$$

where

$$\tilde{S}_{k\ell} = \frac{1}{2}(\frac{\partial\tilde{v}_k}{\partial x_\ell} + \frac{\partial\tilde{v}_\ell}{\partial x_k}) \tag{14}$$

$$II_{\tilde{s}} = \tilde{S}_{k\ell}\tilde{S}_{k\ell}, \tag{15}$$

Pr_T is the turbulent Prandtl number (which assumes a value of approximately 1/2), and C_R and C_I are dimensionless constants which were found to assume the values of 0.012 and 0.0066, respectively, by correlating with the results of direct numerical simulations of compressible isotropic turbulence. This model may be viewed as a compressible analogue of the linear combination model of Bardina, et al.[5]. The subgrid scale stress model (12) was found to correlate well with the results of direct numerical simulations of compressible isotropic turbulence for average Mach numbers $0 \leq M_0 \leq 0.6$ (for average Mach numbers $M_0 \geq 0.4$ there can be localized supersonic regions in this flow[4]). Correlation coefficients in the range of 80-95% were obtained at the tensor level independent of the average Mach number (see Table 1). These direct simulations of isotropic turbulence were performed using Fourier collocation methods on a 96^3 grid at a Reynolds number of $Re_\lambda \doteq 40$ based on the Taylor microscale. The initial energy spectrum was chosen to match that measured by Comte-Bellot and Corrsin[6], and the results (including those to be shown later in Fig. 1) were then non-dimensionalized with respect to a reference length scale and velocity scale of $10/\pi$ cm and 1 cm/sec, respectively (the physical properties of air at room temperature were used for the reference density and viscosity). The rms density fluctuations $\rho_{rms} \equiv \langle \rho'^2 \rangle^{1/2} / \langle \rho \rangle$ for $M_0 = 0.1$, $M_0 = 0.4$, and $M_0 = 0.6$ were 0.0034, 0.0358, and 0.0739 respectively, where $\langle \cdot \rangle$ denotes the spatial average.

In contrast to these compressible subgrid-scale models based on Favre-filtering, Yoshizawa[1] represents the subgrid scale Reynolds stress $\overline{v_k'' v_\ell''}$ by the Smagorinsky model (derived formally to the first-order using a two-scale DIA method; see equation (81) of Yoshizawa[1])

$$-\overline{v_k'' v_\ell''} = -\frac{2}{3} K \delta_{k\ell} + \nu_e \left(\frac{\partial \overline{v}_k}{\partial x_\ell} + \frac{\partial \overline{v}_\ell}{\partial x_k} \right) \tag{16}$$

where

$$K = \frac{1}{2} \overline{v_k'' v_k''} \tag{17}$$

$$\nu_e = C_{uu2}^2 \, \Delta^2 (2 \, \overline{S}_{mn} \overline{S}_{mn})^{1/2} \tag{18}$$

and C_{uu2} is a dimensionless constant that was found to assume a value of 0.16. However, by taking the trace of (16) it follows that

$$\underset{\sim}{\nabla} \cdot \underset{\sim}{\overline{v}} = 0 \tag{19}$$

which is strictly true only for incompressible turbulence. Hence, as alluded to earlier, the subgrid scale model (16) of Yoshizawa[1] is only appropriate for weakly compressible turbulent flows (this limitation arises since a small compressibility expansion was employed which requires the density fluctuations to be small.) There is an additional problem with the Smagorinsky model (16) even when it is restricted to flows with small density changes as pointed out by Bardina, et al.[5] This model neglects the kinematic Leonard stress $L_{k\ell}$ and Cross stress $C_{k\ell}$ given by

$$L_{k\ell} = \overline{\bar{v}_k \bar{v}_\ell} - \bar{v}_k \bar{v}_\ell, \quad C_{k\ell} = \overline{v_k'' \bar{v}_\ell} + \overline{\bar{v}_k v_\ell''} \tag{20}$$

(the total kinematic subgrid scale stress $\tau_{k\ell} \equiv L_{k\ell} + C_{k\ell} + R_{k\ell}$ where $R_{k\ell} \equiv \overline{v_k'' v_\ell''}$ is the kinematic Reynolds stress). For flows at low Mach numbers $M_0 \lesssim 0.1$, density changes are extremely small and the difference between Favre filtered fields and ordinary filtered fields is negligible. Hence, at low Mach numbers, the model derived by Yoshizawa[1] would correspond to equation (12) with the scale similarity part (i.e., the first term on the right-hand side of (12)) neglected. In particular, it would correspond to the model

$$_D\tau_{k\ell} = 2C_R\bar{\rho}\Delta^2 II_{\tilde{s}}^{1/2}(\tilde{S}_{k\ell} - \frac{1}{3}\tilde{S}_{mm}\delta_{k\ell}) \tag{21}$$

for the deviatoric part $_D\tau_{k\ell}$ of the subgrid scale stress tensor. The computations conducted by Erlebacher, et al.[4] indicate that such a model correlates poorly with the results of direct numerical simulations of compressible isotropic turbulence at low Mach numbers. To be specific, correlations at the tensor level (i.e., correlations of exact versus modeled subgrid scale stress tensors) for $M_0 = 0.1$ were only of the order of 30% as compared to the approximate value of 85% for the more complete model given by (12) (see Table 1 and 2). This improvement in the case of compressible flows is comparable to the improvement obtained by the linear combination model for incompressible flows (see Bardina, et al.[5]).

A distinguishing feature of compressible turbulence models is the existence of an isotropic subgrid scale stress which cannot simply be absorbed into the pressure term as is customarily done for incompressible flows. The isotropic part of Yoshizawa's model, in the limit of low Mach numbers for which the difference between Favre and ordinary filters are negligible, is given by

$$ {}_{I}\tau_{k\ell} = -\frac{2}{3} C_I \bar{\rho} \Delta^2 II_{\underset{\sim}{s}} \delta_{k\ell} \tag{22} $$

which differs from the Erlebacher, et al.[4] model by the absence of the isotropic part of the Leonard and Cross stress contributions. However, this model correlates even more poorly than the deviatoric part ${}_{D}\tau_{k\ell}$ of the subgrid scale stress tensor when compared with the results of direct numerical simulations of isotropic compressible turbulence. A scatterplot of the modeled (Eq. (22)) versus exact isotropic subgrid-scale stress ${}_{I}\tau_{kk}/3$ is shown in Figure 1 which was obtained from a 96^3 direct simulation of isotropic compressible turbulence at $M_0 = 0.1$. The correlation coefficient for this case is 15%. This correlation improves to the 85% level when the Leonard and Cross stresses are included.[4] It must be kept in mind however, that direct numerical simulations (Erlebacher, et al.[4]) indicate that the isotropic Reynolds stress affects the correlations by at most a few percent for $M_0 < 0.4$.

In conclusion, it has been pointed out that the Smagorinsky-type subgrid scale model developed by Yoshizawa[1] from the DIA for compressible large-eddy simulations is not applicable to turbulent flows with large density fluctuations and correlates somewhat poorly with the results of direct numerical simulations of compressible isotropic turbulence at small Mach numbers. In order to overcome these limitations, we believe that models should be based on Favre filtered fields (where no restrictions are placed on the density fluctuations) and the Leonard and Cross stresses must be accounted for. The compressible subgrid scale models recently developed by the authors[4] appear to be more general in this regard and are currently under study in a research program involving the large-eddy simulation of compressible turbulent shear flows.

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	$M_0 = 0.0$		$M_0 = 0.6$	
	L+C+R	C+R	L+C+R	C+R
D	93	82	93	81
OD	80	85	79	84
V	46	72	46	71
S	56	73	56	74

Table 1. Comparison of correlation coefficients of the exact subgrid scale stress $\tau_{k\ell} \equiv L_{k\ell} + C_{k\ell} + R_{k\ell}$ versus its model[4] (given by Eq. (12)) obtained from a 96^3 direct simulation of compressible isotropic turbulence ($D \equiv$ diagonal tensor level, $OD \equiv$ off-diagonal tensor level, $V \equiv$ vector level, $S \equiv$ scalar level, $L_{k\ell} \equiv -\bar{\rho}(\widetilde{\tilde{v}_k\tilde{v}_\ell} - \tilde{v}_k\tilde{v}_\ell)$, $C_{k\ell} = -\bar{\rho}(\widetilde{v_k''\tilde{v}_\ell} + \widetilde{\tilde{v}_k v_\ell''})$, $R_{k\ell} = -\bar{\rho}\widetilde{v_k''v_\ell''}$, $M_0 \equiv$ Average Mach number over the computational domain).

M_0		0.1	0.4	0.6
${}_D\mathbf{R}$	D	31	31	31
	OD	26	26	25
	V	22	22	22
	S	45	45	45

Table 2. Comparison of correlation coefficients between the exact and the modeled deviatoric subgrid scale Reynolds stress (given by Eq. (21)) obtained from a 96^3 direct simulation of compressible isotropic turbulence (${}_DR_{k\ell} \equiv -\bar{\rho}(\widetilde{v_k''v_\ell''} - \frac{1}{3}\widetilde{v_m''v_m''}\,\delta_{k\ell})$).

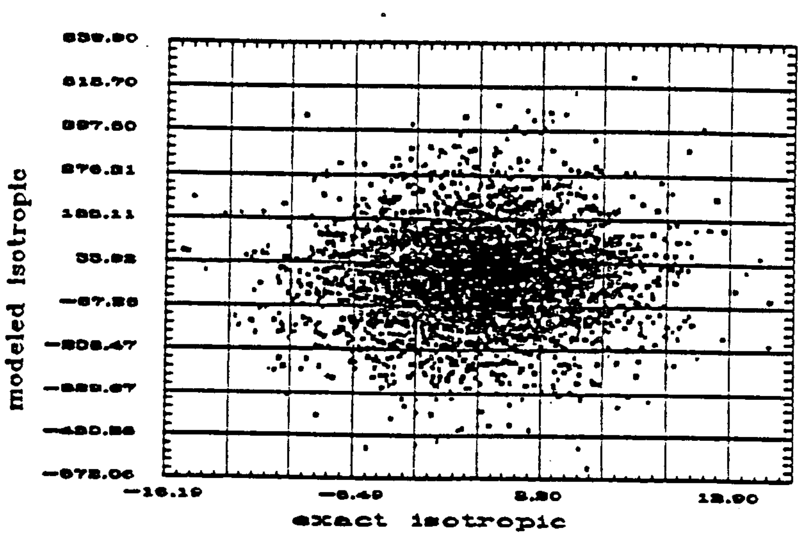

Figure 1. Scatterplot of the isotropic modeled[1] versus the exact subgrid scale stress ${}_I\tau_{kk}/3$ obtained from a 96^3 direct simulation of compressible isotropic turbulence at $M_0 = 0.1$.

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16. Abstract

A subgrid-scale model recently derived by Yoshizawa for use in the large-eddy simulation of compressible turbulent flows is examined from a fundamental theoretical and computational standpoint. It is demonstrated that this model, which is only applicable to compressible turbulent flows in the limit of small density fluctuations, correlates somewhat poorly with the results of direct numerical simulations of compressible isotropic turbulence at low Mach numbers. An alternative model, based on Favre-filtered fields, is suggested which appears to reduce these limitations.

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