A self-contained mapping closure approximation for scalar mixing

By Guo-Wei He † AND Zi-Fan Zhang ‡

1. Objective and motivation

Scalar turbulence exhibits interplays of coherent structures and random fluctuations over a broad range of spatial and temporal scales. This feature necessitates a probabilistic description of the scalar dynamics, which can be achieved comprehensively by using probability density functions (PDFs). Therefore, the challenge is to obtain the scalar PDFs (Lundgren 1967; Dopazo 1979). Generally, the evolution of a scalar is governed by three dynamical processes: advection, diffusion and reaction. In a PDF approach (Pope 1985), the advection and reaction can be treated exactly but the effect of molecular diffusion has to be modeled. It has been shown (Pope 1985) that the effect of molecular diffusion can be expressed as conditional dissipation rates or conditional diffusions. The currently used models for the conditional dissipation rates and conditional diffusions (Pope 1991) have resisted deduction from the fundamental equations and are unable to yield satisfactory results for the basic test cases of decaying scalars in isotropic turbulence, although they have achieved some success in a variety of individual cases. The recently developed mapping closure approach (Pope 1991; Chen, Chen & Kraichnan 1989; Kraichnan 1990; Klimenko & Pope 2003) provides a deductive method for conditional dissipation rates and conditional diffusions, and the models obtained can successfully describe the shape relaxation of the scalar PDF from an initial double delta distribution to a Gaussian one. However, the mapping closure approach is not able to provide the rate at which the scalar evolves. The evolution rate has to be modeled. Therefore, the mapping closure approach is not closed. In this Letter, we will address this problem.

The evolution rate of scalar is a key quantity in modeling turbulent mixing for both conserve and reactive scalars (Cha & Trouillet 2003). It specifies the characteristic time scale of scalar evolution. It has been shown that the decay rate of scalar depends on the relative length scale ratio of the initial scalar and velocity fields (Warhaft & Lumley 1978; Sreenivasan, Tavoularis, Henry & Corrsin 1980; Durbin 1982; Eswaran & Pope 1988; Mell, Kosály & Riley 1991), and recently, the asymptotic decay of scalar turbulence has been extensively studied (Eyink & Xin 2000; Chaves, Eyink, Frisch & Vergassola 2001; Chertkov & Lebedev 2003). Nearly all existing models for scalar mixing, ranging from the simple (conditional) moment approaches to the full PDF approaches, require information on the time scales. These models are mainly based on the assumption of a direct proportionality between the scalar time scales and the turbulence time scales (Fox 1995). Moreover, they exclude the effects of chemical reaction on the time scales of scalar evolution. The mapping closure approach of time-dependent reference fields (Girimaji 1992) can provide the time scale externally, which highlights an attack line to this problem.

† Permanent address: LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing, 100080, China; Email: hgw@lnm.imech.ac.cn
‡ LNM, Institute of Mechanics, Chinese Academy of Sciences.

We develop here a mapping closure approximation (MCA) approach for the time scale of scalar evolution. The MCA approach is based on multi-point joint PDFs. In the mapping closure approach (Pope 1991; Chen, Chen & Kraichnan 1989), an unknown random field is mapped from a known random Gaussian field so that the evolution of the unknown random field can be described by the mapping function. The mapping function is obtained from the transport equation for the unknown random field and the Gaussian closure. Since the mapping function is constructed at the level of one-point PDFs, it is not able to provide the information on two-point statistics, such as the time scales (He, Rubinstein & Wang 2002). In the MCA approach, the mapping functions are constructed at the levels of multi-point joint PDFs. The mapping function based on the two-point joint PDFs could provide the correct information on time scales.

2. Main results

We consider the simple case of a reactive scalar advected by a stochastic velocity field:

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = \Gamma \nabla^2 \varphi + Q(\varphi), \tag{2.1}$$

where the velocity field $\mathbf{u}$ obeys $\nabla \cdot \mathbf{u} = 0$ and is independent of the scalar field. Without the loss of generality, it may be prescribed as a known homogeneous and isotropic Gaussian field. Γ is a molecular diffusivity, $Q(\varphi)$ mimics a one-species chemical reaction.

In the MCA approach, the scalar field is mapped from a known random field by a mapping function

$$\varphi(\mathbf{x}, t) = X(\theta(\mathbf{x}, t), t). \tag{2.2}$$

Here, the known random field $\theta(\mathbf{x}, t)$ is taken as a Gaussian reference field. Its one-point and two-point joint PDFs are defined by

$$g_1(\eta) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{\eta^2}{2}\right], \tag{2.3}$$

$$g_2(\eta_1, \eta_2, r, t) \equiv g(\eta_1, \eta_2, \rho(r, t)) = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left[-\frac{\eta_1^2 + \eta_2^2 - 2\rho\eta_1\eta_2}{2(1-\rho^2)}\right], \tag{2.4}$$

where

$$\rho(r, t) = \frac{\langle \theta(\mathbf{x}, t)\theta(\mathbf{x} + \mathbf{r}, t\rangle}{\langle \theta^2(\mathbf{x}, t)\rangle}. \tag{2.5}$$

Here r is the magnitude of separation vector $\mathbf{r}$. The mapping function is required to represent the one-point and two-point joint PDFs of the scalar φ via the following equations

$$f_1(\psi, t) = g_1(\eta)\left[\frac{\partial X(\eta, t)}{\partial \eta}\right]^{-1}, \tag{2.6}$$

$$f_2(\psi_1, \psi_2, r, t) = g_2(\eta_1, \eta_2, r, t)\left[\frac{\partial X(\eta_1, t)}{\partial \eta_1}\frac{\partial X(\eta_2, t)}{\partial \eta_2}\right]^{-1}. \tag{2.7}$$

In the classic mapping closure approach (Pope 1991; Chen, Chen & Kraichnan 1989),

the mapping function X is only required to represent the one-point PDF of the scalar φ via equation (2.6). Differentiating equation (2.6) with respect to t yields

$$\frac{\partial f_1}{\partial t} + \frac{\partial}{\partial \psi}\left[f_1 \frac{\partial X}{\partial t}\right] = 0. \tag{2.8}$$

Meanwhile, the transport equation for the one-point PDF, $f_1(\psi, t)$, can be derived by the test function method (Gotoh & Kraichnan 1993; Kimura & Kraichnan 1993) as

$$\frac{\partial f_1}{\partial t} + \frac{\partial}{\partial \psi}\left[f_1 \left\langle \Gamma \nabla^2 \varphi + Q(\varphi) \mid \psi \right\rangle\right] = 0. \tag{2.9}$$

Thus, comparing the two equations (2.8) and (2.9) with the substitution of (2.2), we obtain the exact result

$$\frac{\partial X}{\partial t} = \Gamma \left\langle \nabla^2 \varphi \mid \varphi = X(\eta, t) \right\rangle + Q(\varphi). \tag{2.10}$$

The conditional moment in (2.10) can be evaluated from the mapping function (2.2) and the Gaussianity (2.3) and (2.4) of the reference field θ (Panchev 1971)

$$\Gamma \left\langle \nabla^2 \varphi \mid \varphi = X(\eta, t) \right\rangle = -C\rho''(0,t)\Gamma \left[\frac{\partial^2 X}{\partial \eta^2} - \eta \frac{\partial X}{\partial \eta}\right], \tag{2.11}$$

where the prime denotes the derivative with respect to separation r. As a result, the transport equation for the mapping function (2.2) becomes

$$\frac{\partial X}{\partial t} = -C\rho''(0,t)\Gamma \left[\frac{\partial^2 X}{\partial \eta^2} - \eta \frac{\partial X}{\partial \eta}\right] + Q(X). \tag{2.12}$$

It is easily shown from the Gaussianity (2.3) and (2.4) that $\langle (\nabla\theta)^2 \rangle = -C\rho''(0,t)$, where $C = 2$ for a two-dimensional physical space and $C = 3$ for a three-dimensional physical space. Equation (2.12) has been obtained in (Chen, Chen & Kraichnan 1989), where $-C\rho''(0,t)$ is represented by the variance $\langle (\nabla\theta)^2 \rangle$. However, the correlation $\rho(r,t)$ in equation (2.12) still remains to be unknown and has to be input externally. For example, it is set using the results from direct numerical simulation in (Chen, Chen & Kraichnan 1989). Therefore, equation (2.12) is unclosed.

The two-point correlation $\rho(r,t)$ cannot be obtained from the one-point PDF $g_1(\eta)$. Rather, it has to be calculated from the two-point joint PDF $g_2(\eta_1, \eta_2, r, t)$. Hence, we propose to invoke the two-point joint PDF (2.4), which is not used in the classic mapping closure approach. By differentiating (2.7) with respect to t, we obtain

$$\frac{\partial f_2}{\partial t} + \frac{\partial}{\partial \psi_1}\left[f_2 \frac{\partial X_1}{\partial t}\right] + \frac{\partial}{\partial \psi_2}\left[f_2 \frac{\partial X_2}{\partial t}\right] = \frac{f_2}{g_2}\frac{\partial g_2}{\partial t}. \tag{2.13}$$

The transport equation for the two-point joint PDF f_2 derived from the test function method (Gotoh & Kraichnan 1993; Kimura & Kraichnan 1993) has the form

$$\begin{aligned} &\frac{\partial f_2}{\partial t} + \nabla_{\mathbf{r}} \cdot [f_2 \langle (\mathbf{u}_2 - \mathbf{u}_1) \mid \psi_1, \psi_2 \rangle] = \\ &-\frac{\partial}{\partial \psi_1}[f_2 \langle \Gamma \nabla^2 \varphi_1 + Q(\varphi_1) | \psi_1, \psi_2 \rangle] - \frac{\partial}{\partial \psi_2}[f_2 \langle \Gamma \nabla^2 \varphi_2 + Q(\varphi_2) | \psi_1, \psi_2 \rangle]. \end{aligned} \tag{2.14}$$

Subtracting (2.13) from (2.14) leads to

$$\frac{f_2}{g_2}\frac{\partial g_2}{\partial t} + \nabla_{\mathbf{r}} \cdot [f_2 \langle (\mathbf{u}_2 - \mathbf{u}_1) \mid \psi_1, \psi_2 \rangle] = \frac{\partial}{\partial \psi_1}[f_2 H_1] + \frac{\partial}{\partial \psi_2}[f_2 H_2], \tag{2.15}$$

where

$$H_k = \Gamma \langle \nabla^2 \varphi_k \mid \psi_k \rangle - \Gamma \langle \nabla^2 \varphi_k \mid \psi_1, \psi_2 \rangle. \tag{2.16}$$

The first term in (2.16) is the conditional diffusion on a single given scalar and is calculated in equation (2.11). The second term is the conditional diffusion on two given scalars at two different locations and, again, can be evaluated using the mapping function (2.2) and the Gaussianity (2.3) and (2.4) of the reference field θ (Panchev 1971)

$$\begin{aligned}
&\langle \nabla^2 \varphi_k | \psi_1, \psi_2 \rangle = \frac{\partial^2 X_k}{\partial \eta_k^2} \left\langle (\nabla \theta_k)^2 \right| \eta_1, \eta_2 \rangle + \frac{\partial X_k}{\partial \eta_k} \left\langle \nabla^2 \theta_k \right| \eta_1, \eta_2 \rangle \\
&= \frac{\partial^2 X_k}{\partial \eta_k^2} \left\{ -C\rho''(0,t) + \frac{\rho'^2(r,t)}{(1-\rho^2(r,t))^2} + \left[(\eta_l - \rho(r,t)\eta_k)^2 - 1 + \rho^2(r,t) \right] \right\} + \\
&\frac{\partial X_k}{\partial \eta_k} \frac{1}{1-\rho^2(r,t)} \left[\left(\rho''(r,t) + \frac{\rho'(r,t)}{r} \right) (\eta_l - \rho(r,t)\eta_k) + C\rho''(0,t)(\eta_k - \rho(r,t)\eta_l) \right]
\end{aligned} \tag{2.17}$$

where $l = 1$ for $k = 2$ and $l = 2$ for $k = 1$. Multiplying (2.15) by ψ_1 and ψ_2 and then taking the mean with substitution of (2.2), (2.4), (2.7) and (2.17), we obtain the transport equation for $\rho(r,t)$ as follows

$$\begin{aligned}
&\frac{\partial \rho(r,t)}{\partial t} + \nabla_{\mathbf{r}} \cdot \langle (\mathbf{u}_1 - \mathbf{u}_2) X_1 X_2 \rangle \left\langle \frac{\partial X_1}{\partial \eta_1} \frac{\partial X_2}{\partial \eta_2} \right\rangle^{-1} = 2\Gamma \cdot \\
&\left[\rho''(r,t) + \frac{\rho'(r,t)}{r} - C\rho(r,t)\rho''(0,t) + \rho'^2(r,t) \left\langle \frac{\partial^2 X_1}{\partial \eta_1^2} \frac{\partial^2 X_2}{\partial \eta_2^2} \right\rangle \left\langle \frac{\partial X_1}{\partial \eta_1} \frac{\partial X_2}{\partial \eta_2} \right\rangle^{-1} \right]
\end{aligned} \tag{2.18}$$

Equations (2.12) and (2.18) form a closed system for the mapping function, where equation (2.12) describes the evolution of the shape of the mapping function and (2.18) specifies the rate at which the mapping function evolves. In equation (2.18), the second term on the left-hand side corresponds to advection, the first three terms on the right-hand side correspond to diffusion and the last term on the right-hand side corresponds to the effect of nonlinear mapping. The last term vanishes if the mapping function is linear. We note that $\rho(r,t)$ is the correlation function of the reference field and is dependent on the mapping function.

The realizability condition of equation (2.18) is $|\rho(r,t)| \leq 1$. For the pure diffusion processes with the initial Gaussian distributions of positive correlations, the diffusion term $\rho^{''}(r,t) + \rho^{'}(r,t)/r$ and the damping term $-C\rho^{''}(0,t)\rho(r,t)$ decrease the amplitudes of the correlation $\rho(r,t)$, so that the solution of equation (2.18) is realizable.

The mapping equation (2.12) is closed using the two-point joint PDF constraint (2.7), from which the correlation equation (2.18) is derived. Another possibility for the closure is to use the constraint of the joint PDF for the scalar and its derivative (Chen, Chen & Kraichnan 1989), which leads to an unclosed equation for $\rho(0,t)$ and its spatial derivatives. It points to another direction to go beyond the one-point mapping (2.2) for different purpose.

The performance of the MCA models (2.12) and (2.18) are evaluated against direct nu-

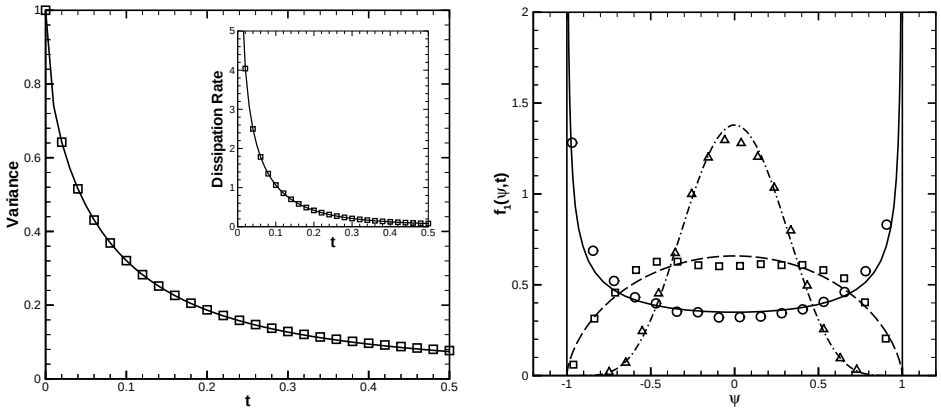

FIGURE 1. Pure diffusion for the conserved scalar with a double-delta initial field. The left: variance and dissipation vs time. Solid lines for MCA and squares for DNS; The right: probability density function. Solid, dashed and dash-dotted lines for MCA at time $0.05, 0.15$ and 0.5, and circles, squares and deltas for DNS at the same time, respectively.

merical simulation. The scalar equation (2.1) and the MCA modeled system of equations (2.12) and (2.18) are numerically solved in a cyclic square of side 2π, using second-order Adams-Bashforth scheme in time and fourth-order central finite-difference scheme in space. In all the cases, the non-dimensional molecular diffusivity $\Gamma = 0.01$. Boundary conditions are periodic in space, except that the ones in the direction of the reference field are obtained by extrapolation. The initial fields for (2.1) are double-delta distributions or isotropic Gaussian distributions with their energy spectra $E_\varphi(k) \propto k^{-17/3}$. Thus, the initial mapping for (2.12) and the initial correlation for (2.18) can be calculated from their definitions.

The velocity field is a given homogeneous isotropic Gaussian process with spectrum of the form $E(k) \propto k^{-5/3}$. We will here present the results for the rapidly changed velocity. That is, the velocity fields are set to change at each time step (Kimura & Kraichnan 1993). In order to isolate the effects of the MCA models on diffusivity and reaction, the advection term in equation (2.18) are calculated directly from the DNS without invoking any models. The analytical treatment on this term can be found in (Kimura & Kraichnan 1993).

Figure 1 compares the evolutions of the variance $\langle \varphi^2(\mathbf{x}, t)\rangle$ and the PDF $f_1(\psi, t)$ obtained by DNS of equation (2.1) with an integration of the MCA models (2.12) and (2.18) for the case of pure diffusion: $\mathbf{u} = 0$ and $Q = 0$. The initial condition is set as a double delta distribution. The results illustrate that the MCA models represent the relaxation of the double delta PDF to the Gaussian PDF not only in its shape but also at the correct rate of evolutions.

In Fig. 2, the same plots are made for the diffusion-reaction equation: $\mathbf{u} = 0$ and $Q(\varphi) = -20\varphi|\varphi|$, with the initial Gaussian distribution. The MCA models are also in agreement with the DNS results. It shows that the MCA models can represent the effects of both diffusion and reactions.

Further comparisons are made in Fig. 3 for the advection-diffusion equation with the same initial condition as used in Fig. 2, where the Péclet number is about 101. Evidently the MCA models are in good agreement with the decay rate of the scalar.

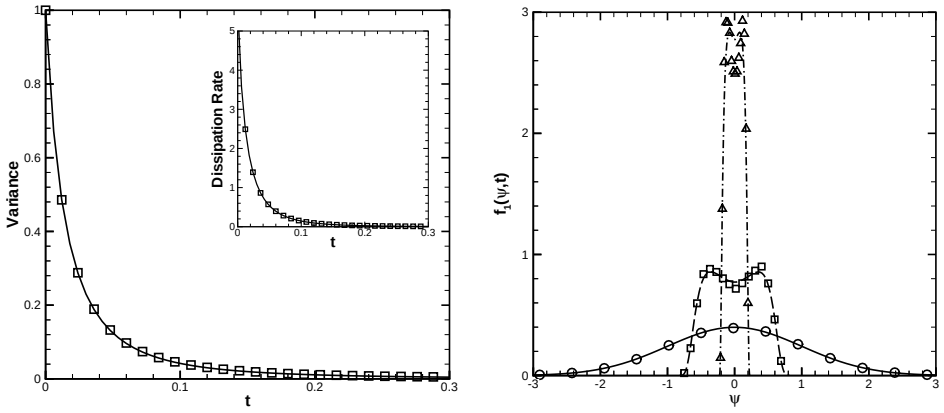

FIGURE 2. Reaction-diffusion for the initial Gaussian scalar. The left: variance and dissipation vs time. Solid lines for MCA and squares for DNS; The right: probability density function. Solid, dashed and dash-dotted lines for MCA at time $0.0, 0.05$ and 0.2, and circles, squares and deltas for DNS at the same time, respectively.

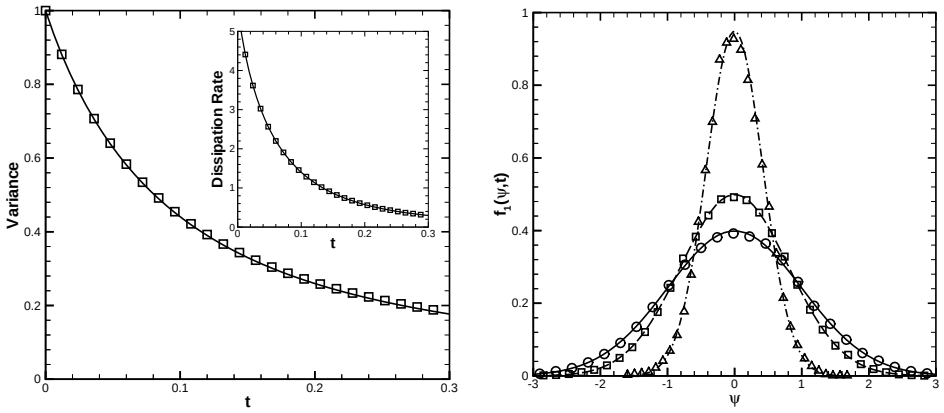

FIGURE 3. Advection-diffusion for the initial Gaussian scalar. The left: variance and dissipation vs time. Solid lines for MCA and squares for DNS; The right: probability density function. Solid, dashed and dash-dotted lines for MCA at time $0.0, 0.05$ and 0.3, and circles, squares and deltas for DNS at the same time, respectively.

In this Letter, the two-point joint PDF is represented by a known two-point joint Gaussian PDF and a mapping function. The correlation of the joint Gaussian PDF and the mapping function evolve under their dynamics. Therefore, the representation of the two-point joint PDF evolves with the dynamics of equation (2.1) via the correlation and mapping function. If it happens that $\rho(r,t) = 0$, equation (2.7) is simplified to $f_2(\psi_1, \psi_2, t) = f_1(\psi_1, t) f_1(\psi_2, t)$. This is the stochastic ansatz in the BBGKY hierarchy in statistical mechanics (Balescu 1975), where the correlations are specified a priori and then fixed. The MCA approach does not invoke this kind of a priori assumption. Moreover, a general N-point ($N > 2$) joint PDF can also be obtained using the known two-point joint Gaussian PDF and the mapping function (2.2), since it can be similarly represented

by the mapping function (2.2) and the N-point joint Gaussian PDF. The latter is fully determined by its two-point joint PDF. In this sense, the MCA approach is self-contained.

3. Conclusion and future work

A self-contained MCA approach is developed for modeling scalar mixing in a stochastic velocity field. It differs from the classic mapping closure approach in that the MCA approach makes use of two-point PDFs to represent the time-evolving correlations of the reference fields and thus the scalar fields. Unlike usual treatments in the BBGKY hierarchy (Balescu 1975), where the representations are specified a priori, the representations in the MCA approach are allowed to evolve in coordinate with the dynamics of scalar mixing. The results obtained using the new approach are in good agreement with the DNS results for the three cases of pure diffusion, diffusion-reaction and advection-diffusion. The approach is under further development for more complex situations including multi-scalar mixing and inhomogeneous scalar fields, using time-evolving Gaussian or non-Gaussian reference fields.

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