Two-point closure strategy in the mapping closure approximation approach

Guo-Wei He[1,2,*] and Zi-Fan Zhang[1]
[1]*Laboratory for Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*
[2]*Center for Turbulence Research, NASA Ames Research Center and Stanford University, Moffett Field, California 94035-1000, USA*
(Received 14 June 2003; revised manuscript received 17 February 2004; published 20 September 2004)

A two-point closure strategy in mapping closure approximation (MCA) approach is developed for the evolution of the probability density function (PDF) of a scalar advected by stochastic velocity fields. The MCA approach is based on multipoint statistics. We formulate a MCA modeled system using the one-point PDFs and two-point correlations. The MCA models can describe both the evolution of the PDF shape and the rate at which the PDF evolves.

DOI: 10.1103/PhysRevE.70.036309 PACS number(s): 47.27.Qb, 47.70.Fw, 82.40.Bj

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 [1–4]. Generally, the evolution of a scalar is governed by three dynamical processes: advection, diffusion, and reaction. In a PDF approach [4], the advection and reaction can be treated exactly but the effect of molecular diffusion has to be modeled. It has been shown [4] 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 [5] 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 [5–11] 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 δ 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 paper, we will address this problem.

The evolution rate of scalar is a key quantity in modeling turbulent mixing for both conserved and reactive scalars [12]. 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 [13–17], and recently, the asymptotic decay of scalar turbulence has been extensively studied [18–20]. 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 [21]. Moreover, they exclude the effects of chemical reaction on the time scales of scalar evolution. The mapping closure approach of time-dependent reference fields [8] can provide the time scale externally, which highlights an attack line to this problem.

We develop here a mapping closure approximation (MCA) approach for the time scale of scalar evolution. In the classic mapping closure approach [5,7], 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. In the MCA approach, the mapping functions are constructed at the levels of multipoint statistics. The mapping function based on the two-point correlations could provide the necessary information on time scales.

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

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \varphi = \Gamma \nabla^2 \varphi + Q(\varphi), \tag{1}$$

where the velocity field $\mathbf{u}$ is incompressible, homogeneous, and isotropic; Γ is a molecular diffusivity and $Q(\varphi)$ mimics a one-species chemical reaction.

In the MCA approach, a surrogate field is introduced by the mapping of a known random field

$$\varphi^s(\mathbf{x},t) = X[\theta(\mathbf{x},t),t]. \tag{2}$$

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

$$g_1(\eta) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{\eta^2}{2}\right], \tag{3}$$

$$g_2(\eta_1,\eta_2,r,t) \equiv g_2[\eta_1,\eta_2,\rho(r,t)] = \frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left[-\frac{\eta_1^2+\eta_2^2-2\rho\eta_1\eta_2}{2(1-\rho^2)}\right], \tag{4}$$

where

*Author to whom correspondence should be addressed. Electronic address: ghe@ctr.stanford.edu; hgw@lnm.imech.ac.cn

$$\rho(r,t) = \langle \theta(\mathbf{x},t)\theta(\mathbf{x}+\mathbf{r},t)\rangle, \tag{5}$$

and r is the magnitude of separation vector $\mathbf{r}$. The one-point and two-point PDFs of the surrogate field can be calculated as follows:

$$f_1^s(\psi,t) = g_1(\eta)\left[\frac{\partial X(\eta,t)}{\partial \eta}\right]^{-1}, \tag{6}$$

$$f_2^s(\psi_1,\psi_2,r,t) = g_2(\eta_1,\eta_2,r,t)\left[\frac{\partial X(\eta_1,t)}{\partial \eta_1}\frac{\partial X(\eta_2,t)}{\partial \eta_2}\right]^{-1}. \tag{7}$$

It is ideal that the surrogate field could represent both one-point and two-point joint PDFs, $f_1(\psi,t)$ and $f_2(\psi_1,\psi_2,r,t)$, of the scalar field. However, for the present purpose on time scales, the surrogate field is only required to represent the one-point PDF and two-point correlation

$$f_1(\psi,t) = f_1^s(\psi,t), \tag{8}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_2(\psi_1,\psi_2,r,t)\psi_1\psi_2 d\psi_1 d\psi_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_2^s(\psi_1,\psi_2,r,t)\psi_1\psi_2 d\psi_1 d\psi_2. \tag{9}$$

The above constraints will be used to determine the mapping function X and the correlation ρ. Therefore, the PDF $f_2^s(\psi_1,\psi_2,r,t)$ thus obtained is an approximation to the scalar PDF $f_2(\psi_1,\psi_2,r,t)$.

In the classic mapping closure approach [5,7], the mapping function X is only required to represent the one-point PDF of the scalar via Eqs. (6) and (8). Differentiating Eq. (6) with respect to t yields

$$\frac{\partial f_1^s}{\partial t} + \frac{\partial}{\partial \psi}\left[f_1^s\frac{\partial X}{\partial t}\right] = 0. \tag{10}$$

Meanwhile, the transport equation for the one-point PDF, $f_1(\psi,t)$, can be derived by the test function method [22,23] as

$$\frac{\partial f_1}{\partial t} + \frac{\partial}{\partial \psi}[f_1\langle \Gamma\nabla^2\varphi + Q(\varphi)|\psi\rangle] = 0. \tag{11}$$

Thus, comparing two Eqs. (10) and (11) with the substitution of Eqs. (2) and (8), we obtain

$$\frac{\partial X}{\partial t} = \Gamma\langle \nabla^2\varphi|\varphi = X(\eta,t)\rangle + Q(\varphi). \tag{12}$$

The conditional moment in Eq. (12) can be evaluated from the mapping function (2) and the Gaussianity (3) and (4) of the reference field θ [24]. As a result, the transport equation for the mapping function (2) becomes

$$\frac{\partial X}{\partial t} = -C\rho''(0,t)\Gamma\left[\frac{\partial^2 X}{\partial \eta^2} - \eta\frac{\partial X}{\partial \eta}\right] + Q(X). \tag{13}$$

It is easily shown from the Gaussianity (3) and (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 (13) has been obtained in Ref. [7], where $-C\rho''(0,t)$ is represented by the variance $\langle(\nabla\theta)^2\rangle$. However, the correlation $\rho(r,t)$ in Eq. (13) still remains unknown and has to be input externally. For example, it is set using the results from direct numerical simulation in Ref. [7]. Therefore, Eq. (13) 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 statistics. Hence, we propose to invoke the two-point correlation (9), which is not used in the classic mapping closure approach. By differentiating Eq. (7) with respect to t, we obtain

$$\frac{\partial f_2^s}{\partial t} + \frac{\partial}{\partial \psi_1}\left[f_2^s\frac{\partial X_1}{\partial t}\right] + \frac{\partial}{\partial \psi_2}\left[f_2^s\frac{\partial X_2}{\partial t}\right] = \frac{f_2^s}{g_2}\frac{\partial g_2}{\partial t}. \tag{14}$$

The transport equation for the two-point joint PDF f_2 can be derived from the test function method [22,23],

$$\frac{\partial f_2}{\partial t} + \nabla_{\mathbf{r}}\cdot[f_2\langle(\mathbf{u}_2-\mathbf{u}_1)|\psi_1,\psi_2\rangle] = \frac{\partial}{\partial \psi_1}[f_2\langle \Gamma\nabla^2\varphi_1 + Q(\varphi_1)|\psi_1,\psi_2\rangle] - \frac{\partial}{\partial \psi_2}[f_2\langle \Gamma\nabla^2\varphi_2 + Q(\varphi_2)|\psi_1,\psi_2\rangle]. \tag{15}$$

Multiplying the difference of Eqs. (14) and (15) by ψ_1 and ψ_2 and then taking the integration of the result with respect to ψ_1 and ψ_2 with substitution of Eq. (9), we obtain

$$\int\int\left(\frac{f_2^s}{g_2}\frac{\partial g_2}{\partial t} + \boldsymbol{\nabla}_{\mathbf{r}}\cdot[f_2^s\langle(\mathbf{u}_2-\mathbf{u}_1)|\psi_1,\psi_2\rangle] - \frac{\partial}{\partial \psi_1}[f_2^s H_1] - \frac{\partial}{\partial \psi_2}[f_2^s H_2]\right)\psi_1\psi_2 d\psi_1 d\psi_2 = 0, \tag{16}$$

where $H_k = \Gamma\langle\nabla^2\varphi_k|\psi_k\rangle - \Gamma\langle\nabla^2\varphi_k|\psi_1,\psi_2\rangle$ can be also evaluated using the mapping function (2) and the Gaussianity (3) and (4) of the reference field θ [24]. Substituting Eqs. (2), (4), and (7), into Eq. (16), we obtain the transport equation for $\rho(r,t)$ as follows:

$$\frac{\partial \rho(r,t)}{\partial t} + \nabla_{\mathbf{r}}\cdot\langle(\mathbf{u}_1-\mathbf{u}_2)X_1X_2\rangle\left\langle\frac{\partial X_1}{\partial \eta_1}\frac{\partial X_2}{\partial \eta_2}\right\rangle^{-1} = 2\Gamma\left[\rho''(r,t) + \frac{\rho'(r,t)}{r} - C\rho(r,t)\rho''(0,t) + \rho'^2(r,t)\times\left\langle\frac{\partial^2 X_1}{\partial \eta_1^2}\frac{\partial^2 X_2}{\partial \eta_2^2}\right\rangle\left\langle\frac{\partial X_1}{\partial \eta_1}\frac{\partial X_2}{\partial \eta_2}\right\rangle^{-1}\right]. \tag{17}$$

Equations (13) and (17) form a closed system for the mapping function, where Eq. (13) describes the evolution of the shape of the mapping function and Eq. (17) specifies the rate at which the mapping function evolves. In Eq. (17), 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 **u** term in Eq. (17) can be treated by the direct interaction or the perturbation method. The model obtained is exact for the conserved scalar advected by a stochastic decorrelated time velocity field. For lack of space, we only give the result as follows:

$$\nabla_{\mathbf{r}} \cdot \langle (\mathbf{u}_1 - \mathbf{u}_2) X_1 X_2 \rangle = h_{ij}(\mathbf{r},t) \frac{\partial^2}{\partial r_i \, \partial r_j} \langle X[\theta(\mathbf{x},t),t] \times X[\theta(\mathbf{x}+\mathbf{r},t),t] \rangle, \tag{18}$$

where

$$h_{ij}(\mathbf{r},t) = 2 \int_0^t \langle u_i(\mathbf{x},t)[u_j(\mathbf{x},t) - u_j(\mathbf{x}+\mathbf{r},t+s)] \rangle ds. \tag{19}$$

The model for the **u** term in Eq. (17) can be also obtained using the scalar-velocity joint PDFs [4].

The realizability condition of Eq. (17) is $|\rho(r,t)| \leqslant 1$. 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 Eq. (17) is realizable.

The mapping equation (13) is closed using the two-point statistics constraint (9), from which the correlation equation (17) is derived. Another possibility for the closure is to use the constraint of the joint PDF for the scalar and its derivative [7], 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) for different purpose.

The performance of the MCA models (13) and (17) are evaluated against the direct numerical simulations (DNS) of the three basic test cases: diffusion equations, diffusion-reaction equations, and advection-diffusion equations. Equation (1) and the MCA models (13) and (17) 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 nondimensional 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 (1) are double-δ distributions or isotropic Gaussian distributions with their energy spectra $E_\varphi(k) \propto k^{-17/3}$. Thus, the initial mapping for Eq. (13) and the initial correlation for Eq. (17) can be calculated from their definitions. The velocity field is a given homogeneous isotropic Gaussian process, decorrelated in time [23], with spectrum of the form $E(k) \propto k^{-5/3}$. In order to isolate the effects of the MCA models on diffusivity and reaction, the advection term in Eq. (17) are calculated directly from the DNS without invoking any models.

Figure 1 compares the evolutions of the variance $\langle \varphi^2(\mathbf{x},t) \rangle$ and the PDF $f_1(\psi,t)$ obtained from Eq. (1) with those from the MCA models (13) and (17) for the diffusion equation: $\mathbf{u}=0$ and $Q=0$. The initial condition is set as a double-δ distribution. The results illustrate that the MCA models represent the relaxation of the double-δ PDF to the Gaussian PDF not only in its shape but also at the correct rate of evolutions.

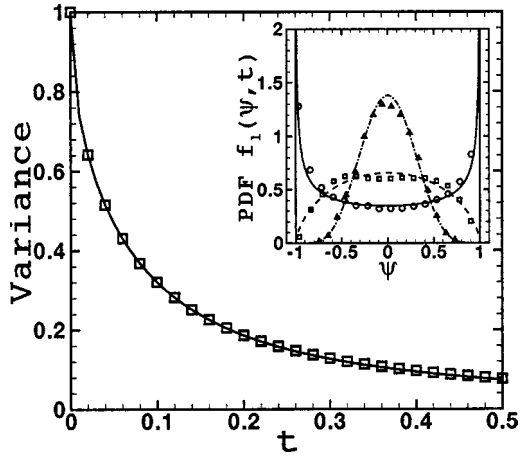

FIG. 1. The scalar variance as a function of time for the diffusion equation: the solid line is from the MCA model and the squares are from DNS. The inset shows the scalar PDFs: the solid, dashed and dash-dotted lines are from the MCA model at $t=0.05, 0.15$, and 0.5, respectively, and the circles, squares, and triangles are from DNS at the corresponding times.

In Fig. 2, the scalar variance and dissipation rate are plotted for the diffusion-reaction equation: $\mathbf{u}=0$ and $Q(\varphi) = -20\varphi|\varphi|$, with the initial Gaussian distribution. The scalar dissipation rate is an important quantity for the mixing models [4]. The MCA model 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 can predict the scalar decay rates. They can still make a good approximation for the higher Péclet number of order 10^2 attained in our numerical simulations.

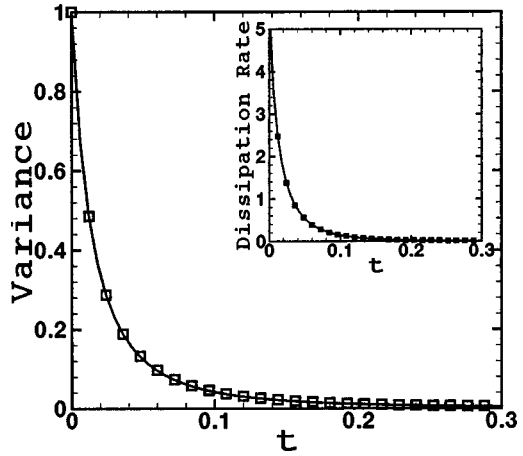

FIG. 2. The scalar variance and dissipation rate (inset) as the functions of time for the reaction-diffusion equation: the solid line is from the MCA model and the squares are from DNS.

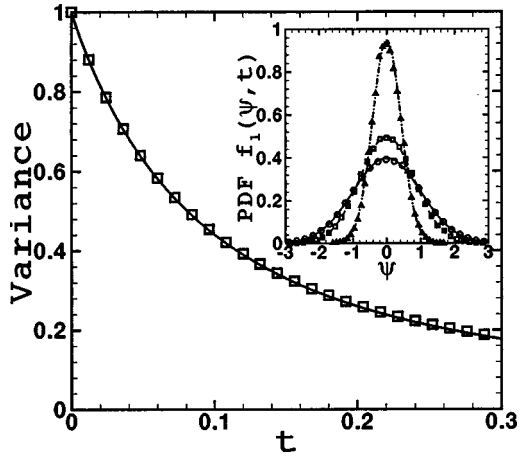

FIG. 3. The scalar variance as a function of time for the advection-diffusion equation: the solid line is from the MCA model and the squares are from DNS. The inset shows the scalar PDFs: the solid, dashed, and dash-dotted lines are from the MCA model at $t=0, 0.05$, and 0.3, respectively, and the circles, squares, and triangles are from DNS at the corresponding times.

A two-point closure strategy in the 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 statistics to determine the time-evolving correlations of the reference fields and thus the scalar fields. Unlike usual treatments in the Bogoliubov-Born-Green-Virkwood-Yvon hierarchy [25], where the representations are specified *a priori*, the representations in the MCA hierarchy are allowed to evolve in coordinate with the dynamics of scalar mixing. Especially, the MCA models obtained are completely closed for the diffusion equations, the diffusion-reaction equations and the advection-diffusion equations of stochastic decorrelated velocity fields. The results from the MCA models are in agreement with the DNS results for the above three basic test cases. The approach is under further development for more complex situations including multiscalar mixing and inhomogeneous scalar fields, using time-evolving Gaussian or non-Gaussian reference fields.

G.-W.H. thanks R. H. Kraichnan for thoughtful comments and stimulating discussions on the manuscript, G. Kosály for the discussions on time scales, M. Wang for his help on the manuscript preparation, Y. L. Bai, R. Rubinstein, M. F. Xia and J. B. Zhang for helpful discussions. This work was supported by the Special Funds for Major Basic Research Project No. G. 2000077305, People's Republic of China and National Natural Science Foundation of China under the Project No. 10325211.

[1] T. S. Lundgren, Phys. Fluids **10**, 969 (1967).
[2] T. S. Lundgren, Phys. Fluids **12**, 485 (1969).
[3] C. Dopazo, Phys. Fluids **22**, 20 (1979).
[4] S. B. Pope, Prog. Energy Combust. Sci. **11**, 119 (1985).
[5] S. B. Pope, Theor. Comput. Fluid Dyn. **2**, 255 (1991).
[6] R. H. Kraichnan, Bull. Am. Phys. Soc. **34**, 2298 (1989).
[7] H. Chen, S. Chen, and R. H. Kraichnan, Phys. Rev. Lett. **63**, 2657 (1989).
[8] S. S. Girimaji, Phys. Fluids A **4**, 2875 (1992).
[9] R. H. Kraichnan, Phys. Rev. Lett. **65**, 575 (1990).
[10] A. Y. Klimenko and S. B. Pope, Phys. Fluids **15**, 1907 (2003).
[11] G.-W. He and R. Rubinstein, J. Turbul. **4**, 029 (2003).
[12] C. M. Cha and P. Trouillet, Phys. Fluids **15**, 1375 (2003).
[13] Z. Warhaft and J. L. Lumley, J. Fluid Mech. **88**, 659 (1978).
[14] K. R. Sreenivasan, S. Tavoularis, R. Henry, and S. Corrsin, J. Fluid Mech. **100**, 597 (1980).
[15] P. A. Durbin, Phys. Fluids **25**, 1328 (1982).
[16] V. Eswaran and S. B. Pope, Phys. Fluids **31**, 506 (1988).
[17] W. E. Mell, G. Kosály, and J. J. Riley, Phys. Fluids A **3**, 2474 (1991).
[18] G. L. Eyink and J. Xin, J. Stat. Phys. **100**, 679 (2000).
[19] M. Chaves, G. Eyink, U. Frisch, and M. Vergassola, Phys. Rev. Lett. **86**, 2305 (2001).
[20] M. Chertkov and V. Lebedev, Phys. Rev. Lett. **90**, 034501 (2003).
[21] R. O. Fox, Phys. Fluids **7**, 1082 (1995).
[22] T. Gotoh and R. H. Kraichnan, Phys. Fluids A **5**, 445 (1993).
[23] Y. Kimura and R. H. Kraichnan, Phys. Fluids A **5**, 2264 (1993).
[24] S. Panchev, *Random Functions and Turbulence* (Pergamon, Oxford, 1971).
[25] R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics* (Wiley, New York, 1975).