Statistical Closure to Derive a Subgrid-Scale Modeling for Large Eddy Simulations of Three-Dimensional Turbulence

Jean-Pierre Chollet

ATMOSPHERIC ANALYSIS AND PREDICTION DIVISION
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH
BOULDER, COLORADO
A subgrid-scale modeling for the velocity field of three-dimensional turbulence has been derived from a two-point closure by Chollet and Lesieur (1981); this model has been used in both two-point closure computations and direct numerical simulations of large scales. The same method is extended to the passive scalar, deriving an eddy diffusivity from the transfer of scalar variance through a given wave number $k_C$. Some specific terms of the transfers are used to determine the modifications that the eddy quantities undergo because of the closeness of $k_C$ to dissipative or large scales. The eddy quantities can be split into two different contributions—an eddy viscosity (or diffusivity) and a higher-order dissipativity, the latter term corresponding to interactions between wave numbers in the neighborhood of the given wave number $k_C$. Drastic differences between the dynamics of three- and two-dimensional turbulence are pointed out. The eddy quantities are used to parameterize the small scales of velocity and scalar fields, first in computations using the same two-point closure, then in direct numerical simulation of large scales.

Jean-Pierre Chollet
3 October 1982
Contents

1. Introduction ............................................. 1
2. Eddy viscosity, diffusivity, and Prandtl number from EDQNM closure .......................... 3
3. Influence of dissipative and large scales .............. 8
4. Eddy viscosities (diffusivities) and high-order dissipativities .......................... 12
5. Use of eddy viscosity and diffusivity in subgrid-scale modeling .......................... 17
   5.1 Subgrid-scale modeling in (EDQNM) closure computations .......................... 17
   5.2 Subgrid-scale modeling in large eddy simulations .................................. 19
6. Conclusion ............................................. 22
References .............................................. 24
Figures and Captions .................................... 26
Introduction

A subgrid-scale model handles the statistical properties of the interactions between small and large scales, and the two-point closures in spectral space are quite convenient for a coherent derivation of such a model. Eddy viscosities can be derived from closure calculations (Kraichnan, 1976; Leslie and Quarini, 1979) and then used to parameterize the small scales in closure computations and in large eddy simulations (Chollet and Lesieur, 1981).

The same kind of derivation is extended in section 1 to the passive scalar despite the lack of consensus as to the value of adjustable closure constants (Herring et al., 1982). We use two sets of constants to clear up the effects associated with their values; one of these sets seems to be in better agreement with the usual numerical or experimental values. To obtain results of general interest, we calculate the numerical values for inertial and inertial-convective $k^{-5/3}$ spectra ranging over the whole interval of computed wave numbers. In section 2, representative terms of the transfer of energy or scalar variance are used to gain some insight into the modifications that these eddy quantities undergo in case the wave number $k_c$ is not so far from the scales of molecular dissipation or of energy production in the usual cases of spectra going to zero at zero wave number.

An interpretation through the addition of an eddy viscosity (diffusivity) and a higher-order dissipativity is suggested in section 3. The parameterization studied here in three-dimensional turbulence is briefly compared to the same problem studied by Basdevant et al. (1981)
2

in two-dimensional turbulence. In section 4, the eddy viscosities and
diffusivities are used to parameterize the small scales of velocity and
passive scalar fields in both closure computations and large eddy
simulations.
2. Eddy viscosity, diffusivity, and Prandtl number from EDQNM closure

We consider a passive scalar, that is, any quantity convected by the velocity field (e.g., a slight fluctuation of temperature or a tracer concentration), provided it does not react on the velocity field. We use a two-point statistical closure with the hypothesis of homogeneity and isotropy, the Eddy Damped Quasi Normal Markovianized closure (EDQNM) which is extensively described for both the velocity and the scalar fields in Larcheveque et al. (1980) and Herring et al. (1982). The spectra of kinetic energy $1/2 \langle u^2 \rangle$ and scalar variance $\langle \theta^2 \rangle$ are defined by

$$
1/2 \langle u^2 \rangle = \int_0^\infty E(k) \, dk \quad \text{and} \quad \langle \theta^2 \rangle = \int_0^\infty E_\theta(k) \, dk \quad (1.1)
$$

The evolution of spectra is governed by

$$
\frac{\partial E(k,t)}{\partial t} + 2 \nu k^2 E(k,t) = T(k,t) + f(k,t) \quad (1.2)
$$

$$
\frac{\partial E_\theta(k,t)}{\partial t} + 2Dk^2 E_\theta(k,t) = T_\theta(k,t) + f_\theta(k,t) \quad (1.3)
$$

where $\nu$ is the molecular viscosity of the fluid; $D$ is the molecular diffusivity of the passive scalar; $f(k,t)$ and $f_\theta(k,t)$ are the spectra of external forcing for the velocity field and the scalar field, respectively; $T(k,t)$ is the energy transfer at wave number $k$; and $T_\theta(k,t)$ is the scalar transfer at wave number $k$. 
The EDQNM yields
\[ T(k,t) = \Delta \int dpdq \theta_{kpq} \frac{x+y+z^3}{q} \left[ k^2E(p,t)E(q,t) - p^2E(q,t)E(k,t) \right] \] (1.4)
and
\[ T_\theta(k,t) = \Delta \int dpdq \frac{kp}{q^3} \theta_{kpq} (1-z^2) E(q,t) \left[ k^2E_\theta(p,t) - p^2E_\theta(k,t) \right] \] (1.5)

Here \( \Delta \) is the domain such that the wave numbers \( k, p, q \) form a triangle (see Fig. 1) and \( x, y, z \) are the cosines of the angles of the triangle \( kpq \).

The relaxation time \( \theta_{kpq} \) associated with the energy transfer is
\[ \theta_{kpq} = \frac{-(\mu_k + \mu_p + \mu_q)t}{1-e^{-(\mu_k + \mu_p + \mu_q)t}} \] (1.6)

where
\[ \mu_k = \lambda \left\{ \int_0^k p^2E(p)dp \right\}^{1/2} + k^2 \] (1.7)
\( \lambda \) is equal to 0.361 in order to fit the experimental values of the Kolmogorov constant (André and Lesieur, 1977).

The relaxation time \( \theta'_{kpq} \) associated with the scalar transfer is
\[ \theta'_{kpq} = \frac{-(\mu'_k + \mu'_p + \mu'_{pq})t}{1-e^{-(\mu'_k + \mu'_p + \mu'_{pq})t}} \] (1.8)

where
\[ \mu'_k = \lambda' \left\{ \int_0^k p^2E(p)dp \right\}^{1/2} + Dk^2 \] (1.9)
\( \nu_k'' = \lambda'' \int_0^k p^2 E(p) dp \)\(^{1/2} + \nu k^2 \).  \hspace{1cm} (1.10)

For a discussion of these relaxation times and the determination of the values of the constants \( \lambda, \lambda', \lambda'' \), see Herring et al. (1982). There is actually no undisputable reason for a definite choice of \((\lambda', \lambda'')\); we are considering in this section the two sets \((\lambda'=\lambda''=\lambda)\) and \((\lambda'=0, \lambda''=3.61\lambda)\).

Extending the derivation of an eddy viscosity from energy equations to the derivation of an eddy diffusivity from scalar variance equations, we consider a wave number \( k_c \) at which the transfers \( T(k) \) and \( T_\theta(k) \) is split into two conceptually distinct parts. We denote by \( T^>(k) \) and \( T^>_\theta(k) \) that portion of (1.4) or (1.5) that has wave numbers \( p \) or (and) \( q \) greater than \( k_c \) (Fig. 1).

These transfers can be rewritten formally within the formulation of an eddy viscosity
\[ \nu(k|k_c,t) = - \frac{T^>(k,t)}{(2k^2 E(k,t))} \] \hspace{1cm} (1.11)

and eddy diffusivity
\[ D(k|k_c,t) = - \frac{T^>_\theta(k,t)}{(2k^2 E_\theta(k,t))} . \] \hspace{1cm} (1.12)

As \( \nu(k|k_c) \) and \( D(k_c) \) depend on the values of \( E(k) \) and \( E_\theta(k) \) over the whole range of wave numbers, to obtain results of some general interest, we consider inertial-convective \( k^{-5/3} \) spectra over the range of computed wave numbers \((k_{\text{min}}, k_{\text{max}})\), corresponding to high Reynolds number flows. Only the case of a molecular Prandtl number equal to unity is considered since the concept of eddy diffusivity and eddy viscosity is meaningless for scales dominated by dissipative or conductive
effects. The eddy quantities are made dimensionless through the eddy viscosity \( [E(k_c)/k_c]^{1/2} \) characteristic of a \( k^{-5/3} \) inertial range; subsequently, we will use only these nondimensional quantities.

\[
\nu_t^+ = \nu_t (k|k_c|/(E(k_c)/k_c))^{1/2}
\]

\[
D_t^+ = D_t (k|k_c|/(E(k_c)/k_c))^{1/2}.
\] (1.13)

The eddy viscosities are plotted on Fig. 2 for the (numerical) wave number discretizations corresponding to \( F = 4, 16, 64 \). Here the wave numbers are logarithmically discretized \( k_L = k_{\text{min}} 2^{(L-1)/F}, F \) being the number of modes per factor of 2. Fig. 2 is identical to the corresponding one in Chollet and Lesieur (1981) except for the higher estimated value of \( F \). We notice some kind of discontinuity around \( k_c/a (a = 2^{1/F-1}) \), where the computation of the transfer switches from a numerical integration of local terms to a calculation of analytical formulation of non-local terms [see Chollet and Lesieur (1981) for details]. Tightening the discretization by increasing the value of \( F \), and hence computing a larger part of the transfer as local terms, does not smooth this discontinuity. The straight lines are constant values obtained through non-local transfer when there is some slight oscillation if the same values are computed through the local terms (higher values of \( F \)). The discrepancies between various curves corresponding to different values of \( F \) seem to be generated by some filtering problems at the close neighborhood of wave number \( k_c \), related to the way of considering \( p,q > k_c \) or \( p,q \geq k_c \). These remarks hold also for the eddy diffusivities and the eddy Prandtl number which are studied below.
The first set of constants \((\lambda=\lambda'=\lambda'')\) gives an eddy diffusivity curve with a very noticeable discontinuity (Fig. 3a). The asymptotic value (when \(k \to 0\)) of the eddy Prandtl number is, for infinite Reynolds and Peclet numbers (Larcheveque et al., 1980)

\[
\Pr_t = \frac{\lambda' + \lambda''}{6\lambda}
\]  

whose numerical value is \(1/3\), as observed in Fig. 3b. This value seems unrealistically low if compared to experimental values of the eddy Prandtl number. This could explain the overestimation of scalar variance spectra calculated by Vignon et al. (1979) with this set of constants.

The second set of constants \((\lambda'=0, \lambda''=3.61\lambda)\) (Fig. 4) seems to be better supported by theoretical arguments (Herring et al., 1982). From (1.14), the value of the eddy Prandtl number is 0.602, as observed in Fig. 4b, and is in better agreement with experimental values. We notice a nearly constant value of this Prandtl number with only a slow decrease (less than 15 percent) next to \(k=k_c\). The choice of the constants \((\lambda, \lambda', \lambda'')\) is important when comparing the eddy diffusivities and Prandtl numbers calculated with the two sets of constants (Figs. 3 and 4): (i) The asymptotic eddy diffusivities \((k \ll k_c)\) differ by a factor of 1.8. (ii) The shape of the curves in the vicinity of \(k = k_c\) involving more local effects is quite different; the eddy Prandtl number can either increase (Fig. 3b) or decrease (Fig. 4b).
3. Influence of dissipative and large scales

A close look at some terms of the transfers of energy and scalar variance (1.4) and (1.5) provides further information on the evolution of the eddy viscosity and eddy diffusivity relations in the particular cases of wave number \( k_C \) close to the range of molecular dissipation or close to the energetic scales for a realistic spectrum (with zero energy at zero wave number). Our aim is not to give quantitative values for numerical corrections but only at understanding the general behavior; we also consider only dominant terms of the transfers, with inertial and inertial-convective \( k^{-5/3} \) spectra over the ranges of interest.

When the wave number \( k_C \) is close enough to the Kolmogorov dissipation wave number \( k_C \), the local part of the transfer is presumably not significantly modified. The non-local part corresponding to interactions \( k \ll p - q \) (so-called eddy viscous in Lesieur and Schertzer, 1978) is affected since \( p \) or \( q \in [k_C, k_S] \) instead of \([k_C, \infty)\).

The corresponding transfer is:

\[
T(k) = -2\nu_t k^2 E(k)
\]

with

\[
\nu_t = \frac{1}{15} k_c \int_{k_S}^{k_C} \theta_{pp} \left[ 5E(p) + p \frac{\partial E}{\partial p} \right] dp .
\]  

(2.1)

With the spectra \( E(k) = K_0 e^{2/3} k^{-5/3} \) for \( 0 < k < k_C \) and \( E(k) = 0 \) for \( k > k_S \), (2.1) is rewritten

\[
T(k) = -2\nu_t k^2 E(k)
\]
\[
\frac{\nu_t}{\nu_t^\infty} = 1 - \frac{k_s}{k_c}^{4/3} \left\{ 1 - \frac{2}{\sqrt[3]{3} K_0^{1/2}} \ln \frac{1 + \frac{\sqrt{3}}{2} K_0^{1/2}}{1 + (\frac{k_c}{k_s})^{4/3} \frac{\sqrt{3}}{2} K_0^{1/2}} \right\}
\]

where

\[
\nu_t^\infty = \frac{1}{6\sqrt{3}} k_0^{1/2} \epsilon^{1/3} k_c^{-4/3}
\]

\(\nu_t^\infty\) is the value of \(\nu_t\) for \(k_s \rightarrow \infty\) (zero viscosity). \(K_0\) is the Kolmogorov constant (=1.40).

From the curve plotted in Fig. 5, we observe a significant damping of \(\nu_t/\nu_t^\infty\) when \(k_c > 0.01\) ks. Consequently, the alteration of \(\nu_t^* (k/k_c)\) can be interpreted as a translation of the curve of Fig. 2 toward lower values, whose amplitude is given by formula (2.2) (Fig. 5). The cusp of Fig. 2 should be preserved as due to local interactions which would not be under the influence of \(k_s\) for \(k\) smaller than about 0.3 \(k_s\).

In largest scales, we model the transfer with the non-local terms which are the most significant in this range of wave number.

\[
T(k) = A_k^4 - 2\nu_t k^2 E(k)
\]

where

\[
A = \frac{14}{15} k_c^{\infty} \int_{opp} E^2(p) dp
\]

(see Lesieur and Schertzer, 1978).
If we write $A$ in terms of $T^+_{4}(k)$ and then

$$\nu_{t4}^{+}(k/k_c) = - \frac{T^+_{4}}{2k^2E(k)} \left( \frac{E(k_c)/k_c}{k^2} \right)^{-1/2}$$

with $E(k) = k_0 e^{2/3} k^{-5/3}$, for $k_c < k < \infty$ we get

$$\nu_{t4}^{+}(k/k_c) = - \frac{7}{75} \frac{1}{\lambda^3} \frac{k^2}{E(k)} \frac{E(k_c)}{k_c^2}$$

(2.6)

which is negative since the energy is transferred to larger scales.

Then the resulting $\nu_{tg}^{+}$ is (with $\lambda = 0.361$)

$$\nu_{tg}^{+} = \nu_{t}^{+} - 0.149 \frac{k^2}{E(k)} \frac{E(k_c)}{k_c^2}$$

(2.7)

where $\nu_{t}^{+}$ is the function used elsewhere (i.e., in Fig. 2).

We notice that (i) when $k \rightarrow 0$, $\nu_{t4}^{+} \rightarrow \infty$ if $E(k) - k^s$ and $s > 2$, therefore $\nu_{tg}^{+}$ negative values; (ii) when $k \rightarrow k_c$, $\nu_{t4}^{+} \rightarrow 0.149$, which means a smoothing of the cusp.

The same kind of results can be obtained for the passive scalar.

If modeling the transfer of scalar variance through the only term

$$T_0(k) = -2D_t k^2 \Theta_0(k)$$

(2.8)

with

$$D_t = \frac{2}{3} k_c \int_{k_c}^{k_s} \Theta_{opp} E(p) dp$$

for an inertial range from $k_c$ to $k_s$, $D_t/D_t^{\infty}$ has just the same formulation as $\nu_t/\nu_t^{\infty}$ (2.2) when $(\lambda' + \lambda'')/2$ takes the place of $\lambda$. 

Depending on the set of constants, the curves associated with the eddy viscosity and diffusivity, respectively, can differ or be identical (Fig. 5).

For large scales, we add to the transfer modeled by the eddy diffusivity $D_t^+$ (Fig. 3a or 4a) a term corresponding to $T_\theta = A_\theta k^4$ where

\[
A_\theta = \frac{4}{3} \int_{k_c}^{\infty} \frac{E(p) E_\theta(p)}{p^2} \, dp
\]  

(2.9)

which can be reformulated as a negative eddy diffusivity

\[
D_{t4}^+ = -\frac{2}{15\sqrt{3}} \frac{1}{\lambda' + \lambda'''} \frac{E_\theta(k_c)}{E_\theta(k)} \cdot \frac{k^2}{k_c^2} .
\]  

(2.10)

$D_{tg}^+ = D_t^+ + D_{t4}^+$ takes negative values when $k+O$ (if $E(k) - k_s$ and $s > 2$); at $k=k_c$ the decreases of $D_t^+$ whose amplitude is -0.118 (with $\lambda' = 0, \lambda''' = 3.61 \lambda$) features the smoothing of the cusp.
4. Eddy viscosities (diffusivities) and high-order dissipativities

For practical use in numerical codes, $\nu_t^+(k/k_c)$ of Fig. 2 must be formulated analytically to take full advantage of the vectorization capabilities of the computer. To be consistent with the dynamics of the interactions of three-dimensional turbulence, as pointed out in section 2, we consider $\nu_t^+(k/k_c)$ as an addition of two terms

$$v_t^+(k/k_c) = v_t^+(0) + v_t^{\text{cusp}}(k/k_c) \quad (3.1)$$

The first term $v_t^+(0)$ has a constant value (some oscillations due to numerical effects are observed in Fig. 2). This term is associated with interactions in which $k$ goes from 0 to $k_c$, hence it can be viewed as non-local; it corresponds to a time-dependent eddy viscosity through the energy at the cut-off $E(k_c,t)$:

$$v_t^+(0|k_c,t) = v_t^+(0) \left[\frac{E(k_c)}{k_c}\right]^{1/2} \quad (3.2)$$

It gives rise to a transfer which is obviously $k$-dependent, increasing like $k^{1/3}$ with a $k^{-5/3}$ spectrum. Considering the numerical results for the highest discretization used in Fig. 2 ($F=64$), we study the cusp range $v_t^{\text{cusp}}(k/k_c)$ of the eddy viscosity $v_t^+$.

In log linear coordinates (Fig. 6a) $v_t^{\text{cusp}}(k/k_c)$ could be adjusted to an exponential. In log-log coordinates as used in Fig. 6b, a straight line signifies a power law, which is of special interest as pointed out below.
The formula

\[ \nu_{\text{t cusp}} = a\left(\frac{k}{k_c}\right)^b \]  \hspace{1cm} (3.3)

seems to be a good approximation for \(0.5 < \frac{k}{k_c} < 0.85\). To detail the values of the exponent \(b\), we draw on Fig. 8a

\[ b = \frac{\partial(\ln \nu_{\text{t cusp}}^+)}{\partial(\ln \left(\frac{k}{k_c}\right))} \]  \hspace{1cm} (3.4)

It appears that there is no exact fitting to a power law \((b=\text{constant})\) for any range of wave numbers; nevertheless, some \(b=4\) could be considered a good approximation.

A log-log regression with a least-square adjustment gives

\[ \nu_{\text{t cusp}}^+ = 0.47236 \left(\frac{k}{k_c}\right)^{3.742} \text{ for } 0.4 < \frac{k}{k_c} < 0.9 \]  \hspace{1cm} (3.5)

(with a correlation coefficient of 0.998).

It is not possible to fit the whole range of wave numbers with this law, which is without noticeable effect in the low \(k\) where the contribution of the cusp to \(\nu_{\text{t cusp}}^+\) is negligible, but is quite significant in the neighborhood of \(\frac{k}{k_c} = 1\) \((k/k_c > 0.9)\). Nevertheless, we know that the cusp should be smoothed in practical cases where \(k_c\) is not far from the integral scales.

The power laws are easy to implement in numerical codes; moreover, they allow some interpretation of the contribution of the cusp to the subgrid-scale model. At least as a first approximation

\[ \nu_{\text{t cusp}} = \left(\frac{k}{k_c}\right)^4 \]

or

\[ \nu_{\text{cusp}}(k|k_c,t) = a(k|k_c)^4 \left[\frac{E(k_c,t)}{k_c}\right]^{1/2} \]  \hspace{1cm} (3.6)
where $a$ is a constant value (about 0.52 from the adjustments). The corresponding transfer is written:

$$T_{cusp}(k,t) = -2k^2E(k,t)a(k/k_c)^4[E(k_c,t)/k_c]^{1/2}.$$  \hspace{1cm} (3.7)

This transfer $-k^6$ can be viewed as a tri-Laplacian operator $(\nabla^2)^3$.

Accordingly, the subgrid-scale transfer is interpreted as a sum of an eddy viscosity and a (at least one) high-order dissipativity; these two terms are time-dependent through the energy at the cut-off $E(k_c,t)$.

For two-dimensional turbulence, Basdevant et al. (1981) have claimed that the use of high-order dissipativities $-(-\nabla^2)^m$ must be preferred to the subgrid model derived from an EDQNM closure by Basdevant et al. (1978). They chose a high value ($m=8$) to provide a large ratio of enstrophy to energy dissipation. This is a major difference between two and three dimensions. In two dimensions, the cut-off is in the range corresponding to the cascade of enstrophy, and the so-called negative eddy viscosity is associated with a transfer of enstrophy and not a transfer of energy. In three dimensions, we handle an equation for the energy. Energy is the quantity that cascades in the range $-k_c$ and the eddy viscosity, whose value is positive in this cascading range, is associated--as is usual--with the energy flux. This eddy viscosity can be interpreted using the usual concept of mixing length when considering a spectrum at large $k$ damping a spike of energy at large scales (Lesieur and Chollet, 1980).

In two dimensions, the parameterization derived from the EDQNM closure is dominated by the non-local interactions, $p \ll k - q$ which requires a good isotropy for all scales, including the largest ones. In
three dimensions, the parameterization is mainly local, the contribution of the interactions $k \ll p,q$ is significant but depends on small scales which can be more easily assumed to be isotropic.

The same derivation can be extended to the eddy diffusivity $D_{t+cusp}$ for the passive scalar. We will keep the two sets of constants $[(\lambda' = 0, \lambda'' = 3.61 \lambda) \text{ and } (\lambda' = \lambda'' = \lambda)]$ to emphasize the sensibility of the eddy diffusivity laws to the choice of the closure constants (Fig. 7a, 7b, 8b).

If our parameterization transfer can be interpreted as a sum of an eddy viscosity and a $(v^2)^3$ dissipativity, the same formulation in physical space can be used. Nevertheless, we have to translate the energy at the cut-off $E(k_c,t)$ and the cut-off wave number $k_c$ into terms depending on physical variables. $k_c$ must be related to the mesh size in physical space; the sharp filter we use in spectral space has to be associated with the corresponding filter in physical space (Leslie and Quarini, 1979); moreover, the filtering depends on the finite-difference scheme in physical space.

$E(k_c)$ is used as a convenient formulation of the dissipation rate of energy $\epsilon$ in an inertial range. $\epsilon$ has to be expressed in terms of variables describing the velocity field in physical space.

$$[E(k_c)/k_c]^{1/2} = K_0^{1/2} \epsilon^{1/3} k_c^{-4/3}$$ (3.8)

with the same assumptions but in terms of variables in physical space

$$\epsilon = 2\nu_t <s_{ij} s_{ij}>$$

where
\[ s_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

is the rate of strain. Consequently, the factor \([E(k_c)/k_c]^{1/2}\) can be formulated in terms of \(\langle s_{ij}s_{ij} \rangle\) and \(k_c = \frac{2\pi}{\Delta x}\) in both eddy viscosity and higher order dissipativity terms.

\[
[E(k_c)/k_c]^{1/2} - K_0^{1/2} \langle s_{ij}s_{ij} \rangle^{1/2} K_0^{1/2} \left( \frac{\Delta x}{2\pi} \right)^{4/3} 
\]

(3.9)

Note that a spectral formulation of a subgrid-scale eddy viscosity can be used in quite a few new numerical codes, most of whose computations are in spectral space.
5. Use of eddy viscosity and diffusivity in subgrid-scale modeling

5.1 Subgrid-scale modeling in (EDQNM) closure computations

The eddy viscosity and diffusivity previously derived from the consideration of some particular interactions can be used to parameterize the small scales of a three-dimensional turbulence, when the wave numbers \( k > k_c \) are not explicitly computed. First, we use this model in closure computations where the numerical schemes, the value of \( F \), and the set of constants \( (\lambda, \lambda', \lambda'') \) are the same as in the derivation of the eddy viscosity and diffusivity. We consider only the set \( (\lambda' = 0, \lambda'' = 3.61\lambda) \).

Then we present some results of stationary calculations which need very short computing times when using an iterative procedure. Contrary to the case of injection in a very narrow band as used in Chollet and Lesieur (1981), the external forcing is introduced here with a distribution \(-k^4 e^{-2(k^2)}\) which makes the spectra even smoother. If the Reynolds number is high enough and if the cut-off \( k_c \) belongs to the inertial range and is far enough from the dissipative range and the largest scales, the use of values corresponding to Figs. 2 and 4 from \( k^{-5/3} \) spectra can be justified.

In Fig. 9, the compensated spectra \((-k^{5/3} E(k))\) are used as a test which is more severe than the log-log spectra to observe possible discrepancies between the spectrum for a complete calculation including explicitly the dissipative scales and the spectrum for the calculation using the subgrid model for \( k > k_c \); these spectra are quite the same. The discretization corresponds to \( F = 8 \).
In Fig. 10, the energy fluxes \( \Pi(k) = -\int_0^k T(k) \, dk \) shows how the parameterized flux increases when \( k \) goes to \( k_c \) to compensate the loss of flux from the terms which are explicitly computed on \([0, k_c]\).

The second test deals with free-decaying turbulence; the initial energy and scalar variance spectra are confined to large scales \( E(k, 0) - E(k, 0) - k^4 e^{-2k^2} \). The discretization corresponds to \( F=4 \).

When comparing the spectra for complete calculation (including dissipative scales) to spectra for parameterized calculation (Figs. 11 and 12), there is an identity of these spectra as long as no significant energy has reached \( k_c \) (\( t=2.5 \)); then the parameterization underestimates the spectrum (\( t=5 \)). As early as \( t=7.5 \) there is no significant difference. At \( t=5 \), The underestimation is due to (i) the eddy quantities \( v_t^+ \) and \( D_t^+ \) are derived from a \( k^{-5/3} \) spectrum, which induces an overestimation of the energy beyond \( k_c \); (ii) To derive \( v_t^+ \) and \( D_t^+ \), we have used \( \theta_{kpq} \) and \( \theta'_{kpq} \) which do not depend on time; the transfers (1.4) and (1.5) are evaluated with \( \theta_{kpq} \) which depends explicitly on time (see (1.6) and (1.7)), especially when starting at \( t=0 \). The results are very similar for energy and scalar variance.

In Fig. 13, the evolution of energy and scalar variance with time are given for the complete calculation and for the parameterized run. In the latter case, one curve (\(- - -\)) corresponds to crude results, the other (\(- \cdot -\)) takes into account scales \( k > k_c \) through a \( k^{-5/3} \) extrapolation beyond \( k_c \); this curve matches the curve from the complete run quite well, except for an ephemeral period of time during which there is already a significant amount of energy beyond \( k_c \) but the \( k^{-5/3} \) inertial range is not yet established. These results are
all the more significant in that the Reynolds number is not very high (initial value $R_I=32800$) and there could be some effect of either dissipative scales or large scales.

The amount of computation required by the EDQNM closure numerical code is usually small enough not to need subgrid-scale modeling; therefore, a reference solution, including the dissipative scales, can be computed. We can also validate the subgrid-scale model by closely comparing the solution from the parameterized computation to the reference solution. Besides, the subgrid model is useful to perform decay experiments over a few hundred large eddy turnover times with virtually infinite Reynolds numbers since there are no explicit dissipative scales.

5.2 Subgrid-scale modeling in large eddy simulations

We are only interested in high Reynolds number turbulence, and a reference solution, including the dissipative scales, is far beyond the capabilities of the most powerful computers. Any attempt to validate this eddy viscosity at low Reynolds number is irrelevant, as pointed out in section 2. Consequently, we restrict ourselves to checking the $k^{-5/3}$ inertial and inertial-convective spectra.

The eddy viscosity defined in section 1 has already been used in large eddy simulations by Chollet and Lesieur (1981) in a spectral dealiased code SPRBOX (Siggia, 1981); some simplifications of this eddy viscosity were tried. Here we use a faster numerical aliased code which is derived from the code written by Meneguzzi et al. (1981) for the computations of magnetic and velocity fields. The resolution is $32^3$. 
The eddy viscosity corresponds to the law $v_t^+(k/k_c)$ (Fig. 2) derived from an inertial spectrum $k^{-5/3}$ and with an analytical formulation of the cusp to preserve the capabilities of vectorization. The experiments of decay start from a velocity field whose energy spectrum is $E(k) \sim k^4 \exp(-2k^2/k_i)$.

In Fig. 14, we observe the decay of the energy spectrum which tends to a $k^{-5/3}$ law without noticeable effects of build-up or defect of energy at the neighborhood of the cut-off.

The evolution of the scalar field uses half a convective and half a conservative form of the scalar equation as suggested by Kerr (1981), although we have not systematically analyzed how necessary such a mixing is.

The subgrid-scale modeling of the scalar field is a simplified formulation using a constant value of the eddy Prandtl number; also, the dependency of eddy diffusivity and eddy viscosity with the wave numbers is assumed to be the same, regarding the effects local to $k_c$. In Fig. 15a with an eddy Prandtl number equal to 0.333 ($\lambda' = \lambda'' = \lambda$), the decay of scalar variance is much faster and there is a noticeable discrepancy with a $k^{-5/3}$ law; the transfer of scalar variance beyond $k_c$ is highly overestimated. As the large eddy simulation is completely independent of the EDQNM computation, these results can be viewed as an a posteriori justification of the relevance of the set of EDQNM constants ($\lambda' = 0$, $\lambda'' = 3.61\lambda$). We notice, at least at the beginning of our decay period, a rather artificial $k^{-5/3}$ spectrum over the four or five wave numbers close to the cut-off for both the energy and scalar spectrum.
variance spectra. This is a consequence of the $k^{-5/3}$ spectrum used to derive the eddy viscosity and diffusivity.

On a Cray 1, the computing time required for a time-step is 0.4 sec for the velocity field only and .75 sec for the velocity and scalar fields.
6. Conclusion

The derivation of an eddy viscosity from an EDQNM closure (Chollet and Lesieur, 1981) has been extended to the derivation of an eddy diffusivity for the advection of a passive scalar. The values of closure-constants (λ', λ'') are of main importance; the LES results seem to promote the set (λ' = 0, λ'' = 3.61λ) which, by the way, is better supported by other arguments detailed in Herring et al. (1982). From the formulation of the transfers in the EDQNM closure, we have described how the eddy viscosity and diffusivity are affected by a closeness of the given wave number $k_C$ to the dissipative scale (as happens in low Reynolds number computations) and the large scales (as when using LES even with high resolution 64³, 128³).

In EDQNM closure computations, the comparison between a reference solution and a result using the parameterization is quite satisfactory, provided the wave number discretization is the same in the computation and in the derivation of the eddy quantities. These closure calculations with subgrid-scale modeling are quite convenient for studies of decay based on the evaluation of the large-scale transfers of energy and scalar variance.

The subgrid-scale modeling in large eddy simulations at high Reynolds (or Peclet) numbers gives good inertial and inertial-convective ranges. The eddy quantities have been derived from $k^{-5/3}$ spectra, which is not a source of inaccuracy when $k_C$ is in an inertial range far enough from dissipative or large scales, but it generates an overestimation of the subgrid transfers for spectra steeper than $k^{-5/3}$ (as
at the beginning of a decay experiment) and some artificial $k^{-5/3}$ close to $k_c$. The only way to overcome these difficulties is to compute completely the small scales with an EDQNM closure. Some of our recent preliminary results are quite promising, but such a full coupling is much more time-consuming, depending on the vectorization of the EDQNM part of the calculations.

The eddy viscosity and diffusivity are scalar quantities and are clearly isotropic. The assumption of isotropy has to hold not only for small scales but for all scales under consideration to derive $v_t^+$ and $D_t^+$; nevertheless, the small scales and that part of the large scales which is not too far from the cut-off are the only ones whose isotropy is absolutely required. Various considerations can be suggested by experiments, the homogeneity seems to set up much faster than the isotropy in three-dimensional flows; but in flows where energy cascades from quasi-two-dimensional to three-dimensional structures (e.g., mixing layers), the spatial intermittency of this transition from two-dimensional to three-dimensional could favor an isotropy of small three-dimensional eddies. In any case, we probably have to distinguish between some anisotropic flows (such as flows along rigid boundaries) and the quasi-two-dimensional flows (oceans, atmosphere) where the huge difference between two-dimensional and three-dimensional scales suggests some relevance to a superimposition of the two-dimensional and three-dimensional effects, each with its own subgrid-scale modeling.
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Paris*, T288, 335-338.
Fig. 1 Domain of integration $\Delta$ for interactions between wave numbers of a triad $k, p, q$; shaded area $\Delta_c$, restriction of $\Delta$ such that $p$ of $q > k_c$. 
Fig. 2  Nondimensionalized eddy viscosity $\nu^+_{t}(k/k_c)$ for various wave number discretizations corresponding to $F = 4, 16, 64$.  

--- $F = 64$;  - - - - $F = 16$;  - - - - - - $F = 4$;  

X X X X curve from Kraichnan (1976).
Fig. 3 For the set of constants ($\lambda' = \lambda'' = \lambda = 0.361$) and various wave number discretizations corresponding to $F = 4, 16, 64$.

- F = 64;  
- F = 16;  
- F = 4.

(a) nondimensionalized eddy diffusivity $D_\tau^+(k/k_c)$
(b) eddy Prandtl number $\nu_\tau^+/D_\tau^+(k/k_c)$
Fig. 4  For the set of constants ($\lambda' = 0$, $\lambda'' = 3.61 \lambda$; $\lambda = 0.361$) and various wave number discretizations corresponding to $F = 4, 16, 64$.

- $F = 64$; $\ldots$ $F = 16$; $\cdots$ $F = 4$;

(a) nondimensionalized eddy diffusivity $D_t^+(k/k_c)$
(b) eddy Prandtl number $\nu_t^+/D_t^+(k/k_c)$
Fig. 5  Rate of the eddy viscosity $v_t'(D_t)$ to their asymptotic values $v_t^\infty(D_t^\infty)$, versus $k_c/k_s$, where $k_s$ is the Kolmogorov dissipation wave number (taking no account of local effects around $k_c$).

---: eddy viscosity $v_t/v_t^\infty$

or eddy diffusivity $D_t^+/D_t^\infty$

with ($\lambda' = \lambda'' = \lambda$)

---: eddy diffusivity $D_t^+/D_t^\infty$

with ($\lambda' = 0; \lambda'' = 3.61 \lambda$)
Fig. 6 Cusp of the nondimensionalized eddy viscosity

\( \nu_t^{+ \text{cusp}}(k/k_c) \). K: points from Kraichnan (1976).

(a) \( \ln (\nu_t^{+ \text{cusp}}) \) versus \( k/k_c \)

(b) \( \ln (\nu_t^{+ \text{cusp}}) \) versus \( \ln(k/k_c) \)
Fig. 7 Cusp of the nondimensionalized eddy diffusivity $D_{t_{cusp}}^+(k/k_c)$.
(a) $\ln (D_{t_{cusp}}^+)$ versus $k/k_c$
(b) $\ln (D_{t_{cusp}}^+)$ versus $\ln(k/k_c)$

--- : with $\lambda' = 0$; $\lambda'' = 3.61 \lambda$
--- --- : with $\lambda' = \lambda'' = \lambda$
Fig. 8 Exponent of a power law for the cusp of the eddy viscosity and eddy diffusivity:

(a) $\frac{d(\ln \nu^+_{\text{cusp}})}{d(\ln (k/k_c))}$
(b) $\frac{d(\ln D^+_{\text{cusp}})}{d(\ln (k/k_c))}$

- - - - - - : with $\lambda' = \lambda'' = \lambda$

---

: with $\lambda' = 3.61 \lambda$
Fig. 9  Stationary turbulence, Re = 60000, molecular Prandtl nb. = 1,
wave number discretization corresponding to F = 8

--- --- : complete calculation including dissipative scales
x x x x x : parameterized calculation, $k_c = 16$

(a) compensated spectrum of energy
(b) compensated spectrum of scalar variance
Fig. 10  Stationary turbulence, $R_T = 60000$, molecular Prandtl nb. = 1

---: total flux for the complete calculation
x x x x x: total flux for the parameterized calculation
---------------: flux generated by the subgrid-scale modeling

(a) energy flux
(b) scalar variance flux
Fig. 11  Free-decaying turbulence, energy spectra, initial Reynolds number: $R_I = 32800$, wave number discretization corresponding to: $F = 4$

---: complete calculation (including dissipative scales)

+++ + + : parameterized calculation, $k_c = 16$

----- : initial spectrum

(a)-(d): times: 2.5, 5, 7.5, 10.

(unit of time: large eddy ($k=1$) turnover time)
Fig. 12 Free-decaying turbulence, scalar variance spectra, same conditions as for Fig. 8, Prandtl number = 1.

(a)-(d): times: 2.5, 5., 7.5, 10.
**Fig. 13a Decay of energy with time:**

- Complete calculation: 
  \[
  \frac{1}{2} \langle u^2 \rangle = \int_0^\infty E(k) \, dk
  \]

- Parameterized calculation, \( k_c = 16 \)
  \[
  \frac{1}{2} \langle u^2 \rangle = \int_0^{k_c} E(k) \, dk
  \]

- Parameterized calculation, \( k_c = 16 \), with a 
  \( k^{-5/3} \) extrapolation of spectrum beyond \( k_c \).

\[
\frac{1}{2} \langle u^2 \rangle = \int_0^{k_c} E(k) \, dk + \frac{3}{2} \, \frac{k}{c} \, E(k) \, .
\]

**Fig. 13b Decay of scalar variance with time:**

- Complete calculation: 
  \[
  \langle \theta^2 \rangle = \int_0^\infty E_\theta(k) \, dk
  \]

- Parameterized calculation, \( k_c = 16 \)
  \[
  \langle \theta^2 \rangle = \int_0^{k_c} E_\theta(k) \, dk
  \]

- Parameterized calculation, \( k_c = 16 \), with a 
  \( k^{-5/3} \) extrapolation of spectrum beyond \( k_c \).

\[
\frac{1}{2} \langle \theta^2 \rangle = \int_0^{k_c} E_\theta(k) \, dk + \frac{3}{2} \, \frac{k}{c} \, E(k) \, .
\]
Fig. 14 Large eddy simulation with subgrid-scale modeling: Spectrum of kinetic energy:

- --- t = 0.0 s
- o t = 1.0 s
- * t = 2.0 s
Fig. 15 Large eddy simulation with subgrid-scale modeling: Spectrum of scalar variance:

- --- t = 0.0 s
- o t = 0.4 s
- △ t = 0.8 s
- + t = 1.2 s
- * t = 1.6 s
- □ t = 2.0 s

(a) Subgrid-scale modeling with eddy Prandtl number = 0.333

(b) Subgrid-scale modeling with eddy Prandtl number = 0.6