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MAPPING CLOSURE APPROXIMATION FOR REACTIVE SCALARS IN RANDOM FLOWS*

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ABSTRACT: The Mapping Closure Approximation (MCA) approach is developed to describe the statistics of both conserved and reactive scalars in random flows. The statistics include Probability Density Function (PDF), Conditional Dissipation Rate (CDR) and Conditional Laplacian (CL). The statistical quantities are calculated using the MCA and compared with the results of the Direct Numerical Simulation (DNS). The results obtained from the MCA are in agreement with those from the DNS. It is shown that the MCA approach can predict the statistics of reactive scalars in random flows.

KEY WORDS: conserved and reactive scalars, MCA, probability density function, conditional dissipation rate, conditional Laplacian

1 INTRODUCTION

Statistics of a reactive scalar in random flows may be found in problems of great practical and fundamental importance in many fields of science and engineering. The important examples include chemical reaction flows in combustion[1] and porous media[2]. The reactive scalar is usually governed by an advection-diffusion-reaction equation

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} \equiv \frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \kappa \nabla^2 \phi + S(\phi) \qquad (1)$$

Here, the scalar ϕ represents the concentration of species. κ is a molecular diffusivity. The source term S represents the chemical reaction rate. The scalar ϕ is reactive if $S \neq 0$ and conserved if $S = 0$. The velocity field $\boldsymbol{u}(\boldsymbol{x}, t)$ is usually solved from the Navier-Stokes equation. For simplicity in the discussion of this paper, the velocity is assumed as a known homogeneous Gaussian field with a short time correlation. This assumption is reasonable since ϕ is a passive scalar.

The statistical description of reactive scalars is usually achieved by moment and PDF approaches. The moments and PDFs are obtained by solving respective transport equations separately. However, both moment and PDF equations suffer from the closure problems. In the moment equations[2], the unclosed terms are convection and reaction. They are modeled by truncated Taylor series expansions with respect to variances. The truncated Taylor series expansion is only valid for small variances. In the PDF equations[1], the unclosed terms are Conditional Dissipation Rate (CDR) and Conditional Laplacian (CL). They are modeled using the Gaussian assumptions. These models are only valid for near-Gaussian distributions. The closure problems for reactive scalars are very similar to the ones in turbulence. Turbulence models are based on Kolmogorov's universal theory of small scale motions. Unfortunately, such a theory does not exist for reactive scalars in random flows. Therefore, one has to adopt some assumptions a priori. For example, the small variance is assumed in the moment approach and the Gaussian closure is assumed in the PDF approach. The assumptions have to be justified.

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The recently developed mapping closure[3,4], lately named as Mapping Closure Approximation (MCA)[5], provides an alternative approach for PDFs without any ad hoc assumption. The main idea of the MCA is to keep track of the evolution of an unknown random field by using a known reference field and a mapping function. The known reference field is usually chosen to be a Gaussian random field, because we understand the properties of the Gaussian closure. The dynamical evolution of the PDF is described by an evolution equation of the mapping function; the latter is obtained directly from the original governing equation under the Gaussian closure. In mapping equations, the unclosed terms, CDR and CL, can be calculated in the successive approximation by the mapping function itself and Gaussian closure so that we do not need any ad hoc models. The recent work on MCA can be found in Refs.[6~10].

The models of CDR and CL have direct applications to Large Eddy Simulation (LES) of turbulent reacting flows. In the LES based on the PDF[11] and conditional moment closure[12], the CDR and CL have to be modeled. Although there are extensive studies on CDR and CL for conserved scalars, there is very little work on CDR and CL for reactive scalars[1]. Unlike conserved scalars, reactive scalars are related with nonlinear reaction, in addition to advection and diffusion. MCA has been shown to be able to predict the CDR and CL for conserved scalars. In this paper we will show that MCA can predict these quantities for reactive scalars. We will use MCA to calculate the PDFs, CDRs and CLs of reactive scalars in random flows. This paper is arranged as follows: in section 2, the MCA approach is described, followed by calculations of the PDFs, CDRs and CLs for both conserved and reactive scalars. The results obtained from MCA are tested quantitatively against computer simulations in section 3. We summarize and discuss the results in section 4.

2 THE MCA APPROACH TO PDF, CDR AND CL

The transport equation for the PDF of reactive scalar can be derived from the advection-diffusion-reaction Eq.(1)

$$\frac{\mathrm{D}P(\phi,t)}{\mathrm{D}t}+\frac{\partial}{\partial\phi}[\kappa\langle\nabla^2\phi|\phi\rangle P(\phi,t)+ S(\phi)P(\phi,t)]=0 \tag{2}$$

Equation (2) includes an unclosed term—Conditional Laplacian (CL) or conditional diffusion

$$\Theta(\phi,t)\equiv\kappa\langle\nabla^2\phi|\phi\rangle \tag{3}$$

Using the test function method, we can also show

$$\langle\nabla^2\phi|\phi\rangle P(\phi,t)=\frac{\partial}{\partial\phi}[\langle(\nabla\phi)^2|\phi\rangle P(\phi,t)] \tag{4}$$

Submitting Eq.(4) into Eq.(2), we obtain an alternative form of the PDF transport equation

$$\frac{\mathrm{D}P(\phi,t)}{\mathrm{D}t}+\frac{\partial^2}{\partial\phi^2}[\kappa\langle(\nabla\phi)^2|\phi\rangle P(\phi,t)]+ \frac{\partial}{\partial\phi}[S(\phi)P(\phi,t)]=0 \tag{5}$$

which includes another unclosed term—Conditional Dissipation Rate (CDR)

$$\chi(\phi,t)\equiv\kappa\langle(\nabla\phi)^2|\phi\rangle \tag{6}$$

In the PDF transport equation, the effects of chemical reactions appear in closed form. This closed form constitutes the primary advantage of the PDF approach over others. However, the unclosed terms, either CDR or CL, still remain to be modelled a priori. The MCA approach is introduced to evaluate the CDR and CL and calculate the PDF.

In the MCA approach, an unknown random field $\phi(\boldsymbol{x},t)$ is represented by a mapping of a known random field $\theta(\boldsymbol{x})$, where $\theta(\boldsymbol{x})$ might be chosen as a homogeneous Gaussian field. Namely, it is assumed that the representation

$$\phi(\boldsymbol{x},t)=X(\theta(\boldsymbol{x}),t) \tag{7}$$

holds true only in the sense of statistics: the unknown random field $\phi(\boldsymbol{x},t)$ has the same statistics, such as PDF and conditional moment, as its surrogate $X(\theta(\boldsymbol{x}),t)$. The representation (7) implies

$$P(\phi,t)=P_0(\theta)\Big[\frac{\partial X(\theta,t)}{\partial\theta}\Big]^{-1} \tag{8}$$

where $P_0(\theta)$ is the Gaussian PDF of θ. The mapping Eq.(7) exists 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[4]. It is also required to be one-to-one and monotonic to ensure that Eq.(8) is correct.

Differentiating Eq.(8) with respect to t yields

$$\frac{\partial P(\phi,t)}{\partial t}+\frac{\partial}{\partial\phi}\Big[\Big\langle\frac{\mathrm{D}X}{\mathrm{D}t}\Big|\phi\Big\rangle P(\phi,t)\Big]=0 \tag{9}$$

The comparison of Eq.(9) with Eq.(2) gives the transport equation of the mapping function X

$$\frac{\partial X}{\partial t} = \kappa\langle\nabla^2\phi|\phi\rangle + \langle S(\phi)|\phi\rangle \tag{10}$$

The conditional moments in Eq.(10) can be evaluated from the mapping function (7) and the Gaussianity for the reference field θ

$$\begin{aligned}\Theta(\phi,t) &= \kappa\langle\nabla^2\phi|\phi\rangle = \kappa\langle\nabla^2 X|\theta\rangle \\ &= \kappa\langle(\nabla\theta)^2\rangle\Big[-\frac{\theta}{\langle\theta^2\rangle}\frac{\partial X}{\partial\theta} + \frac{\partial^2 X}{\partial\theta^2}\Big]\end{aligned} \tag{11}$$

$$\langle S(\phi)|\phi\rangle = \langle S[X(\theta)]|\theta\rangle = S[X(\theta)] \tag{12}$$

Then, the transport equation of the mapping function (7) is

$$\begin{aligned}\frac{\partial X}{\partial t} =& \kappa\langle(\nabla\theta)^2\rangle\Big[-\frac{\theta}{\langle\theta^2\rangle}\frac{\partial X}{\partial\theta} + \frac{\partial^2 X}{\partial\theta^2}\Big] + \\ & S[X(\theta)]\end{aligned} \tag{13}$$

The solution of Eq.(13) can be used to calculate the PDF $P(\theta,t)$ via Eq.(8), the CL $\Theta(\theta,t)$ via Eq.(11) and the CDR $\chi(\theta,t)$ via

$$\begin{aligned}\chi(\phi,t) &= \kappa\langle(\nabla\phi)^2|\phi\rangle \\ &= \kappa\langle(\nabla\theta)^2\rangle\Big[\frac{\partial X}{\partial\theta}\Big]^2\end{aligned} \tag{14}$$

Other statistics, such as mean and variance, can also be calculated using the scalar PDFs. The mapping Eq.(13) plays a key role in the calculation of the scalar statistics. Its numerical algorithms will be discussed in the next section. However, for a conserved scalar, $S = 0$, the mapping Eq.(13) is analytically solvable. The results for initial Gaussian and double-delta distributions are summarized as follows[4,14]:

(1) The initial double-delta PDF

$$P(\phi,0) = \begin{cases} A & \text{if } \phi = 0 \\ 1-A & \text{if } \phi = 1 \\ 0 & \text{if } \phi \neq 0 \text{ or } 1 \end{cases} \tag{15}$$

where $0 \leq A \leq 1$. The corresponding initial mapping function is of the form

$$X(\theta,0) = \begin{cases} 0 & \text{if } \theta \leq \gamma \\ 1 & \text{if } \theta > \gamma \end{cases} \tag{16}$$

where $\gamma = \sqrt{2}\mathrm{erf}^{-1}(2A-1)$. The exact solution of Eq.(13) with the initial condition (16) is solved as

$$X(\vartheta,t) = \frac{1}{2}\Big[1 + \mathrm{erf}\Big(\frac{\vartheta - \gamma\mathrm{e}^{\tau}}{\sqrt{2}\Sigma}\Big)\Big] \tag{17}$$

where

$$\begin{aligned}\vartheta &= \frac{\theta}{\sqrt{\langle\theta^2\rangle}} \\ \tau &= \kappa\frac{\langle(\nabla\theta)^2\rangle}{\langle\theta^2\rangle}t \\ \Sigma &= \sqrt{\exp(2\tau)-1}\end{aligned} \tag{18}$$

Using the solution (17), we can calculate the CDR, CL and PDF

$$\begin{aligned}\chi(\phi,t) &= \kappa\frac{\langle(\nabla\theta)^2\rangle}{\langle\theta^2\rangle}\frac{1}{2\pi\Sigma^2(\tau)}\cdot \\ &\quad \exp\big(-2\big[\mathrm{erf}^{-1}(2\phi-1)\big]^2\big) \\ &= \chi(0.5,t)\exp\big(-2\big[\mathrm{erf}^{-1}(2\phi-1)\big]^2\big)\end{aligned} \tag{19}$$

$$\begin{aligned}\Theta(\phi,t) &= \frac{\kappa}{\sqrt{\pi}}\frac{\langle(\nabla\theta)^2\rangle}{\langle\theta^2\rangle}[1+\Sigma^{-2}(\tau)]\cdot \\ &\quad \exp\big(-2\big[\mathrm{erf}^{-1}(2\phi-1)\big]^2\big)[\mathrm{erf}^{-1}(1-2\phi) - \\ &\quad \sqrt{1-\exp(-2\tau)}\mathrm{erf}^{-1}(1-2\langle\phi\rangle)]\end{aligned} \tag{20}$$

$$\begin{aligned}P(\phi,t) &= \Sigma(\tau)\exp(-[\Sigma(\tau)\mathrm{erf}^{-1}(2\phi-1) - \\ &\quad \mathrm{e}^{\tau}\mathrm{erf}^{-1}(2\langle\phi\rangle-1)]^2 + [\mathrm{erf}^{-1}(2\phi-1)]^2)\end{aligned} \tag{21}$$

(2) The initial Gaussian PDF

$$P(\phi,0) = \frac{1}{\sqrt{2\pi}}\exp\Big(-\frac{\phi^2}{2}\Big) \tag{22}$$

The corresponding initial mapping function is $X(\theta,0) = \theta$. The solution of Eq.(13) is $X(\theta,t) = \theta\exp(-\tau)$. Therefore, the CDR, CL and PDF are calculated as follows

$$\chi(\phi,t) = \kappa\langle(\nabla X)^2|\theta\rangle = \kappa\langle(\nabla\theta)^2\rangle\mathrm{e}^{-2\tau} \tag{23}$$

$$\Theta(\phi,t) = \kappa\langle\nabla^2 X|\theta\rangle = -\kappa\frac{\langle(\nabla\theta)^2\rangle}{\langle\theta^2\rangle}X \tag{24}$$

$$P(\phi,t) = \frac{1}{\sqrt{2\pi}\exp(-\tau)}\exp\Big(-\frac{X^2}{2\exp(-2\tau)}\Big) \tag{25}$$

3 COMPARATIVE ASSESSMENTS OF THE MCA

The objective of this section is to evaluate the performance of the MCA via comparative assessments against the DNS. We performed the DNS for the scalar equation (1) in a cyclic square of side 2π. The Eq.(1) is discretized spatially, using the fourth-order central-finite-difference scheme, with $N = 512$ computational grids. It is integrated in time using an Euler scheme for the first time step and second-order Adams-Bashforth scheme for all subsequent time steps. The incompressible random velocity $\boldsymbol{u}(\boldsymbol{x},t)$ is numerically constructed as an isotropic

and homogeneous Gaussian field of zero mean and unity variance, with a specified energy spectrum $(k/k_0)^4 \exp[-(k/k_0)^2]$, where $k_0 = 4$. The velocity field is temporally frozen for the case that the convection time scale $(\epsilon k^2)^{-1/3}$ is much longer than the diffusion time scale $(\kappa k^2)^{-1}$.

The mapping Eq.(13) is solved by numerical integration, using the same procedure as used in Eq.(1). The boundary conditions for the mapping function X are obtained by extrapolation in the direction of the reference field θ.

The initial conditions are chosen as the Gaussian and double-delta distributions. The former is simulated for random mixing and the latter for binary mixing. The chemical reactions are modelled by the quadratic form of $S(\phi) = -20\phi|\phi|$ and the cubic form of $S(\phi) = -20(\phi^3 - 0.5\phi)$, whose combination represents quite general nonlinear reactions. The molecular diffusion $\kappa = 0.005$ is much smaller than the nonlinear reaction. The models from the MCA are calibrated to a case where nonlinear effects are dominant and the moment approach does not work well.

In the figures, the coordinate axes are re-scaled as follows

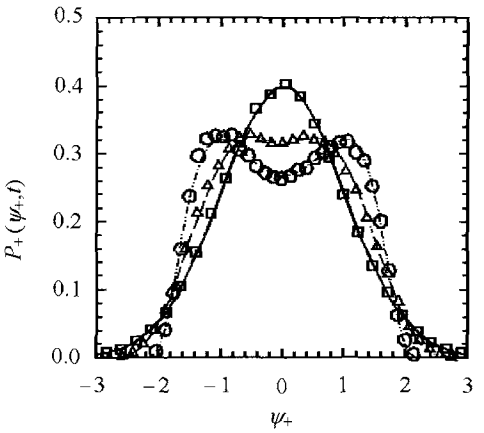
$$\begin{aligned} \Psi_+(\boldsymbol{x},t) &= \frac{\phi(\boldsymbol{x},t) - \langle\phi\rangle}{\sigma(t)} \\ P_+(\phi,t) &= \sigma(t) \cdot P(\phi,t) \\ \Theta_+(\phi,t) &= \frac{\Theta(\phi,t)}{\hat{\Theta}(t)} \\ \chi_+(\phi,t) &= \frac{\chi(\phi,t)}{\hat{\chi}(t)} \end{aligned} \tag{26}$$

where

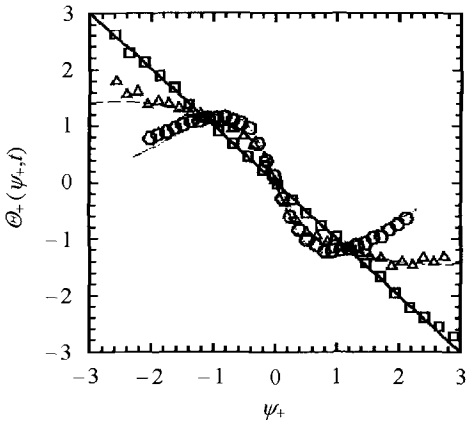
$$\begin{aligned} \sigma(t) &= \langle(\phi - \langle\phi\rangle)^2\rangle^{1/2} \\ \hat{\Theta}(t) &= \Big[\int_{-\infty}^{+\infty} \Theta^2(\phi,t)P(\phi,t)\mathrm{d}\phi\Big]^{1/2} \\ \hat{\chi}(t) &= \int_{-\infty}^{+\infty} \chi(\phi,t)P(\phi)\mathrm{d}\phi \end{aligned} \tag{27}$$

The renormalization implies that an external time scale is used to rescale relaxation time of the mapping function. The time scale can be provided by the variances of the mapping function and its derivative.

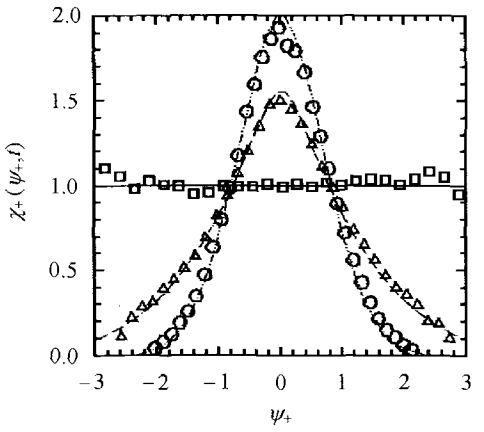
We first make comparative assessments for initial Gaussian scalars. In Figs.1 and 2, the quantities



(a) PDF

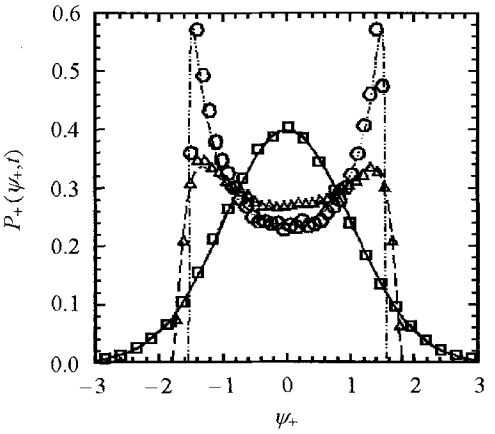


(b) Conditional diffusion

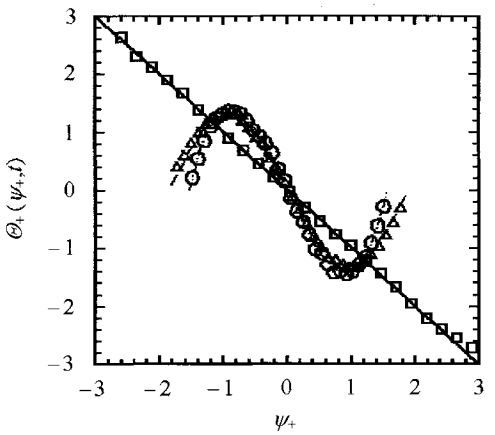


(c) Conditional dissipation rate

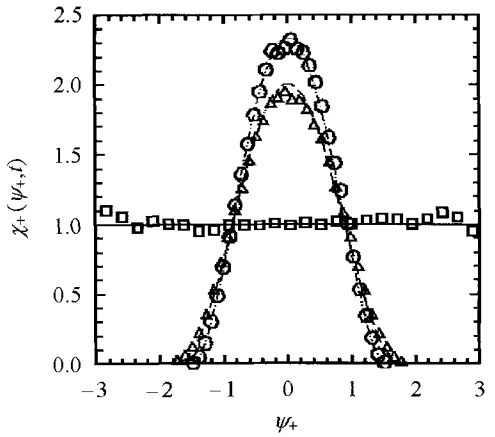
Fig.1 Statistics of the reactive scalar of initial Gaussian field with reaction $S(\phi) = -20\phi|\phi|$. Squares, triangles and circles are for DNS and solid, dash and dash-dotted lines are for MCA at the variances $\sqrt{\langle\phi^2\rangle} = 1.0$, 0.5 and 0.2, respectively



(a) PDF



(b) Conditional diffusion

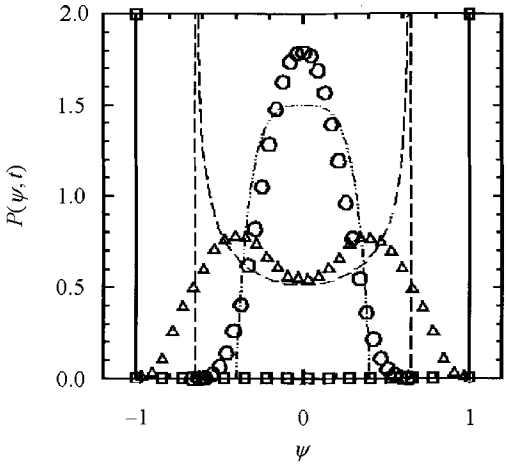


(c) Conditional dissipation rate

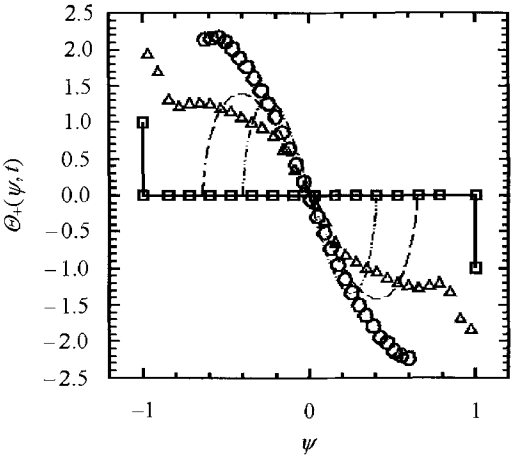
Fig.2 Statistics of the reactive scalar of initial Gaussian field with reaction $S(\phi) = -20(\phi^3 - 0.5\phi)$. Squares, triangles and circles are for DNS and solid, dash and dash-dotted lines are for MCA at the variances $\sqrt{\langle\phi^2\rangle}$ = 1.0, 0.5 and 0.2, respectively

including PDF, CL and CDR are shown for the reactive scalars of the quadratic and cubic nonlinear reactions separately. The nonlinear terms distort their shapes: the PDFs depart from the initial Gaussian distribution and become symmetric β-distribution. The CLs look like sinusoidal distributions due to significant distortions of nonlinear reaction for large ϕ. The CDRs become parabolic instead of being a constant. The results from the MCA are in agreement with those from the DNS, and the nonlinear distortions are well predicted by the MCA.

We further make comparative assessments for initial binary scalars in Figs.3 and 4. Even for the

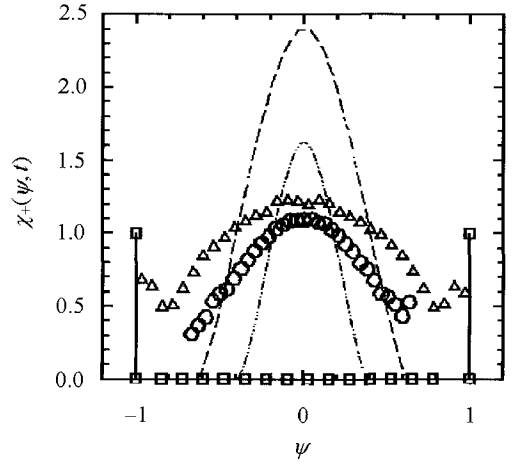


(a) PDF



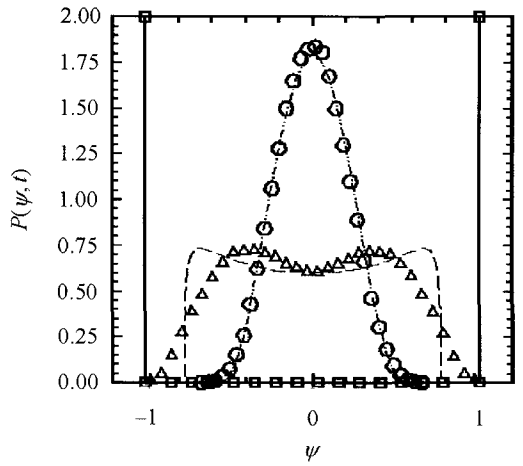
(b) Conditional diffusion

Fig.3 Statistics of the reactive scalar of initial double-delta field with reaction $S(\phi) = -20\phi|\phi|$. Squares, triangles and circles are for DNS and solid, dash and dash-dotted lines are for MCA at the variances $\sqrt{\langle\phi^2\rangle}$ = 1.0, 0.2 and 0.04, respectively

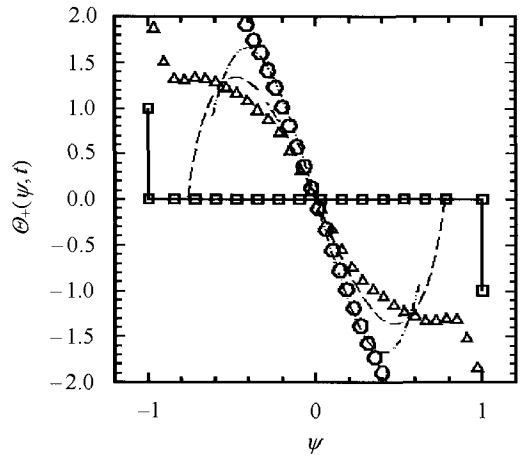


(c) Conditional dissipation rate

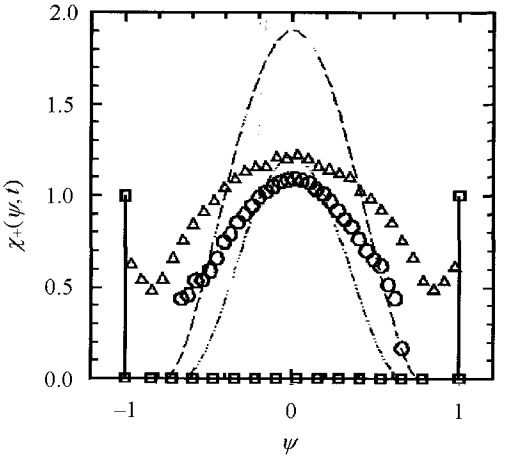
Fig.3 Statistics of the reactive scalar of initial double-delta field with reaction $S(\phi) = -20\phi|\phi|$. Squares, triangles and circles are for DNS and solid, dash and dash-dotted lines are for MCA at the variances $\sqrt{\langle\phi^2\rangle}$ = 1.0, 0.2 and 0.04, respectively (continued)



(a) PDF



(b) Conditional diffusion



(c) Conditional dissipation rate

Fig.4 Statistics of the reactive scalar of initial double-delta field with reaction $S(\phi) = -20(\phi^3 - 0.5\phi)$. Squares, triangles and circles are for DNS and solid, dash and dash-dotted lines are for MCA at the variances $\sqrt{\langle\phi^2\rangle}$ = 1.0, 0.2 and 0.04, respectively

binary initial distributions, the PDFs from the MCA are in good agreement with those from the DNS. The MCA also predicts the evolution of the CLs although there are slight differences in the tails. The MCA predictions of the CDRs are qualitatively correct but with some magnitude differences. The magnitude differences are due to the fact that the current mapping is an amplitude approximation in the sense of a first-order accuracy, which is expected to be improved by a higher-order approximation[5].

The comparative assessments indicate that the MCA can predict the statistics of the initial Gaussian scalars with or without reactions. The MCA predictions of initial binary scalars on PDFs and CLs are also in agreement with those of the DNS, but have some magnitude differences on CDRs with those of the DNS.

4 CONCLUSIONS AND DISCUSSIONS

It is demonstrated that the MCA can be used to describe the statistics of reactive scalars in random flows. Typically, the approach can predict the shapes of the PDFs, CDRs and CLs for both conserved and reactive scalars. In the MCA approach, the effects of reactions are in closed form. Therefore, the MCA can keep track of nonlinear distortions from the reaction terms so that it correctly describes the shapes of the statistics. The rescaling time in the plots implies an external time scale. The time scale could

be provided by the variances of the mapping and its derivative. Therefore, the mapping for the joint PDF of scalar and its derivative is a natural choice for this purpose. Although the present paper is restricted to the quadratic and cubic nonlinear reactions, the MCA can be applied to nonlinear reactions of general forms.

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