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Subgrid-Scale Turbulent Micromixing: Dynamic Approach

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When numerically simulating the behavior of unsteady large scales in turbulent mixing problems, subgrid diffusion of chemical species (turbulent micromixing) requires a closure. A dynamic model is proposed to estimate micromixing from the known properties of the resolved large-eddy field. The dynamic procedure also provides a direct estimation of the micromixing time. A reference scalar field is invoked in the closure, and the physical model is based on basic properties of mass transfer by diffusion. Direct numerical simulation (DNS) is utilized to validate the ability of the closure to capture the relaxation of probability density functions for three-dimensional homogeneous freely decaying turbulence and a two-dimensional mixing layer. The dynamic closure for diffusion is shown to reproduce DNS results, and then a standard test case for micromixing models is computed using large-eddy simulation.

Nomenclature

D	= diffusion coefficient
$\mathcal{D}(Z^*)$	= conditional filtered value of diffusive budget $D\nabla^2 Z$
$E(k)$	= energy spectrum
$\mathcal{F}_{R_1,R_2,(\bar{Z})}(\bar{Z}^*)$	= function relating Z^* to $\bar{Z}^*$
f_{τ_t}	= mixing frequency
$G(\underline{x}; \bar{\Delta})$	= subgrid filter
k	= wave number
$\bar{P}_{sg}(Z^*; \underline{x}, t)$	= subgrid probability density function (PDF) of Z
R_1	= ratio of filter sizes, $\hat{\Delta}/\bar{\Delta}$
R_2	= ratio between filter size and δ_r, $\bar{\Delta}/\delta_r$
t	= time
$\boldsymbol{u}$	= velocity vector
$\underline{x}$	= spatial position
Z	= mixture fraction
Z^r	= reference mixture fraction field
Γ_{R_1,R_2}	= ratio of $\mathcal{D}$ defined for different filtering levels
$\bar{\Delta}$	= subgrid filter size and uniform grid spacing for large-eddy simulation
$\hat{\Delta}$	= test filter size, $(>\bar{\Delta})$
δ_m	= thickness of the mixing layer
δ_r	= uniform grid spacing utilized to define the reference field
$\delta(Z - Z^*)$	= fine-grained PDF
$\langle\,\rangle$	= Reynolds average

Subscripts

1, 2	= mixing layer streams

Superscripts

$\bar{}$	= subgrid filtering
$\hat{}$	= test filtering, $(\hat{\Delta} > \bar{\Delta})$
$*$	= composition space

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Introduction

WHEN fuel and oxidizer are not perfectly premixed before entering a turbulent combustion chamber, large-scale unsteady movements lead to an incomplete mixing between the reactants, whereas micromixing mechanisms bring fuel and oxidizer into contact within thin reaction zones. The description of both unsteady large scales and micromixing mechanisms is a crucial issue of turbulent combustion modeling.[1]

In nonreactive flows, it is believed that, in opposition to large eddies, small-scale motion is dominated by properties that weakly depend on flow geometries. Based on these considerations, large-eddy simulation (LES) is characterized by an exact simulation of the large scales of the flow, whereas the dissipation of energy is modeled at smaller scales. This corresponds to a direct estimation of the large-eddy field from the solution of local volume averaged transport equations, whereas small-scale stresses are approximated. LES implicitly assumes that the behavior of large scales is not directly related to the mechanism utilized to capture the energy transferred toward smaller scales. Moreover, the properties of the large scales are supposed to fix the dissipation.[2] LES is now accepted as an effective tool for nonreactive flows,[3–5] and dynamic simulations in which model parameters are determined from the resolved large eddies have been widely used.[6,7]

Using time averaged quantities, the probability density function (PDF) has been shown to be an attractive formalism to compute nonpremixed turbulent combustion.[8–10] The main advantage of the PDF is that chemical effects appear in a closed form within the transport equation for the joint PDF of reactive species. Thus, it is possible to account for the fluctuations of species and temperature when including chemical effects. However, a closure is needed to capture turbulent micromixing.[10,11] In the work of Gao and O'Brien,[12] Cook and Riley,[13] Réveillon and Vervisch,[14] and the references therein, the PDF formalism has been extended to LES. The objective was to describe the subgrid statistics of a conserved scalar field (nonreactive). In those works, a presumed shape for the PDF was jointly used with infinitely fast chemistry hypothesis; however, presumed PDFs are difficult to handle when finite-rate chemistry needs to be described.[8] Here we propose a closed transport equation for calculating this PDF, the unknown turbulent micromixing being estimated from the knowledge of the resolved large-eddy field.

Both direct numerical simulations (DNS) and LES are performed to estimate the validity of the proposed procedure. Two flow configurations have been retained; they correspond to well-documented mixing problems: the isotropic freely decaying turbulence and the mixing layer. A previously developed finite difference DNS code[15] is used. Following the methodology of Poinsot et al.,[16] it is sixth-order accurate in space and third-order accurate in time.

First, we investigate the properties of subgrid micromixing needing to be captured by the closure. Then, a dynamic micromixing model is constructed, and from DNS results we discuss its capability to reproduce subgrid diffusion along with the corresponding characteristic mixing time. Finally, the closed PDF transport equation is solved for the mixing in isotropic turbulence of an initially segregated field.

Subgrid Micromixing

Introduction

The description of the diffusion flame is usually done by introducing combinations of species mass fraction that are conserved through reaction zones.[17] In this spirit, the mixture fraction $Z(\underline{x}, t)$ is a conserved scalar widely utilized to characterize mixing between fuel and oxidizer in nonpremixed turbulent flames ($Z = 1$ in pure fuel and $Z = 0$ in pure air). To focus on large scales, all spatial fluctuations smaller than a length $\bar{\Delta}$ are damped using a filtering operation, or local volume average. It is defined from a convolution between the turbulent signal and a filter $G(\underline{x}; \bar{\Delta})$ of width $\bar{\Delta}$, and such that

$$\int_{-\infty}^{+\infty} G(\underline{x}; \bar{\Delta})\, \mathrm{d}\underline{x} = 1$$

The convolution operation between the turbulent signal $Z(\underline{x}, t)$ and the filter $G(\underline{x}; \bar{\Delta})$ may be written[18] as

$$\bar{Z}(\underline{x}, t) = \int_{-\infty}^{+\infty} Z(\underline{x}', t) G(\underline{x} - \underline{x}'; \bar{\Delta})\, \mathrm{d}\underline{x}'$$

The PDF of the passive scalar Z is introduced to capture the statistical properties of mixing at large scales. This PDF is obtained from a filtering operation applied to the function $\delta[Z(\underline{x}', t) - Z^*]$, called fine-grained PDF,[19] defined by letting $\delta_{Z^*} \to 0$ in the expressions

$$\delta[Z(\underline{x}', t) - Z^*] = 1/\delta_{Z^*} \quad \text{if} \quad -\delta_{Z^*}/2 < Z(\underline{x}', t) - Z^* < \delta_{Z^*}/2$$

$$\delta[Z(\underline{x}', t) - Z^*] = 0 \qquad \text{otherwise}$$

At the subgrid level $\bar{P}_{sg}(Z^*; \underline{x}, t)$ is defined as

$$\bar{P}_{sg}(Z^*; \underline{x}, t) = \int_{-\infty}^{+\infty} \delta[Z(\underline{x}', t) - Z^*] G(\underline{x}' - \underline{x}; \bar{\Delta})\, \mathrm{d}\underline{x}'$$

and $Z(\underline{x}, t)$ is isotropic in the case of the freely decaying turbulence, or statistically homogeneous in the streamwise direction of the temporal mixing layer. From the transport equation for Z, $\partial Z/\partial t = -\boldsymbol{u} \cdot \nabla Z + D\nabla^2 Z$, the transport equation for the subgrid PDF may be written[20] as

$$\frac{\partial \bar{P}_{sg}(Z^*; \underline{x}, t)}{\partial t} = -\frac{\partial}{\partial Z^*}\left[\overline{(-\boldsymbol{u} \cdot \nabla Z(\underline{x}, t) \mid Z = Z^*)} \bar{P}_{sg}(Z^*; \underline{x}, t)\right] - \frac{\partial}{\partial Z^*}\left[\overline{(D\nabla^2 Z(\underline{x}, t) \mid Z = Z^*)} \bar{P}_{sg}(Z^*; \underline{x}, t)\right] \tag{1}$$

in which the unclosed terms of the form $\overline{(A \mid Z = Z^*)}$ are conditional filtered mean values. The first term on the right-hand side of Eq. (1) is the advection term, which vanishes for a homogeneous and isotropic turbulence, and it will not be considered here. The other term represents micromixing effects; it may be cast in the following form:

$$\begin{aligned}\bar{\mathcal{D}}(Z^*) &= \overline{(D\nabla^2 Z(\underline{x}, t) \mid Z = Z^*)} \bar{P}_{sg}(Z^*; \underline{x}, t) \\ &= \int_{-\infty}^{+\infty} D\nabla^2 Z(\underline{x}', t) \delta(Z(\underline{x}', t) - Z^*) G(\underline{x}' - \underline{x}; \bar{\Delta})\, \mathrm{d}\underline{x}' \\ &= \overline{D\nabla^2 Z(\underline{x}, t) \delta(Z(\underline{x}, t) - Z^*)}\end{aligned} \tag{2}$$

Hereafter $\mathcal{D}$ is referred to as the micromixing term. In an LES simulation, the flow is fully resolved for scales larger than $\bar{\Delta}$; within this range a test filter with a characteristic width $\hat{\Delta} > \bar{\Delta}$ is introduced. The basic idea, discussed and tested in the following, is to estimate the unknown quantity

$$\bar{\mathcal{D}}(Z^*) = \overline{D\nabla^2 Z(\underline{x}, t) \delta(Z(\underline{x}, t) - Z^*)} \tag{3}$$

found in Eq. (1) from the test micromixing term

$$\hat{\mathcal{D}}(\bar{Z}^*) = \widehat{D\nabla^2 \bar{Z}(\underline{x}, t) \delta(\bar{Z}(\underline{x}, t) - \bar{Z}^*)} \tag{4}$$

which is known from the resolved large-eddy field $\bar{Z}$. $\bar{\mathcal{D}}(Z^*)$ and $\hat{\mathcal{D}}(\bar{Z}^*)$ control the evolution via Eq. (1) of PDFs defined at the two subgrid levels $\bar{\Delta}$ and $\hat{\Delta}$, respectively; those filtered diffusion terms are representative of micromixing effects relative to the filter width.

Properties of Subgrid Micromixing Terms

DNSs of three-dimensional freely decaying isotropic turbulence have been carried out. The DNS solver has already been validated in different situations.[15,21,22] The initial Z field is characterized by its energy spectrum and a nearly bimodal PDF[23]; its Schmidt number is set to unity. The initial turbulent Reynolds number based on the integral length scale is about 50. Starting from the synthetic initial condition, the flow is allowed to evolve toward a situation where basic properties of turbulence are verified; results are presented from this instant in a nondimensional time constructed with the initial eddy turn-over time.

The DNS field $Z(\underline{x}, t)$ is filtered, and the resulting large-eddy quantities (PDF, conditional filtered means) are averaged over the computational domain. The large-eddy mixing problem is then characterized by the time evolution of the ensemble mean of the subgrid PDF $\langle \bar{P}(Z^*, t)\rangle = \langle \bar{P}_{sg}(Z^*; \underline{x}, t)\rangle$, which is expressed from Eq. (1) in the form

$$\frac{\partial \langle \bar{P}(Z^*, t)\rangle}{\partial t} = -\frac{\partial}{\partial Z^*}[\langle \bar{\mathcal{D}}(Z^*)\rangle] \tag{5}$$

First, mean values of the micromixing term $\langle \bar{\mathcal{D}}(Z^*)\rangle$ [Eq. (3)] and of the test mixing term $\langle \hat{\mathcal{D}}(\bar{Z}^*)\rangle$ [Eq. (4)] are extracted from 65^3 DNS. Both $\langle Z\rangle = 0.5$ and $\langle Z\rangle = 0.3$ are considered to study cases featuring symmetric and nonsymmetric shape for the PDF. As expected[24] $\langle \bar{\mathcal{D}}(Z^*)\rangle$ and $\langle \hat{\mathcal{D}}(\bar{Z}^*)\rangle$ present maximum and minimum values, which are symmetrically located with respect to the means $Z^* = \langle Z(\underline{x}, t)\rangle$ and $\bar{Z}^* = \langle \bar{Z}(\underline{x}, t)\rangle$.

However, comparison of the two filtered micromixing terms lead to the following conclusions (Fig. 1).

1) Different amplitudes are found for the extrema of $\langle \bar{\mathcal{D}}(Z^*)\rangle$ and $\langle \hat{\mathcal{D}}(\bar{Z}^*)\rangle$.

2) These extrema move toward the mean when the test filter is applied, i.e., the maximum value of $\langle \bar{\mathcal{D}}(Z^*)\rangle$ and $\langle \hat{\mathcal{D}}(\bar{Z}^*)\rangle$ are found for different values of Z^*.

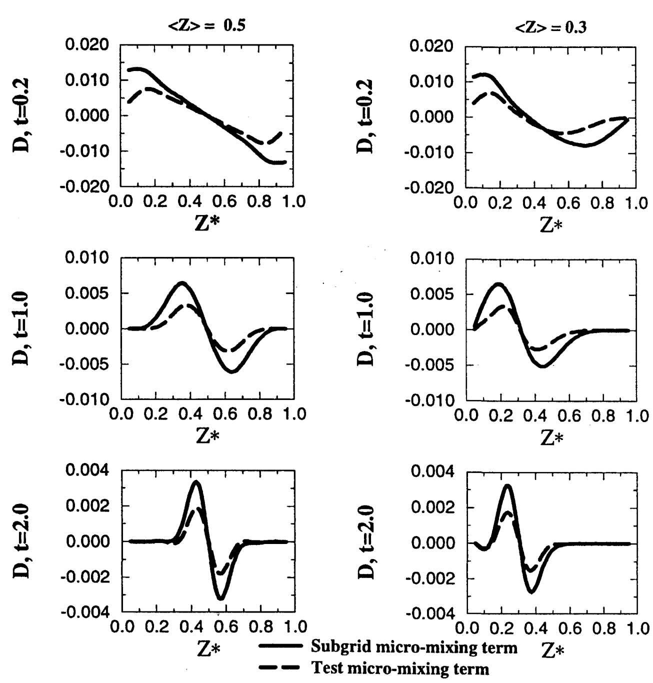

Fig. 1 Micromixing term: ——, $\langle \bar{\mathcal{D}}(Z^*)\rangle$ level $\bar{\Delta}$ and – – –, $\langle \mathcal{D}(\bar{Z}^*)\rangle$ level $\hat{\Delta}$; DNS of isotropic turbulent mixing $\langle Z\rangle = 0.5$ (left) and $\langle Z\rangle = 0.3$ (right); time evolution from top to bottom.

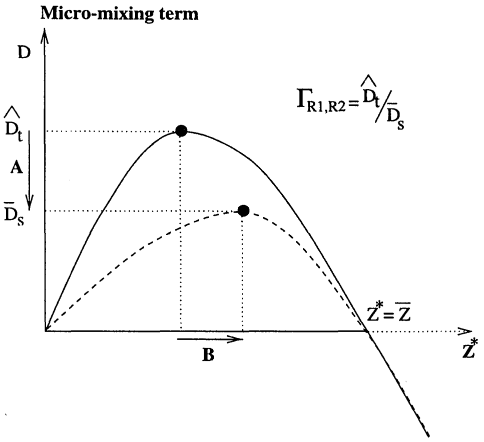

Fig. 2 Impact of the filtering operation on the micromixing term: ——, $\langle\bar{\mathcal{D}}(Z^*)\rangle$ level $\bar{\Delta}$ and - - -, $\langle\hat{\mathcal{D}}(\bar{Z}^*)\rangle$ level $\hat{\Delta}$; A, diffusive amplitude shift and B, recall effect toward the mean.

Both points 1 and 2 are simply because the filtering process on average decreases the gradient of the mixture fraction Z. Figure 2 shows the effect of filtering on micromixing terms.

Dynamic Model for Turbulent Micromixing

To estimate $\langle\bar{\mathcal{D}}(Z^*)\rangle$, we formulate the hypothesis that points 1 and 2 just discussed can be reproduced from the properties of the filtering operations applied to a prescribed reference scalar field $Z^r(\underline{x})$.

One may write

$$\langle\bar{\mathcal{D}}[\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)]\rangle = \frac{1}{\Gamma_{R_1,R_2}}\langle\hat{\mathcal{D}}(\bar{Z}^*)\rangle \tag{6}$$

where the parameter $R_1 = \hat{\Delta}/\bar{\Delta}$ is the ratio of the test ($\hat{\Delta}$) to subgrid ($\bar{\Delta}$) filter widths, whereas $R_2 = \bar{\Delta}/\delta_r$ is the ratio of the subgrid filter width to the uniform grid spacing δ_r. Γ_{R_1,R_2} and $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ may be determined as follows using points 1 and 2 discussed earlier.

1) Γ_{R_1,R_2} is utilized to capture the difference in magnitude between the amplitude of micromixing estimated at the subgrid ($\bar{\Delta}$) and test ($\hat{\Delta}$) levels (Fig. 2). It is defined from the ratio

$$\Gamma_{R_1,R_2} = \frac{\max_{0<\bar{Z}^*<1}\langle\hat{\mathcal{D}}(\bar{Z}^*)\rangle}{\max_{0<Z^*<1}\langle\bar{\mathcal{D}}(Z^*)\rangle} \tag{7}$$

2) The function $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ with

$$Z^* = \mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*) \tag{8}$$

is also introduced to map the known micromixing term computed at test level ($\hat{\Delta}$ and $Z = \bar{Z}^*$) to the corresponding one presumed at subgrid level ($\bar{\Delta}$ and $Z = Z^*$). The role of $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ is to mimic the shift toward the mean observed for the extrema when moving from $\langle\hat{\mathcal{D}}(\bar{Z}^*)\rangle$ to $\langle\bar{\mathcal{D}}(Z^*)\rangle$ (Fig. 2).

To determine Γ_{R_1,R_2} and $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$, it is assumed that Eq. (6) is a generic relationship between micromixing terms defined for different subgrid levels. Then, Γ_{R_1,R_2} and $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ may be determined from Eqs. (7) and (8) by using a reference scalar field $Z^r(\underline{x})$.

Figure 3 shows the time evolution of Γ_{R_1,R_2} computed from DNS (three-dimensional isotropic mixing). Despite the dramatic evolution of the statistical properties of the mixture fraction field Z leading to a rapid decay of the fluctuations (Fig. 3), Γ_{R_1,R_2} can be considered as a parameter depending only on the ratios R_1 and R_2. Similarly, $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ has been extracted from filtered DNS fields (Fig. 4). Results suggest that, in a first approximation, $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ can be considered as only weakly dependent on the statistical properties of Z. Both Γ_{R_1,R_2} and $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ can then be tabulated as functions of R_1, R_2, and $\langle\bar{Z}\rangle$.

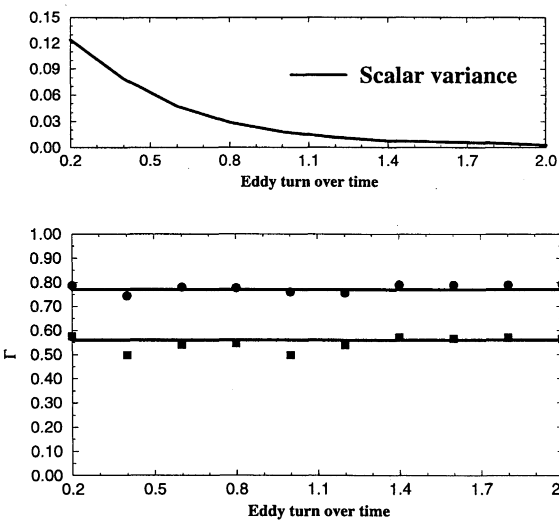

Fig. 3 Isotropic turbulent mixing; top, time evolution of $\langle[\langle Z\rangle - Z(\underline{x},t)]^2\rangle$ and, bottom, comparison of the time evolution of Γ_{R_1,R_2} computed from DNS (● and ■) and from the Γ_{R_1,R_2} database (——). For $R_1 = \hat{\Delta}/\bar{\Delta} = 2$, two cases are considered: ●, $R_2 = \bar{\Delta}/\delta_r = 2$ and ■, $R_2 = 4$.

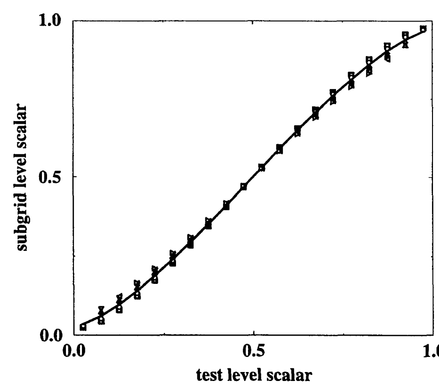

Fig. 4 $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ at various times in DNS of isotropic turbulent mixing (symbols), relation $Z^* = \mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ tabulated from database $Z^r(\underline{x})$, $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*) = 0.02 + 0.46\bar{Z}^* + 1.5\bar{Z}^{*2} - \bar{Z}^{*3}$ (——) for $R_1 = \hat{\Delta}/\bar{\Delta} = 2$, $R_2 = \bar{\Delta}/\delta_r = 2$, and $\bar{Z} = 0.5$.

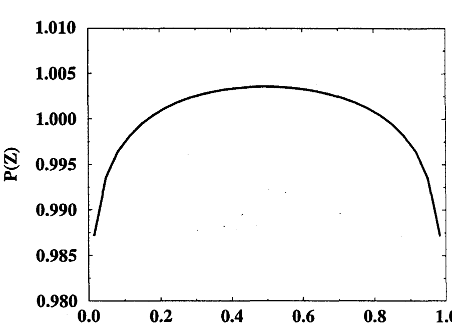

Fig. 5 PDF of the reference scalar field Z^r.

To parametrize $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ and Γ_{R_1,R_2} for imposed filter sizes, a random three-dimensional isotropic reference field $Z^r(\underline{x})$ is chosen whose PDF (Fig. 5) and energy spectrum (Fig. 6) are representative of an intermediate stage in a mixing problem, which started with an initially fully segregated field (double-delta PDF) with mean value $\langle\bar{Z}\rangle$. This is motivated by the necessity of generating databases for Γ_{R_1,R_2} and $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ that may be utilized for situations ranging from fully segregated to fully mixed. In other words, this option allows for moderating the impact on the model of the properties of the reference field Z^r. To apply the closure to nonhomogeneous flows, for given R_1 and R_2, the response of Γ_{R_1,R_2}

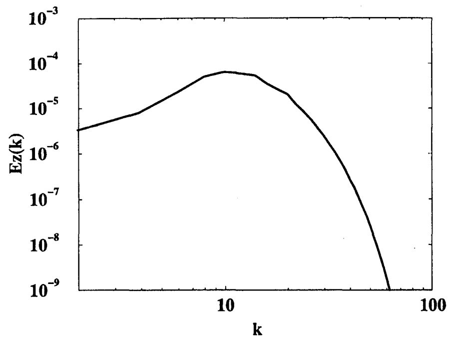

Fig. 6 Spectrum of the reference scalar field Z^r.

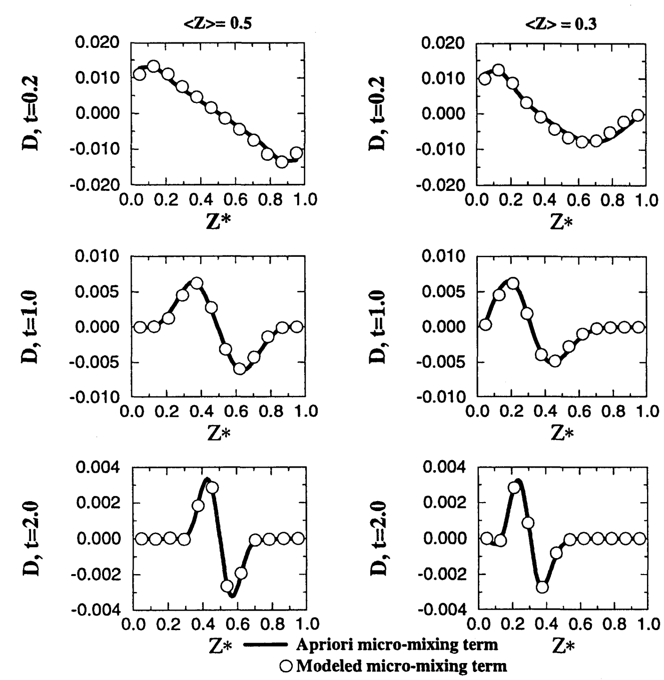

Fig. 7 Isotropic turbulent mixing, subgrid micromixing term $\langle\bar{\mathcal{D}}(Z^*)\rangle$ extracted from DNS (——) and corresponding modeled values (○); $\langle Z\rangle$ = 0.5 (left) and $\langle Z\rangle$ = 0.3 (right).

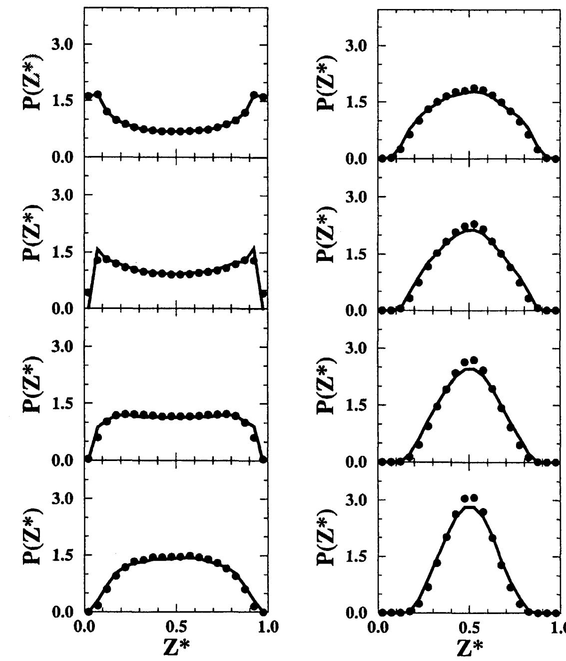

Fig. 8 Time evolution of the subgrid PDF $\langle\bar{P}(Z^*,t)\rangle$ during isotropic turbulent mixing; comparison between the relaxation of the PDF obtained from DNS (●) and computed by solving Eq. (3) (——) in which $\langle\bar{\mathcal{D}}(Z^*)\rangle$ is provided by the subgrid dynamic mixing model.

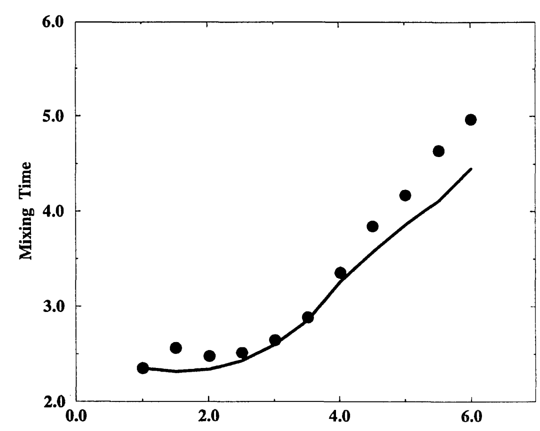

Fig. 9 Isotropic turbulent mixing, subgrid mixing time ($f_{\tau_t}^{-1}$) estimated from the dynamic model via the slope of $\langle\bar{\mathcal{D}}(Z^*)\rangle/\langle P_{sg}(Z^*)\rangle$ at $Z^* \simeq \bar{Z}$ (——) and extracted from DNS (●) as $\langle\overline{\psi^2}\rangle/\langle\overline{D(\partial\psi/\partial x_i)(\partial\psi/\partial x_i)}\rangle$, where $\psi = \bar{Z} - Z$. Scalar mean = 0.5.

and $\mathcal{F}_{R_1,R_2,\langle\bar{Z}\rangle}(\bar{Z}^*)$ to various $\langle\bar{Z}\rangle$ is constructed by linear interpolations between databases generated from Eqs. (7) and (8) for different mean values of the reference field ($\langle Z^r\rangle = \langle\bar{Z}\rangle$).

Test of the Dynamic Micromixing Model

Three-Dimensional Isotropic Turbulent Mixing

The isotropic turbulent mixing case is considered first. To mimic the determination of subgrid micromixing from resolved large scales, $\langle\hat{\mathcal{D}}(\bar{Z}^*)\rangle$, the diffusive term at test level ($\hat{\Delta}$), is extracted from DNS; then it is introduced as an input to the model presuming $\langle\bar{\mathcal{D}}(Z^*)\rangle$. Following this procedure, the validity of the closure can be estimated by comparing modeled values of $\langle\bar{\mathcal{D}}(Z^*)\rangle$ to those directly extracted from DNS. Figure 7 displays the time evolution of $\langle\bar{\mathcal{D}}(Z^*)\rangle$ and the results are encouraging. Because of classical DNS limitations, these validations have to be seen has a preliminary development of the model. A more severe test case is performed when solving the transport equation for the PDF in which the model has been introduced to compute the right-hand side of Eq. (5). Figure 8 shows the relaxation of the PDF during mixing obtained from DNS and from the solution of Eq. (3).

Micromixing models usually need as an input a characteristic mixing time.[25–27] Here the determination of the frequency of mixing is embedded within the dynamic process. To estimate this characteristic mixing time, an analogy is made with the Linear Mean Square Estimation (or Interaction by Exchange with the Mean) closure.[10] It supposes a linear response proportional to the frequency of mixing for the conditional mean value of diffusion $\langle\bar{\mathcal{D}}(Z^*)\rangle/\langle P_{sg}(Z^*)\rangle \simeq f_{\tau_t}(\bar{Z} - Z^*)$. DNS suggests that this closure is valid for LES in the vicinity of the mean value in composition space ($Z^* \simeq \bar{Z}$); notice that this remark would not be valid for a reactive scalar. Then, the magnitude of the slope of $\langle\bar{\mathcal{D}}(Z^*)\rangle$ at the point where $\langle\bar{\mathcal{D}}(Z^*)\rangle \simeq 0$ should be a fair estimation of the characteristic frequency of subgrid micromixing. Figure 9 shows a comparison of the mixing time extracted from DNS and presumed by the model. Because the turbulence is decaying, after four eddy turn-over times most of the subgrid energy has been dissipated, and a deviation between the modeled time scale and the computed one is observed in Fig. 9. A good agreement is found, however, before the subgrid energy decays.

Mixing Layer

Temporal simulations of two-dimensional mixing layers that are statistically homogeneous in the streamwise directions have been performed. The initial streamwise velocity profile is cast in the form

$$u(y) = \tfrac{1}{2}(u_1 + u_2) + \tfrac{1}{2}(u_1 - u_2)\tanh(2y/\delta_m) \qquad (9)$$

To help in the generation of large-scale instabilities, white noise is superimposed to the initial velocity field. The corresponding initial distribution for the mixture fraction is constructed by normalizing Eq. (9). Results are presented in nondimensional units constructed from the velocity difference $(u_1 - u_2)/2$ and the thickness δ_m. In these units $u_1 = 2.5$ and $u_2 = 0.5$. Figure 10 shows the development of the mixing zone; as expected for these two-dimensional flows, the spectrum of the velocity fluctuations follows a k^{-4} behavior (Fig. 11).

The initial laminar diffusive layer is convected and stretched during the growth of the instabilities. The spreading of the points in the scatter plot for the $\overline{D\nabla^2 Z}$ plotted vs Z^* is an indicator of the intensity of multiple interactions between vortices and diffusive zones (Fig. 12). The effect of the test filter $(\hat{\Delta})$ when computing $\widehat{D\nabla^2\tilde{Z}^*}$ is also shown in Fig. 13, whereas Fig. 14 shows comparison between the micromixing term presumed by the model and its value extracted from DNS.

The preceding remarks concerning subgrid mixing time scale are applied to the mixing layer configuration. To estimate a local mixing time, Eq. (6) can be utilized for only a few points within mixture fraction space in the vicinity of $Z^* \simeq \tilde{Z}$. Then a linear regression is made to estimate the unknown micromixing term. Result of this procedure is compared against DNS in Fig. 15; this suggests that dynamic mixing closure can be used not only to solve the PDF

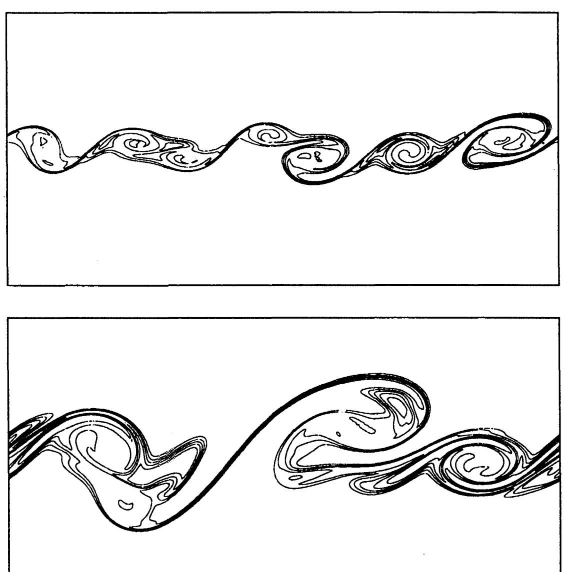

Fig. 10 Two-dimensional mixing layer, isoline for mixture fraction field Z, t = 60 (top) and t = 100 (bottom).

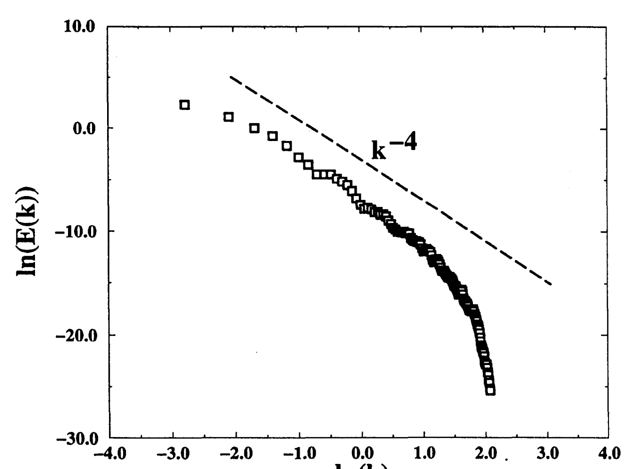

Fig. 11 Two-dimensional mixing layer, energetic spectrum of the velocity field.

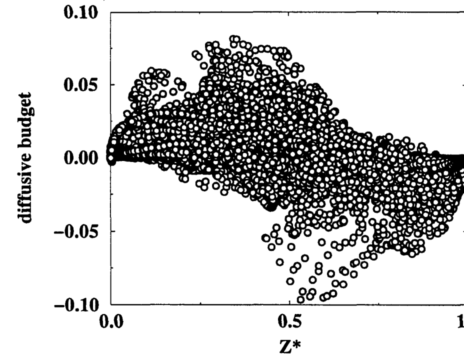

Fig. 12 Two-dimensional mixing layer, scatter plot of $\overline{D\nabla^2 Z(\underline{x}, t)}$ (subgrid level $\bar{\Delta}$).

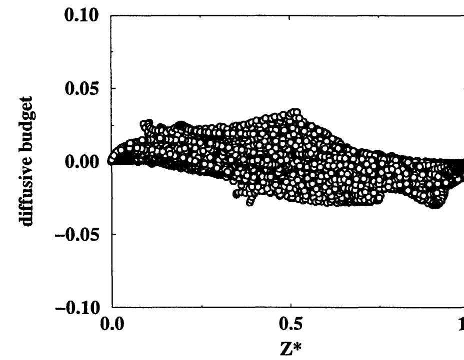

Fig. 13 Two-dimensional mixing layer, scatter plot of $\widehat{D\nabla^2\tilde{Z}(\underline{x}, t)}$ (test level $\hat{\Delta}$).

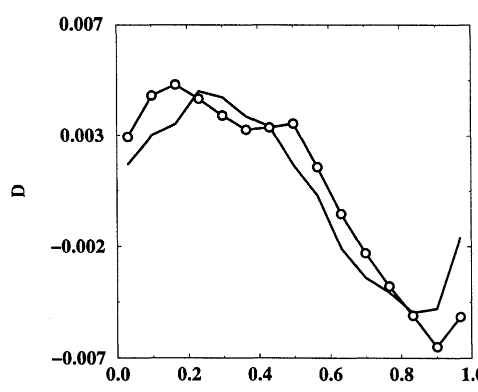

Fig. 14 Two-dimensional mixing layer, micromixing $\langle\bar{\mathcal{D}}(Z^*)\rangle$: ——, DNS and ○, dynamic micromixing model.

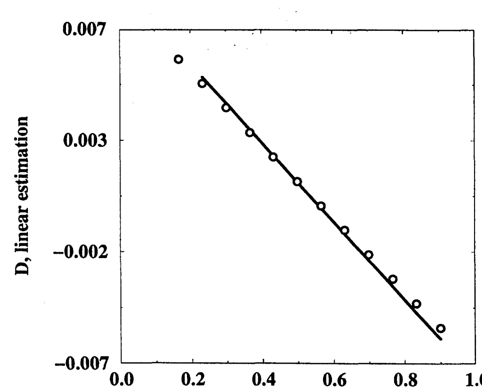

Fig. 15 Two-dimensional mixing layer, linear estimation of the micromixing term $\langle\bar{\mathcal{D}}(Z^*)\rangle$: ——, DNS and ○, dynamic micromixing model.

transport equation, but it is also of great interest to estimate the subgrid characteristic mixing time.

Conclusion

1) An attempt has been made to develop a dynamic closure for small-scale micromixing in the context of LES using PDF. It is based on a direct estimation of subgrid mixing from the knowledge of the resolved large-eddy field. A reference scalar field is used to link subgrid diffusion at different filter sizes.

2) In the case of three-dimensional isotropic freely decaying turbulence including the mixing of an initially segregated mixture fraction field, the dynamic procedure reproduces the correct relaxation of the PDF and it provides a direct estimation of the characteristic subgrid mixing time.

3) For two-dimensional mixing layers, the comparison between DNS results with those obtained from the closure indicates that the dynamic procedure may be an alternative route to compute scalar mixing involving unsteady large eddies.

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