Mapping closure approximation to conditional dissipation rate for turbulent scalar mixing

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1. Motivation and objectives

The probability density function (PDF) approach has been shown to be a useful tool in turbulence research. The systematic approach for determining PDFs is by means of solving the transport equations for PDFs. In the PDF equations for turbulent scalar fields, conditional dissipation rate (CDR) appears as the only unclosed term (Pope (1985)). Recently developed large-eddy simulation schemes for turbulent reactive flow, such as the filtered PDF approach (Colucci, *et al.* (1998)), the conditional moment closure (Bushe & Steiner (1999)), and the Lagrangian flamelet model (Pitsch & Steiner (2000)), also require models for the CDR.

No satisfactory closure model for CDR had been constructed until the mapping closure approach (Kraichnan (1989), Chen, *et al.* (1989)) was formulated. Amplitude mapping closure suggests a CDR model (O'Brien & Jiang (1991)) whose form is separable in scalar and time variables. The model is in good agreement with direct numerical simulation (DNS) for initially symmetric binary mixing but fails in describing asymptotic behavior of the CDR for initially unsymmetric binary mixing (O'Brien & Sahay (1992)). Girimaji (1992) has developed a novel amplitude mapping closure approach in which the reference fields are time-dependent. The CDR model obtained from a time-evolving Gaussian reference field still fails to describe the asymptotic behavior, but the one from a time-evolving Beta reference field can successfully describe the asymptotic behavior. This strongly suggests that the amplitude mapping closure is inadequate to describe the asymptotic behavior by itself.

In the present research, we will develop a novel mapping closure approximation (MCA) to make successive approximations to statistics of a scalar in homogeneous turbulence. This technique will be used to construct a CDR model which accounts for the asymptotic behavior of the CDR. In Section 2.1, we will investigate the asymptotic behavior of the CDR model from amplitude mapping closure and explain the reason why it fails to describe the asymptotic behavior correctly. In Section 2.2, we will outline the MCA technique for successive approximation. In Section 2.3, we will use the MCA technique to formulate a novel CDR model and compare it with DNS results. We will conclude with a summary in Section 3.

2. Accomplishments

2.1. *Asymptotic behaviors of amplitude mapping closure*

In this section, we will show that the CDR model from amplitude mapping closure has incorrect asymptotic behavior for unsymmetric binary mixing. We consider the simple case of a single conserved scalar $Z(x, t)$ in incompressible homogeneous and isotropic

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turbulence. With $u(x,t)$ being the velocity field and κ the molecular diffusivity, the evolution equation for scalar Z is

$$\frac{\partial Z}{\partial t} + \mathbf{u} \cdot \nabla Z = \kappa \nabla^2 Z. \tag{2.1}$$

Here the boundary condition is periodic and the scalar is initially homogeneous and isotropic. Therefore, the scalar $Z(x,t)$ will remain homogeneous and isotropic for all time. We further assume that the scalar is binary (0 or 1) and its initial PDF is a double-delta distribution:

$$P(Z,0) = \begin{cases} A & \text{if } \ Z = 0 \\ 1 - A & \text{if } \ Z = 1 \\ 0 & \text{if } \ Z \neq 0 \text{ or } 1, \end{cases} \tag{2.2}$$

where $0 \le A \le 1$. $A = 0.5$ implies that the binary scalar has the same weights and the corresponding PDF $P(Z,0)$ is symmetric with respect to $Z = 0.5$, while $A \neq 0.5$ implies that the binary scalar has different weights and the corresponding PDF $P(Z,0)$ is unsymmetric. DNS Eswaran & Pope (1988) has shown that the scalar PDF $P(Z,t)$ asymptotically approaches a Gaussian distribution whether the initial double-delta distribution is symmetric or unsymmetric. The mean $\langle Z \rangle = 1 - A$ remains unchanged in turbulent mixing. The CDR $\chi(Z,t) = \kappa \langle (\nabla Z)^2 | Z \rangle$ is nearly parabolic. At early stages, the CDR maximum is located at $Z = 0.5$, the mean of the initial interface of the binary scalar. The maximum then moves and finally approaches the mean $\langle Z \rangle$ of the scalar, accompanied by a distortion of the parabola. Therefore, for an initially symmetric binary scalar ($A = 0.5$), the maximum will remain fixed at $Z = 0.5$, where the mean of the scalar and the mean of the initial interface are coincident. For an initially unsymmetric binary scalar ($A \neq 0.5$), the maximum will shift to the mean $Z = 1 - A$ of the scalar from the mean $Z = 0.5$ of the initial interface.

Amplitude mapping closure assumes

$$Z = X(\phi_0, t), \tag{2.3}$$

where $\phi_0(\mathbf{x})$ is a homogeneous Gaussian random field. The governing equation for the mapping function X is

$$\frac{\partial X}{\partial t} = \kappa \langle \phi_{0x}^2 \rangle \left(-\frac{\phi_0}{\langle \phi_0^2 \rangle} \frac{\partial X}{\partial \phi_0} + \frac{\partial^2 X}{\partial \phi_0^2} \right), \tag{2.4}$$

where ϕ_{0x} is the spatial gradient of the scalar ϕ_0. The initial mapping function corresponding to (2.2) is

$$X(\phi_0, 0) = \begin{cases} 0 & \text{if } \ \phi_0 \le \gamma \\ 1 & \text{if } \ \phi_0 > \gamma, \end{cases} \tag{2.5}$$

where $\gamma = \sqrt{2} erf^{-1}(2A - 1)$. The exact solution of Eq. (2.4) with the initial condition (2.5) is

$$X(\phi_0, t) = \frac{1}{2}\left[1 + erf\left(\frac{\theta_0 - \gamma e^{\tau}}{\sqrt{2}\Sigma}\right)\right], \tag{2.6}$$

where

$$\begin{aligned} \theta_0 &= \frac{\phi_0}{\sqrt{\langle\phi_0^2\rangle}}, \\ \tau &= \kappa\frac{\langle\phi_{0x}^2\rangle}{\langle\phi_0^2\rangle}t, \\ \Sigma &= \sqrt{\exp(2\tau) - 1}. \end{aligned} \tag{2.7}$$

We can calculate the CDR from the exact solution (2.6)

$$\begin{aligned} \chi(Z, t) &= \kappa\frac{\langle\phi_{0x}^2\rangle}{\langle\phi_0^2\rangle}\frac{1}{\sqrt{2\pi}\Sigma}\exp\left(-2\left[erf^{-1}(2Z-1)\right]^2\right) \\ &= \chi(0.5, t)\exp\left(-2\left[erf^{-1}(2Z-1)\right]^2\right). \end{aligned} \tag{2.8}$$

The most striking feature of the CDR model (2.8) is the separability of its form in Z and t. The separability suggests that the CDR's shape remains unchanged although its amplitude decays with time. The CDR maximum is located permanently at $Z = 0.5$ without any shift for either symmetric or unsymmetric initial conditions. The permanent location of the maximum for unsymmetric initial condition (Girimaji (1992), O'Brien & Jiang (1991), O'Brien & Sahay (1992)) is contrary to the known asymptotic behavior of the CDR. Therefore, the CDR model (2.8) from amplitude mapping closure is not able to describe the asymptotic behavior of the CDR. The amplitude mapping closure with a time-evolving Gaussian reference field gives a similar CDR model whose form is separable in t and Z and also fails to describe the shift of the maximum. Therefore, the separation in form is the main reason for the incorrect asymptotic behavior of the CDR model from amplitude mapping closure.

2.2. *Mapping closure approximation*

The basic idea of mapping closure is to represent an unknown random field by mapping of a known random reference field. The statistics of the unknown random field can be calculated from the mapping function and the known reference field. The governing equation for the mapping function can be obtained from the evolution equation of the unknown random field and the governing equation of its PDF.

Amplitude mapping closure assumes that the unknown random field can be mapped by a single known Gaussian reference field: $Z = X(\phi(x'), t)$ and a coordinate transformation $dx'/dx = J(d\phi(x')/dx', t)$ that accounts for turbulent stretching. The assumption Gotoh & Kraichnan (1993) holds if and only if the spatial level crossing frequency at which the unknown random field passes through a given value has a single maximum as a function of that value. Therefore, the existence of the mapping function as well as the coordinate transformation is not ensured for arbitrary unknown random fields. Physically, a turbulent field exhibits eddies of different length and time scales so that it cannot be mapped by a single reference Gaussian field with a compact spectrum. Therefore, it is necessary to introduce more reference fields accounting for different eddies of different time and length scales:

$$Z = X(\phi_0(x,t), \phi_1(x,t), \cdots, \phi_n(x,t); x, t) \tag{2.9}$$

where ϕ_i, $i = 1, \cdots, n$, are reference fields. So far, we have not imposed any constraints on the reference fields so that we have some freedom in choosing the reference fields. For example, ϕ_0 could be Gaussian but ϕ_1 could be a Beta random field.

A one-to-one mapping could be established artificially between $(Z, \phi_1, \cdots, \phi_n)$ and $(\phi_0, \phi_1, \cdots, \phi_n)$. Thus, we can calculate the PDF and the conditional dissipation rate of the scalar

$$P(Z; x, t) = \int P(\phi_0, \phi_1, \cdots, \phi_n) \left(\frac{\partial X}{\partial \phi_0}\right)^{-1} d\phi_1 \cdots d\phi_n, \tag{2.10}$$

$$\langle (\nabla Z)^2 | Z\rangle = \langle (\nabla X)^2 | Z\rangle. \tag{2.11}$$

Here the integration is taken over the entire subspace of the composition $\phi_1, \cdots, \phi_n$. The ensemble average is taken over the level surface on which $(\phi_0, \phi_1, \cdots, \phi_n)$ satisfies the constraint $X(\phi_0(x,t), \phi_1(x,t), \cdots, \phi_n(x,t); x, t) = Z$ for a given Z.

Introduction of more reference fields is expected to improve the approximation accuracy of mapping closure. The reference fields might be chosen to be statistically orthogonal so that more information can be introduced at less expense. MCA provides a successive non-perturbative approximation approach which is different from the Wiener-Hermite expansion (Orszag & Bissonnette (1967)).

2.3. *The model for conditional dissipation rate*

Broad classes of mapping function are admissible to MCA approach. The form to be considered here is

$$Z = Y(\phi_0(x), \phi_1(t); t), \tag{2.12}$$

where $\phi_0(x)$ is a homogeneous random Gaussian field in space and $\phi_1(t)$ an inhomogeneous random Gaussian field in time. Amplitude mapping closure requires $\phi_1(t) = 0$, which fails in the asymptotic behavior of conditional dissipation rate due to lack of an independent time-evolving reference field.

Following the standard method (Gotoh & Kraichnan (1993), Kimura & Kraichnan (1993)), we can formulate the mapping equation:

$$\frac{\partial Y}{\partial t} + \frac{\partial Y}{\partial \phi_1}\langle \frac{d\phi_1}{dt} | Z\rangle = -\langle u\nabla Y | Z\rangle + \kappa \langle \nabla^2 Y | Z\rangle. \tag{2.13}$$

The conditional averages in (2.13) can be evaluated by homogeneity of the velocity and scalar fields and Gaussianity of the reference fields

$$\begin{aligned} &\langle u\nabla Y | Z\rangle = 0, \\ &\langle \frac{d\phi_1}{dt} | Z\rangle = \frac{\phi_1}{2\langle \phi_1^2\rangle}\frac{d\langle \phi_1^2\rangle}{dt}, \\ &\langle \nabla^2 Y | Z\rangle = -\phi_0 \frac{\langle \phi_{0x}^2\rangle}{\langle \phi_0^2\rangle}\frac{\partial Y}{\partial \phi_0} + \langle \phi_{0x}^2\rangle \frac{\partial^2 Y}{\partial \phi_0^2} \end{aligned} \tag{2.14}$$

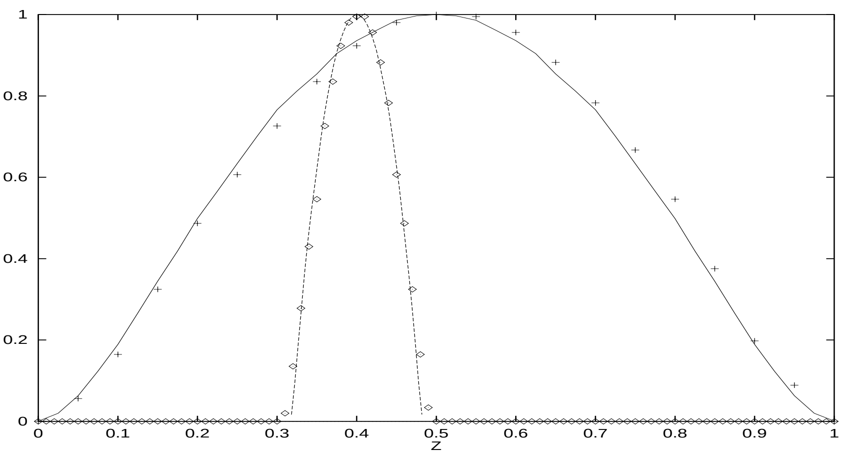

FIGURE 1. Normalized CDRs $\chi(Z,t)/F(t)$ for the initially unsymmetric double-delta distribution with $A = 0.6$. ——— (DNS) and + (model): initial CDRs; - - - - (DNS) and ⋄ (model): final CDRs.

An exact solution can be obtained from (2.13) with the evaluated conditional averages (2.14) and the initial condition (2.5) which requires $\phi_1(0) = 0$

$$Y = \frac{1}{2}\left[1 + erf\left(\frac{\phi_0 - \gamma e^{\tau}}{\sqrt{2}\,\Sigma}\right) + \left(1 - \exp[\phi_1 - \langle\phi_1\rangle + \int_0^t \langle\frac{d\phi_1}{dt}|Z\rangle dt]\right)(2\langle Z\rangle - 1)\right]. \tag{2.15}$$

We will calculate the CDR $\chi(Z,t) = \kappa\langle(\nabla Y)^2|Z\rangle$, where ensemble average is taken over the level surface on which (ϕ_0, ϕ_1) satisfies $Y(\phi_0, \phi_1; t) = Z$. The expression obtained is then simplified by the first-order approximation of its Taylor expansion with respect to $\langle\phi_1(t)\rangle$. This leads to

$$\chi(Z,t) = F(t)\exp\left[-2\left(erf^{-1}[(2Z-1) - (1 - \frac{1}{\sqrt{1 + f_{\phi_1} t}})(2\langle Z\rangle - 1)]\right)^2\right], \tag{2.16}$$

where

$$\begin{aligned} F(t) &= \frac{f_{\phi_0}}{\sqrt{2\pi}\Sigma}, \\ f_{\phi_0} &= \kappa\frac{\langle(\phi_{x0})^2\rangle}{\langle\phi_0^2\rangle}, \\ f_{\phi_1} &= \frac{d\langle\phi_1^2\rangle}{dt}/\langle\phi_1^2\rangle. \end{aligned} \tag{2.17}$$

The time scales f_{ϕ_0} and f_{ϕ_1} are parameters of the present closure which must be input externally. Usually, they are reset at each time using a dynamical scheme, such as $f_{\phi_0} = \kappa\langle(\nabla Z)^2\rangle/\langle Z^2\rangle$ and $f_{\phi_1} = f_{\phi_0}$, so as to give correct evolution of the CDR. The CDR model (2.16) is compared with DNS of the diffusion equation with $\kappa = 1$. In the case of homogeneity, the use of the diffusion equation to validate the CDR model for turbulent mixing has a reasonable justification. Figure 1 shows the initial and final CDRs obtained by the DNS and the CDR model (2.16) for the initially unsymmetric binary scalar with mean $\langle Z \rangle = 0.4$. For exhibiting the shift of the maximum, the CDRs are normalized by their amplitudes $F(t)$ and (2.16) rescaled by the scalar's variances.

The CDR model (2.16) is no longer separable in Z and t. Its shape will shift while its amplitude decays with time. It is easy to verify that $\chi(0.5, 0)/F(t) = 1$ and that $\chi(\langle Z \rangle, \infty)/F(t) = 1$. Therefore, Eq. (2.16) correctly describes asymptotic behaviors of CDR: the CDR's maximum asymptotically approaches $Z = \langle Z \rangle$, while initially being at $Z = 0.5$.

It has been shown that the mapping (2.12) is an appropriate approximation for a scalar gradient field. However, it is not expected that the mapping (2.12) makes the same accurate approximation to the scalar field as it does to the scalar gradient field itself. The reason is that a homogeneous random field is statistically orthogonal to its gradient field. The amplitude mapping (2.3) is an appropriate approximation to scalar fields but fails to approximate its gradient field. Generally speaking, the mapping closure carried out at the level of single-point PDFs is not valid for two-point PDFs such as gradient fields. This is the motivation to develop mapping closure approximation of higher orders.

3. Conclusions and further plans

We have developed a novel model of the conditional dissipation rate for turbulent mixing. The model is able to describe the asymptotic behavior of the CDR for either symmetric or unsymmetric initial double-delta distributions. The amplitude mapping closure has unsatisfactory asymptotic properties for the shift of the CDR's maximum. The problem can be solved using the extended mapping closure approximation developed in this paper. Further research will involve extending the CDR model (2.16) to account for the evolution of scalar variance. MCA can incorporate the effect of multiple time and length scales of practical interest in its predictions using more than one reference field. It provides a useful approach to describe statistics of turbulent mixing.

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