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Realizability conditions for the turbulent stress tensor in large-eddy simulation

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The turbulent stress tensor in large-eddy simulation is examined from a theoretical point of view. Realizability conditions for the components of this tensor are derived, which hold if and only if the filter function is positive. The spectral cut-off, one of the filters frequently used in large-eddy simulation, is not positive. Consequently, the turbulent stress tensor based on spectrally filtered fields does not satisfy the realizability conditions, which leads to negative values of the generalized turbulent kinetic energy k. Positive filters, e.g. Gaussian or top-hat, always give rise to a positive k. For this reason, subgrid models which require positive values for k should be used in conjunction with e.g. the Gaussian or top-hat filter rather than with the spectral cut-off filter. If the turbulent stress tensor satisfies the realizability conditions, it is natural to require that the subgrid model for this tensor also satisfies these conditions. With respect to this point of view several subgrid models are discussed. For eddy-viscosity models a lower bound for the generalized turbulent kinetic energy follows as a necessary condition. This result provides an inequality for the model constants appearing in a 'Smagorinsky-type' subgrid model for compressible flows.

1. Introduction

Most turbulent flows contain too many scales to be solved directly. In order to reduce the number of scales to be solved, the Navier–Stokes equations governing turbulent flow are averaged. Two types of averaging approaches can be distinguished. In the classical approach, also known as the statistical approach, the equations are averaged with a statistical mean or ensemble average (Tennekes & Lumley 1972). In the filtering approach, which is the basis of the large-eddy simulation (LES) of turbulent flow (reviewed by e.g. Rogallo & Moin 1984), the averaging operator is a linear filtering operator, e.g. a local weighted average over a small volume of fluid. In the averaged Navier–Stokes equations additional terms appear, for which a model has to be assumed before the equations can be solved. The additional terms in the momentum equations are spatial derivatives of the turbulent stress tensor. In a large-eddy simulation this tensor is modelled with a subgrid model, so called since the scales which can be represented on the grid are solved explicitly, while the effect of the small 'subgrid scales' is modelled.

In the statistical approach the turbulent stress reduces to the Reynolds stress, which is a statistical central moment, and satisfies the so-called 'realizability conditions' (Du Vachat 1977; Schumann 1977). Unlike the ensemble average in the statistical approach, the averaging operator in the filtering approach does not satisfy the Reynolds rules for the mean (Monin & Yaglom 1971, p. 207). Although for this reason

the turbulent stress in the filtering approach is not equal to the Reynolds stress, several analogies between these two stresses exist. First, the turbulent stress in the filtering approach satisfies the Reynolds equations for the Reynolds stress in the statistical approach (Germano 1992). In addition to this property, which is called the averaging invariance of the turbulent equations, Germano presents an algebraic identity for the turbulent stress, resulting in a dynamic subgrid-scale eddy-viscosity formulation. Invariances or algebraic properties related to the large-eddy-simulation technique and their applications to subgrid modelling are scarcely found in literature. In addition to Germano's work, the work of Speziale (1985) should be mentioned, in which the Galilean invariance of subgrid models is discussed.

In the present paper it will be shown that the realizability conditions for the Reynolds stress in the statistical approach are also valid for the turbulent stress in the filtering approach, if and only if the filter function is positive. The proof of this statement is given in §2, while in §3 the theory is illustrated for three filters commonly used in large-eddy simulation. Furthermore, in §4 it is argued that a consistent subgrid model for the turbulent stress should satisfy the same inequalities as the turbulent stress itself. Whether this requirement is fulfilled is investigated for several existing subgrid models. Moreover, it is shown that for eddy-viscosity models the realizability conditions lead to a lower bound for the generalized turbulent kinetic energy.

2. Realizability conditions

In the large-eddy simulation of turbulent flow, any flow variable f is decomposed into a large-scale contribution $\bar{f}$ and a small-scale contribution f', i.e. $f=\bar{f}+f'$. The filtered part $\bar{f}$ is defined as follows:

$$\bar{f}(\boldsymbol{x}) = \int_{\Omega} G(\boldsymbol{x},\boldsymbol{\xi}) f(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}, \tag{1}$$

where $\boldsymbol{x}$ and $\boldsymbol{\xi}$ are vectors in the infinite flow domain Ω. The filter function G depends on the parameter Δ, called the filter width, and satisfies the condition

$$\int_{\Omega} G(\boldsymbol{x},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} = 1 \tag{2}$$

for every $\boldsymbol{x}$ in Ω. If this filter is applied to the Navier–Stokes equations for incompressible flow, the turbulent stress tensor τ_{ij} appears in the filtered equations,

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j, \tag{3}$$

where u_i is the component of the velocity field in the x_i-direction.

The filtering approach is different from the statistical approach, in which the averaging operator represents the ensemble average and τ_{ij} is equal to the Reynolds stress $\overline{u_i' u_j'}$. Since the averaging operator is a statistical mean, it is well-known that the tensor $\overline{u_i' u_j'}$ is positive semidefinite (Du Vachat 1977; Schumann 1977). If the tensor τ_{ij} is positive semidefinite (or 'positive' for convenience) then the following inequalities hold (Ortega 1987, p. 36):

$$\tau_{ii} \geqslant 0 \qquad \text{for} \quad i \in \{1,2,3\}, \tag{4}$$

$$|\tau_{ij}| \leqslant (\tau_{ii}\tau_{jj})^{1/2} \quad \text{for} \quad i,j \in \{1,2,3\}, \tag{5}$$

$$\det(\tau_{ij}) \geqslant 0. \tag{6}$$

We refer to these three properties as 'realizability conditions'. If the filtering approach is followed, in general $\tau_{ij} \neq \overline{u_i' u_j'}$ and, therefore, we will investigate the conditions under which τ_{ij} is positive semidefinite.

The turbulent stress tensor τ_{ij} in large-eddy simulation is preferably 'positive' for a number of reasons. First, if τ_{ij} is 'positive', the generalized turbulent kinetic energy formally introduced by Germano (1992),

$$k = \tfrac{1}{2}(\tau_{11}+\tau_{22}+\tau_{33}), \tag{7}$$

is a positive quantity at each location of the flow domain for an arbitrary velocity field. This quantity is frequently used in the theory of subgrid modelling and is often required to be positive. As an example, we mention the available k-equation models, which would become ill-defined for negative values of k. Moreover, twice the turbulent kinetic energy is an upper bound for all components of the turbulent stress, i.e. $|\tau_{ij}| \leqslant 2k$ for all i and j, which follows from the estimates given in equation (5). Other analogies between the classical approach with the ensemble average and the filtering approach exist, if τ_{ij} is 'positive'. For example, as in the classical approach, the fractions $\tau_{ij}/(\tau_{ii}\tau_{jj})^{1/2}$ in the filtering approach can be considered as correlation coefficients. The existence of such analogies could be a reason why turbulence models developed for the ensemble averaged equations can often be applied in large-eddy simulation. An example is Smagorinsky's (1963) model, which is quite similar to the classical mixing-length model of Prandtl.

In the following it will be proved that τ_{ij} is positive semidefinite if and only if the filter kernel $G(x,\xi)$ is positive for all x and ξ. As a first step, suppose $G \geqslant 0$. In order to prove that τ_{ij} is 'positive' for all x in the flow domain Ω, a subset Ω_x is defined, being the support of the function $\xi \to G(x,\xi)$. Moreover F_x is the space of real functions on the domain Ω_x. Since $G \geqslant 0$, for $f, g \in F_x$ the expression

$$(f,g)_x = \int_{\Omega_x} G(x,\xi) f(\xi) g(\xi)\,\mathrm{d}\xi$$

defines an inner product on F_x (Rudin 1973, p. 292). Next, we show that the turbulent stress can be written as an inner product. Using the definition of the filter operator, equation (1) and property (2), yields

$$\begin{aligned}
\tau_{ij}(x) &= \overline{u_i u_j}(x) - \bar{u}_i(x)\,\bar{u}_j(x) \\
&= \overline{u_i u_j}(x) - \bar{u}_i(x)\,\bar{u}_j(x) - \bar{u}_j(x)\,\bar{u}_i(x) + \bar{u}_i(x)\,\bar{u}_j(x) \\
&= \int_{\Omega_x} G(x,\xi)\,u_i(\xi)\,u_j(\xi)\,\mathrm{d}\xi - \bar{u}_i(x)\int_{\Omega_x} G(x,\xi)\,u_j(\xi)\,\mathrm{d}\xi \\
&\quad - \bar{u}_j(x)\int_{\Omega_x} G(x,\xi)\,u_i(\xi)\,\mathrm{d}\xi + \bar{u}_i(x)\,\bar{u}_j(x)\int_{\Omega_x} G(x,\xi)\,\mathrm{d}\xi \\
&= \int_{\Omega_x} G(x,\xi)(u_i(\xi)-\bar{u}_i(x))(u_j(\xi)-\bar{u}_j(x))\,\mathrm{d}\xi = (v_i^x, v_j^x)_x,
\end{aligned} \tag{8}$$

with $v_i^x(\xi) \equiv u_i(\xi) - \bar{u}_i(x)$ defined on Ω_x. In this way the tensor τ_{ij} forms a 3×3 Grammian matrix of inner products. Since such a matrix is always positive semidefinite (Ortega 1987, p. 74), τ_{ij} is positive semidefinite and satisfies the realizability conditions. Note that $v_i^x(\xi)$ is not identical to the standard velocity fluctuation $u_i'(\xi) = u_i(\xi) - \bar{u}_i(\xi)$, since $v_i^x(\xi)$ also depends on x. Consequently, (8) is not equal to $\overline{u_i' u_j'}$. Moreover, the relation $\bar{\bar{u}}_i = \bar{u}_i$, which is not true in general, is not used in the derivation.

Filter	Filter function $G(x, \xi)$	Fourier transform $\hat{G}(k)$
Top-hat	$\begin{cases} 1/\Delta^3 & \text{if } \lvert x_i-\xi_i\rvert < \frac{1}{2}\Delta, \\ 0 & \text{otherwise.} \end{cases}$	$\prod_{i=1}^{3} \frac{\sin(\frac{1}{2}\Delta k_i)}{\frac{1}{2}\Delta k_i}$
Gaussian	$\left(\frac{6}{\pi\Delta^2}\right)^{3/2} \exp\left(\frac{-6\lvert x-\xi\rvert^2}{\Delta^2}\right)$	$\exp\left(\frac{-\Delta^2\lvert k\rvert^2}{24}\right)$
Spectral cut-off	$\prod_{i=1}^{3} \frac{\sin(k_c(x_i-\xi_i))}{\pi(x_i-\xi_i)}$ with $k_c = \frac{\pi}{\Delta}$	$\begin{cases} 1 & \text{if } \lvert k_i\rvert < k_c, \\ 0 & \text{otherwise.} \end{cases}$

TABLE 1. Filter functions in physical and spectral space. $\hat{G}(k)$ is the Fourier transform of $G(x,\xi)$ with respect to the vector $x-\xi$.

We proceed to show that $G \geqslant 0$ is not only a sufficient, but also a necessary condition for τ_{ij} to be positive semidefinite. Suppose the condition $G \geqslant 0$ is not fulfilled for a piecewise-continuous filter function G. Then vectors x and $\hat{\xi}$ in Ω and a neighbourhood of $\hat{\xi}$, $V = \{\xi \in \Omega \mid |\xi-\hat{\xi}| < \delta\}$ exist, such that $G(x,\xi) < 0$ for all $\xi \in V$. For a function u_1 on Ω with $u_1(\xi) \neq 0$ if $\xi \in V$ and $u_1(\xi) = 0$ elsewhere, $\tau_{11}(x)$ appears to be negative:

$$\tau_{11}(x) = \overline{u_1^2}(x) - (\bar{u}_1(x))^2 \leqslant \overline{u_1^2}(x) = \int_V G(x,\xi)(u_1(\xi))^2 \, \mathrm{d}\xi < 0.$$

Consequently, the tensor τ_{ij} is not positive semidefinite, which completes the proof that τ_{ij} is positive semidefinite if and only if the filter function G is positive.

3. Filters

In the previous section we have shown that the turbulent stress tensor is positive semidefinite if and only if the condition $G \geqslant 0$ is fulfilled. If this is the case, we call the corresponding filter a *positive filter*. In this section we consider some of the positive and non-positive filters which frequently appear in the literature on large-eddy simulation. Also, turbulent kinetic energies obtained with positive and non-positive filters are compared for a fully developed turbulent flow field.

Typical filters commonly used in large-eddy simulation, the top-hat, Gaussian and spectral cut-off filter, are listed in table 1. The top-hat and Gaussian filters are positive, whereas the spectral cut-off is not. Hence τ_{ij} is 'positive' if the first two filters are applied, but not if the spectral cut-off is applied to the velocity field. For compressible flows the Favre filter is used, $\tilde{u}_i = \overline{\rho u_i}/\bar{\rho}$, where ρ is the density (Erlebacher *et al.* 1992). This filter inherits positivity from the underlying 'bar' filter, but does in general not commute with partial derivatives, unlike the filters listed in table 1.

Next the specific behaviour of the turbulent stress based on the spectral cut-off filter is illustrated. First, as an example the sinusoidal velocity profile $u_1 = \sin(ak_c x_1)$ with $\frac{1}{2} < a < 1$ is considered and the cut-off filter is applied with cut-off wavenumber k_c. Since u_1 is a single Fourier mode, the filter operation is easily performed in Fourier space. This implies

$$\tau_{11} = \overline{\tfrac{1}{2} - \tfrac{1}{2}\cos(2ak_c x_1)} - (\tfrac{1}{2} - \tfrac{1}{2}\cos(2ak_c x_1)) = \tfrac{1}{2}\cos(2ak_c x_1),$$

which is not positive for all x_1. Consequently, for spectrally filtered fields τ_{ij} does not satisfy the realizability conditions.

As a further illustration the generalized turbulent kinetic energy is calculated by

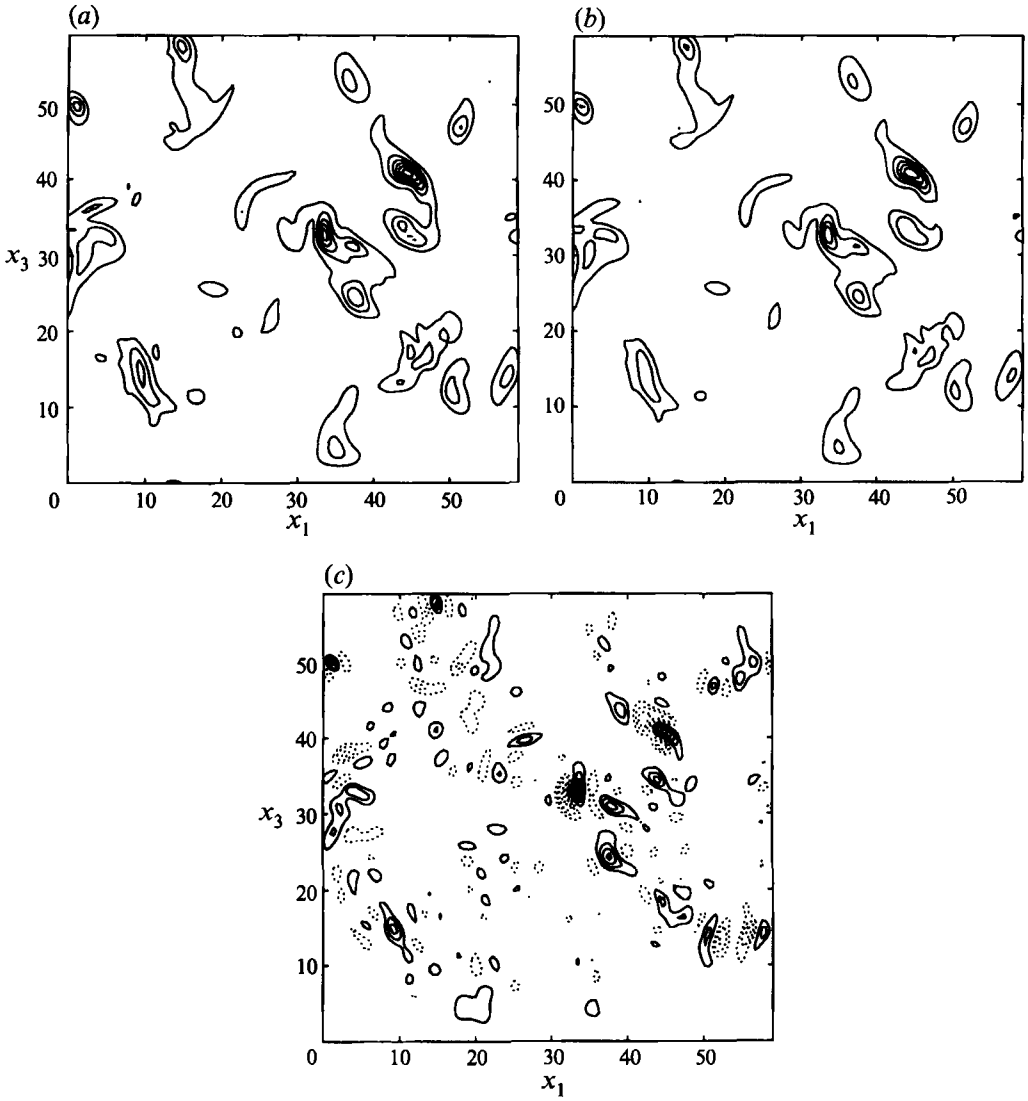

FIGURE 1. Contours of the generalized turbulent kinetic energy in the centreplane of the mixing layer at $t = 80$ for (*a*) the top-hat filter, (*b*) the Gaussian filter and (*c*) the spectral cut-off filter. Solid and dotted contours indicate positive and negative values respectively. The contour increment is 0.04.

filtering a turbulent velocity field. For this purpose we use the database of a direct numerical simulation (in which no turbulence model is adopted) of the temporal mixing layer in three dimensions with a convective Mach number of 0.2 (Vreman, Geurts & Kuerten 1993). At this Mach number the flow can be regarded as incompressible (Sandham & Reynolds 1991). The simulation was performed on a uniform cubic grid with grid spacing h and 128^3 grid points, and an additional simulation on a 192^3 grid confirmed the accuracy of the database. The length in the streamwise direction was chosen equal to four times the wavelength of the most unstable mode given by linear stability theory. The scenario of the simulation showed the roll-up of the spanwise vorticity, resulting in four spanwise rollers at the non-dimensional time $t = 20$. Subsequently, pairing of these rollers was observed, reducing

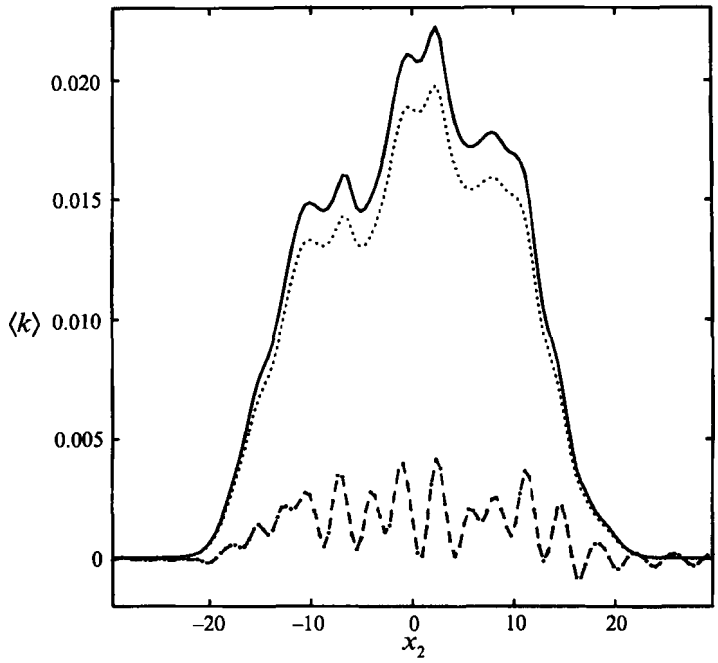

FIGURE 2. The generalized turbulent kinetic energy integrated over the homogeneous directions as a function of the normal coordinate (x_2) for the mixing layer at $t = 80$. Top-hat filter (solid), Gaussian filter (dotted) and spectral cut-off filter (dashed).

the number of rollers to two at $t = 40$. The final pairing was accomplished at $t = 80$, at which time the complicated structure of the flow was highly three-dimensional. In the following the flow field at $t = 80$ is used for the calculation of the generalized turbulent kinetic energy k, defined in equation (7). We compare k obtained with the top-hat and Gaussian filter, as examples of positive filters, to k obtained with the spectral cut-off filter. The filter width Δ, which is the same in the three filter functions, is chosen equal to $4h$, which implies that if a large-eddy simulation of this flow is performed with grid spacing Δ, the grid contains 32^3 cells. In figure 1 contours of k are shown in the centreplane of the shear layer for the three filters. Also, k integrated over the two homogeneous directions of the flow ($\langle k \rangle$) is plotted as a function of the normal coordinate in figure 2. These figures show that the generalized turbulent kinetic energy k is positive everywhere if the top-hat or Gaussian filter is used. However, if the spectral cut-off is employed, k and even $\langle k \rangle$ are negative in some parts of the flow.

As a conclusion, unlike the top-hat and Gaussian filters, the spectral cut-off filter gives rise to a turbulent stress tensor which does not satisfy the realizability conditions. This does not imply that τ_{ij} becomes ill-defined for the spectral cut-off filter. However, certain properties of τ_{ij} which are true for positive filters do not hold for the spectral cut-off. In particular, the generalized turbulent kinetic energy, k, obtained with spectrally filtered velocity fields, can locally be negative. Similarly, the generalized turbulent dissipation rate (Germano 1992, equation (25)),

$$\epsilon = \nu \sum_{i=1}^{3} \sum_{k=1}^{3} \overline{\left(\left(\frac{\partial u_i}{\partial x_k} \right)^2 - \left(\overline{\frac{\partial u_i}{\partial x_k}} \right)^2 \right)},$$

can locally be negative if a spectral filter is used, while it is positive for positive filters. Some consequences of these properties will be discussed in the next section. Finally, the

fact that τ_{ij} based on spectrally filtered fields is not 'positive' might explain the large amount of backscatter for this filter when compared to positive filters (Piomelli *et al.* 1990).

4. Subgrid models

The large-eddy-simulation approach is to close the filtered equations by replacing the exact turbulent stress τ_{ij} with a subgrid model, represented by the tensor m_{ij}. A model which shares some basic properties with the turbulent stress is appealing from a theoretical point of view. For example, since τ_{ij} is a symmetric tensor, the model m_{ij} is preferably symmetric as well, which is true for all existing subgrid models. Secondly, the filtered Navier–Stokes equations are Galilean invariant. As Speziale (1985) has argued, they should retain this property if τ_{ij} is replaced by the model m_{ij}. The observation that τ_{ij} is 'positive' for positive filters is another basic property of the turbulent stress. Therefore, it is reasonable to require the model m_{ij} to be 'positive' as well, if a positive filter is adopted. Such a requirement is based not only on theoretical but also on practical grounds. For example, it provides a useful lower bound for the generalized turbulent kinetic energy when an eddy-viscosity model is adopted, as will be shown below. In the following a number of subgrid models are considered and the question of whether they are 'positive' for positive filters is addressed.

First consider Bardina's scale-similarity model (Bardina, Ferziger & Reynolds 1984):

$$m_{ij} = \overline{\bar{u}_i \bar{u}_j} - \bar{\bar{u}}_i \bar{\bar{u}}_j.$$

This tensor is obtained if the definition of the turbulent stress τ_{ij} (equation (3)) is applied to the filtered velocity field $\bar{u}_i$. The tensor m_{ij} is also called the resolved turbulent stress (Germano 1992) and is clearly 'positive' for positive filters. Another 'positive' tensor is the model by Clark, Ferziger & Reynolds (1979):

$$m_{ij} = \tfrac{1}{12}\Delta^2(\nabla \bar{u}_i \cdot \nabla \bar{u}_j),$$

which was obtained using Taylor expansions. This tensor is positive semidefinite since it can be interpreted as a Grammian matrix with respect to the Euclidian inner product in $\mathbb{R}^3$. Notice that m_{ij} is 'positive', even if the filter is not positive, and, consequently the use of this model in conjunction with e.g. the spectral cut-off filter is not consistent.

The two subgrid models discussed above are not of the eddy-viscosity type. Next we turn to the group of eddy-viscosity models (e.g. Rogallo & Moin 1984). The anisotropic part of the turbulent stress,

$$\tau^a_{ij} = \tau_{ij} - \tfrac{2}{3}k\delta_{ij},$$

is modelled with

$$m^a_{ij} = -\nu_e S_{ij}.$$

The symbol ν_e represents the eddy viscosity and

$$S_{ij} = \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \tfrac{2}{3}(\nabla \cdot \bar{\boldsymbol{u}})\,\delta_{ij}$$

is the strain rate. If the flow is incompressible, the divergence term vanishes, while for compressible flows the bar filter represents the Favre filter. The sum of the anisotropic and isotropic parts is formally written as

$$m_{ij} = -\nu_e S_{ij} + \tfrac{2}{3}k\delta_{ij}. \tag{9}$$

An interesting result is obtained if m_{ij} is required to satisfy the realizability conditions. This requirement implies:

$$m_{12}^2+m_{13}^2+m_{23}^2 \leqslant m_{11}\,m_{22}+m_{11}\,m_{33}+m_{22}\,m_{33}.$$

Equation (9) is substituted in this expression, which yields

$$\nu_e^2(S_{12}^2+S_{13}^2+S_{23}^2) \leqslant \nu_e^2(S_{11}\,S_{22}+S_{11}\,S_{33}+S_{22}\,S_{33})+\tfrac{4}{3}k^2. \tag{10}$$

Here the property that the tensor S_{ij} is trace-less has been employed. This property is also used to rewrite the terms between parentheses in the right-hand side of (10) as follows:

$$\begin{aligned} S_{11}\,S_{22}+S_{11}\,S_{33}+S_{22}\,S_{33} &= \tfrac{1}{2}(S_{11}+S_{22}+S_{33})^2-\tfrac{1}{2}(S_{11}^2+S_{22}^2+S_{33}^2) \\ &= -\tfrac{1}{2}(S_{11}^2+S_{22}^2+S_{33}^2). \end{aligned}$$

Substituting this expression in (10) finally yields

$$k \geqslant \tfrac{1}{2}\sqrt{3}(\nu_e S^{1/2}) \quad \text{with} \quad S=\tfrac{1}{2}\sum_{i,j} S_{ij}^2. \tag{11}$$

The inequality gives a lower bound for the generalized turbulent kinetic energy k when an eddy-viscosity model is adopted in conjunction with a positive filter.

The lower bound for k provides information on the isotropic part of the turbulent stress in the eddy-viscosity formulation. In a large-eddy simulation of incompressible flow the isotropic part is usually added to the filtered pressure, resulting in a modified pressure (Rogallo & Moin 1984). In that case, the large-eddy simulation solves the modified pressure, while the (filtered) pressure itself remains unknown, which is undesirable in applications in which the pressure is an important quantity. The approach involving a modified pressure especially causes problems in the large-eddy simulation of compressible flows, since in the evolution equations for compressible flows the pressure not only appears in the momentum equations but also in the energy evolution equation and in the equation of state. For these reasons subgrid models have been proposed that explicitly prescribe k in order to model the isotropic part of the turbulent stress. For such models inequality (11) is particularly interesting since it implies inequalities for the model coefficients, as shown in the following part of this section.

In fact inequality (11) can be used to suggest a subgrid model for k corresponding to a specific eddy-viscosity model. We will demonstrate this for the Smagorinsky model, which leads to the Yoshizawa model for k. A similar procedure could be followed for e.g. the structure-function eddy-viscosity model (Normand & Lesieur 1992). In a formulation equivalent to that given by Leith (1990) the Smagorinsky eddy viscosity (Smagorinsky 1963) is defined as

$$\nu_e = C_S^2\,\Delta^2\,S^{1/2},$$

where C_S is the Smagorinsky constant. Inequality (11) now reduces to

$$k \geqslant \tfrac{1}{2}\sqrt{3}C_S^2\,\Delta^2 S,$$

which suggests the following subgrid model for k:

$$k = C_k\,\Delta^2 S, \tag{12}$$

where the constant C_k has to satisfy

$$C_k \geqslant \tfrac{1}{2}\sqrt{3}C_S^2. \tag{13}$$

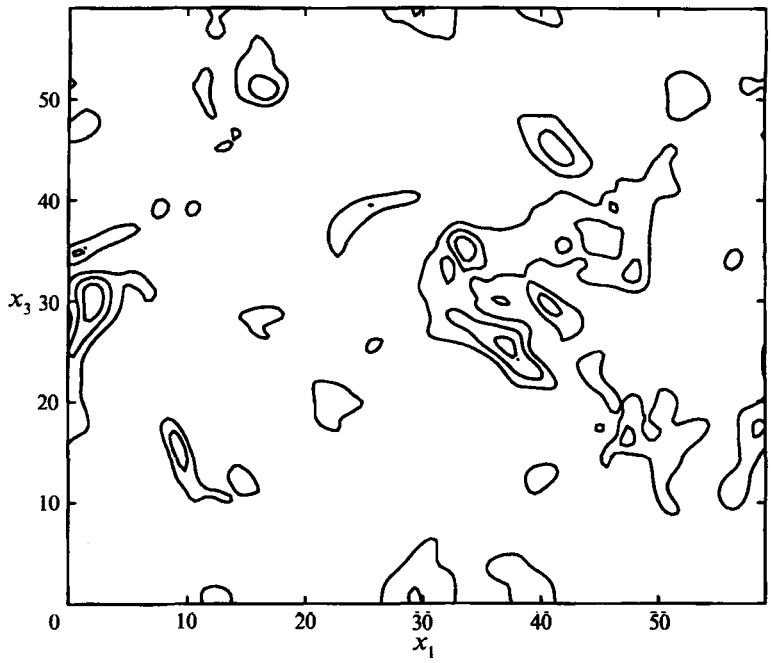

FIGURE 3. Contours of $\frac{1}{2}\sqrt{3}\,\nu_e S^{1/2}$ in the centreplane of the mixing layer at $t = 80$, using the Smagorinsky eddy viscosity with $C_S = 0.16$ and the top-hat filter. Solid and dotted contours indicate positive and negative values respectively. The contour increment is 0.015.

This inequality expresses a necessary condition for realizability, if a positive filter is used. The model for the generalized turbulent kinetic energy k in (12) is similar to the estimates for k given by Lilly (1967), Deardorff (1970), and it is known as the Yoshizawa model (Yoshizawa 1986). Yoshizawa proposes $C_S(= C_{uu2}) = 0.16$ and $C_k(= C_{uu2}^4/C_{uu1}^2) = 0.0886$, where C_{uu1} and C_{uu2} are notations which Yoshizawa uses in his presentation of the model. These values clearly satisfy inequality (13).

The right-hand side of inequality (11) has been evaluated for the Smagorinsky eddy viscosity using the numerical database described in the previous section. Results for the centreplane are shown in figure 3 for the top-hat filter. The agreement with figure 1 (*a*) is reasonable and quantitatively corresponds to a correlation of 0.62. Thus Yoshizawa's model gives a reasonably good prediction of k on the tensor level, which is in agreement with the findings of Erlebacher *et al.* (1987, table 10). The results of averaging the right-hand side of (11) in the homogeneous directions are shown in figure 4, which may be compared with figure 2. For the positive filters (top-hat and Gaussian) we observe that inequality (11) is satisfied and that some global features of $\langle k \rangle$ are present in the lower bound as well. The lower bound is about half the value of k. For the non-positive spectral cut-off, inequality (11) is clearly not satisfied. Since the Yoshizawa model leads to positive values for k, it is suggested that the Yoshizawa model should not be used in conjunction with the spectral cut-off filter, for which the exact k attains negative values. It should be noticed that, on the vector level, i.e. when ∇k is considered, the correlation of the Yoshizawa model is poor (Erlebacher *et al.* 1987; Speziale *et al.* 1988).

The SEZH-model (Erlebacher *et al.* 1992; Zang, Dahlburg & Dahlburg 1992) is the sum of the similarity model and Yoshizawa's model. It was developed using the Gaussian filter, which is positive. The references suggest $C_S(= (C_R/\sqrt{2})^{1/2}) = 0.092$ and

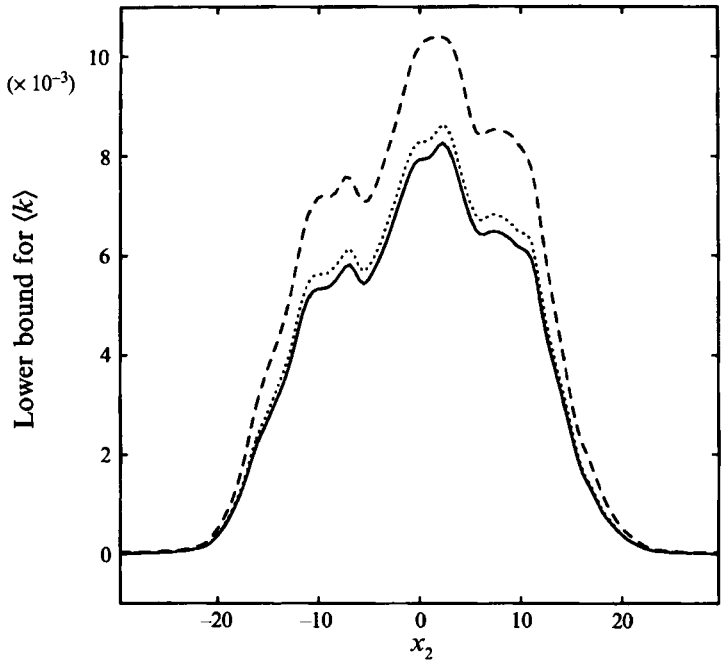

FIGURE 4. $\frac{1}{2}\sqrt{3}\,\nu_e S^{1/2}$ integrated over the homogeneous directions as a function of the normal coordinate (x_2) for the mixing layer at $t = 80$, using the Smagorinsky eddy viscosity with $C_S = 0.16$. Top-hat filter (solid), Gaussian filter (dotted) and spectral cut-off filter (dashed).

$C_k(= C_I/2) = 0.0033$ or even $C_k = 0$. These values do not satisfy (13) and, consequently, the Yoshizawa part of this model is not realizable. However, this does not imply non-realizability of the complete SEZH-model, since the sum of the similarity model and Yoshizawa's model can theoretically still be positive semidefinite. For this reason it is consistent to reformulate the SEZH-model in the following way: rather than modelling the 'positive' tensor $\overline{u_i' u_j'}$, the Yoshizawa model approximates $\tau_{ij} - (\overline{\bar{u}_i \bar{u}_j} - \bar{\bar{u}}_i \bar{\bar{u}}_j)$, which in general is not 'positive'.

An alternative for modelling k is to solve this quantity using an additional partial differential equation for k (Schumann 1975; Horiuti 1985; Moin & Jimenez 1993). In this formulation the eddy viscosity is proportional to $k^{1/2}$, while in the k-equation terms proportional to $k^{1/2}$ and $k^{3/2}$ occur. This model requires positive values for k and the formulation is such that k remains positive during the simulation, i.e. the model is 'realizable'. As for the models by Clark *et al.* and Yoshizawa, it is consistent to use the k-equation models in conjunction with positive filters only, since the exact k is guaranteed to be positive in this case. To employ these models with e.g. the spectral cut-off filter is less attractive, since in that case the original turbulent kinetic energy attains values of both signs, while the model requires positive values only.

5. Conclusions

In this paper the turbulent stress in large-eddy simulations has been shown to satisfy the same realizability conditions as the well-known Reynolds stress in the statistical approach. Positiveness of the filter function is a necessary and sufficient requirement. In particular this implies that the generalized turbulent kinetic energy is positive in all regions of the flow. In view of these considerations, the top-hat and Gaussian filters are

fundamentally different from the spectral cut-off filter. The first two filters (and their corresponding Favre filters for compressible flows) are positive, whereas the spectral cut-off is non-positive and, consequently, in the latter case the realizability conditions are not applicable. Indeed, the generalized turbulent kinetic energy k based on spectrally filtered fields obtained from a numerical simulation appeared to be negative in many regions of the flow. For this reason subgrid models which predict a positive k, e.g. the model by Clark *et al.*, the Yoshizawa model and k-equation models, should be used in conjunction with a positive filter. Bardina's similarity model satisfies the realizability conditions for positive filters only and, consequently, this model can be used in combination with any filter. Imposing realizability for eddy-viscosity models has led to a lower bound for k. Substitution of the Smagorinsky eddy viscosity in this inequality leads to the Yoshizawa model for compressible flow with a corresponding inequality for the model constants.

In conclusion, the fundamental properties of the turbulent stress presented here give an increased understanding of the filtering technique and subgrid modelling within the large-eddy simulation of turbulent flow. If more research is conducted in this direction, such properties may lead to new insights into the theory of subgrid modelling.

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