Testing multiple mapping conditioning mixing for Monte Carlo probability density function simulations

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Mitarai *et al.* [Phys. Fluids **17**, 047101 (2005)] compared turbulent combustion models against homogeneous direct numerical simulations with extinction/recognition phenomena. The recently suggested multiple mapping conditioning (MMC) was not considered and is simulated here for the same case with favorable results. Implementation issues crucial for successful MMC simulations are also discussed. © *2005 American Institute of Physics*. [DOI: 10.1063/1.2147609]

A number of modern turbulent combustion models have been recently tested[1,2] for a homogeneous combustion case and compared against direct numerical simulations (DNS).[3] This case was selected because the combustion is close to extinction/recognition and is sensitive to all the instantaneous properties of the flow, hence, the case tests the capabilities of turbulent combustion models. The purpose of this paper is to implement and validate the recently suggested multiple mapping conditioning (MMC) model[4] using this case. Probabilistic MMC (Refs. 4–6) is used here with a solitary reference variable that is similar to the mixture fraction. MMC maintains localness of mixing interactions and, effectively, unites many existing models, such as conditional moment closure (CMC),[7] Curl's model,[8] and interaction by exchange with the mean (IEM) or conditional mean (IECM) (Ref. 9) into a single methodology. The scalars that are transported for this case are denoted by $Y_I=\{Z,T\}$, where Z is the mixture fraction and T is the normalized temperature defined as in previous publications[1–3] in terms of the absolute temperature T^0 by $T=(T^0-T^0_\infty)/(T^0_f-T^0_\infty)$ with T^0_∞ representing the inlet temperatures and T^0_f representing the adiabatic flame temperature. The probabilistic MMC transport equations are given by[4–6]

$$dY_I=(S[Y_I]+W_I)dt, \tag{1}$$

$$d\xi=A^0dt+(2B)^{1/2}dw, \tag{2}$$

where $S[Y_I]$ represents the effect of the mixing model, w a Wiener process and W_I the source term: $W_I=\{0,\Omega\}$, where $\Omega=\Omega(Z,T)$ is the reaction source term specified in previous publications.[1] A single-step chemical reaction was considered so this system is characterized by Z and T. The coefficients A^0 and B are selected so that the probability density function (PDF) for the reference variable ξ has a standard Gaussian distribution while the magnitude of $B=B(t)$ is determined to match the required average dissipation rate[4]

$$\langle N\rangle=B\left\langle\left(\frac{\partial\langle Z|\xi\rangle}{\partial\xi}\right)^2\right\rangle. \tag{3}$$

Here, $N=D(\nabla Z)^2$ is the scalar dissipation rate and D is the diffusivity. The drift coefficient becomes[4] $A^0=-B\xi$. The diffusion coefficient B is responsible for the decay of the large-scale unconditional fluctuations $Z'\equiv Z-\langle Z\rangle$ and the (major) time scale associated with this process is $\tau_{\rm maj}\sim 1/B$. A more accurate definition of $\tau_{\rm maj}$ is given by the equation

$$\frac{d\langle(Z')^2\rangle}{dt}=-2\langle N\rangle=-2\frac{\langle(Z')^2\rangle}{\tau_{\rm maj}}. \tag{4}$$

Fluctuating ξ induces fluctuations $\langle Y_I|\xi\rangle$, which are called the major fluctuations in MMC. The stochastic deviations from the conditional values $(Y_I)''\equiv Y_I-\langle Y_I|\xi\rangle$ are called the minor fluctuations. In conditional MMC, the minor fluctuations are minimized to follow the first-order CMC approach, where they are neglected. In probabilistic MMC, which is used here, the minor fluctuations are not negligibly small and play a noticeable role. The minor fluctuations are generated from the major fluctuations and are dissipated by the mixing operator S, where all species are treated in the same manner. The overall balance equation for the minor fluctuations is given by[6]

$$\frac{d\langle(Z'')^2\rangle}{dt}=2B\left\langle\left(\frac{\partial\langle Z|\xi\rangle}{\partial\xi}\right)^2\right\rangle-2\frac{\langle(Z'')^2\rangle}{\tau_{\rm min}}, \tag{5}$$

where the minor dissipation time $\tau_{\rm min}$ characterizes the dissipation rate of the operator S.

In the present work, the modified Curl's model[8] is used for the mixing model S and this version of the MMC model can be referred to as MMC-Curl. The minor dissipation time affects the level of the conditional fluctuations $T'''\equiv T-\langle T|Z\rangle$ that represent an important physical quantity and must not be confused with $T''\equiv T-\langle T|\xi\rangle$ that is defined only in the MMC context. The conventional MMC regime is achieved when $\tau_{\rm min}<\tau_{\rm maj}$. Under these conditions, the parameter B (which is linked to $\tau_{\rm maj}$) is selected to match the overall dissipation rate N, while a proper selection[5,6] of $\tau_{\rm min}$ ensures the appropriate level of T'''. (If $\tau_{\rm min}>\tau_{\rm maj}$, then $\tau_{\rm min}$ determines the overall dissipation rate while the correlation

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between Z and ξ rapidly disappears and, without dependence of Z on ξ, there is no significant difference between the MMC-Curl and Curl's models.)

Under the quasisteady conditions of $d\langle(Z'')^2\rangle/dt=0$, Eqs. (3)–(5) yield

$$\langle N\rangle = \langle(Z')^2\rangle/\tau_{\mathrm{maj}} = \langle(Z'')^2\rangle/\tau_{\mathrm{min}},$$

that is,

$$\frac{\tau_{\mathrm{min}}}{\tau_{\mathrm{maj}}} = \frac{\langle(Z'')^2\rangle}{\langle(Z')^2\rangle}. \tag{6}$$

The initial distribution of Z must have the correct level of conditional fluctuations $\langle(Z'')^2\rangle$ as required when their quasisteady state is reached. Physically, if the streams have mixed, conditional fluctuations have been generated, so that if the initial state of the simulation is taken after some mixing has occurred, in order to recreate this state correctly, the conditional fluctuations must also be correctly recreated. If this is not done, the initial period would be consumed with generating conditional fluctuations while the dissipation would not reach the required level during this period. Thus the intensity of mixing is underpredicted until equilibrium is reached, hence the decay rate of the unconditional variance is also underpredicted. The initial level of conditional fluctuations $\langle(Z'')^2|\xi\rangle=\langle N|\xi\rangle\tau_{\mathrm{min}}$ can be set by randomly altering particles' positions in ξ space (after Y_I is assigned) by $\Delta\xi$ so that P_ξ is satisfied. The localized dispersion in ξ space may be approximated by

$$\langle\Delta\xi^2|\xi\rangle \approx \langle(Z'')^2|\xi\rangle \left\langle \left(\frac{\partial\langle Z|\xi\rangle}{\partial\xi}\right)^2 \middle| \xi \right\rangle^{-1}. \tag{7}$$

This approximation is only valid where the derivative is significant; note that adjustment of ξ is not needed in those regions where this is not the case.

In the DNS,[3] the mixture fraction (whose mean was $\langle Z\rangle=1/2$) was initialized as blobs of pure fuel ($Z=1$) and oxidizer ($Z=0$) that mix for a short time before an igniter brings the mixture to chemical equilibrium. The initial physical singularity of the mixture fraction gradients is reflected in MMC by the initial rapid change of $\langle Z|\xi\rangle$ from 0 to 1 near $\xi=0$. For simulations performed here, the number of particles was $n_p=172\,800$ as in the preceding simulations.[2] The computational time step was divided into three fractional steps. The solution order of the fractional steps, with each substep using information from the preceding substeps, was transport in ξ space, mixing of Y_I using S (using the new values of ξ) and the chemical reaction for T. The chemical reaction used is fully defined in Mitarai *et al.*[2] For the mixing substep, pairs of stochastic particles were selected so that their spacing in reference space ξ was small, thus preserving the localness of MMC. Care must be taken that particles do not repetitively mix with only one other particle since they will reach their mean values of scalars after few time steps and would not dissipate any further. For the chemical reaction, a stiff ODE solver was used, with the rate of change of variables being the sum of the chemical reaction rate and the rate from the finite difference of the states before and after the (conservative) mixing substep.

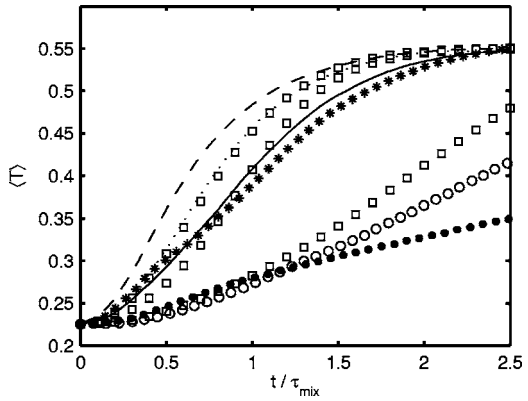

FIG. 1. Mean temperature results $n_p=172800$. MMC (lowest to highest: $\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}=1/1.05$, $1/8$, and $1/100$), □. DNS (Ref. 3), —. Other models (Ref. 2): EMST, ∗; CMC, ···; Curl's model, ○; IEM, ●; FCL, --.

The ratio $\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}$ defined using Eq. (6) was fixed during each individual simulation and different values were used to implement MMC across its suite of applicability with the expectation that the CMC[7] limit is attained at one extreme ($\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}\to 0$) and Curl's model at the other ($\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}\sim 1$). One goal of this work is to learn what value of the ratio corresponds to practical results. Results for the mean temperature are in Fig. 1 showing the selected time scale ratio that best matched the DNS data overall ($\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}=1/8$). Also shown are results that clearly approach the CMC limit ($\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}=1/100$) and Curl's model ($\tau_{\mathrm{min}}/\tau_{\mathrm{maj}}=1/1.05$). The stoichiometric temperature is plotted in Fig. 2. The mechanical mixing time scale, τ_{mix}—based on the scalar dissipation rate—is used to normalize the temporal axis. This quantity was used to be consistent with the reporting of other results[2] and played no part in the MMC modeling.

The Lagrangian modified flamelet model,[1] which has been specifically suggested to treat this case, matched the reported averaged temperatures from the DNS (Ref. 3) the best (the curve virtually coincides with the DNS curve so is not shown in Fig. 1). However, the simplified conditions near the bounds of Z space lead to particles in the middle of Z space not completely extinguishing. We tested MMC and the results from all other models were taken from Mitarai *et al.*[2] Among general mixing models, the EMST model[10] predicted

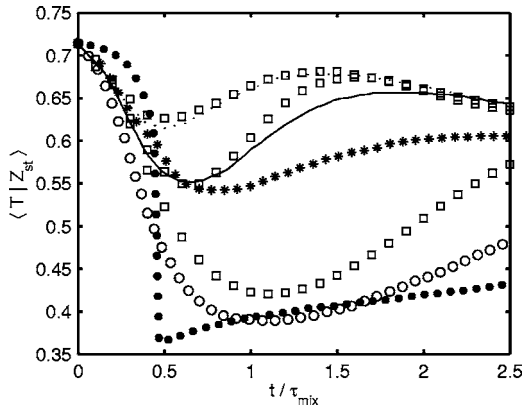

FIG. 2. Stoichiometric temperature results. As per Fig. 1.

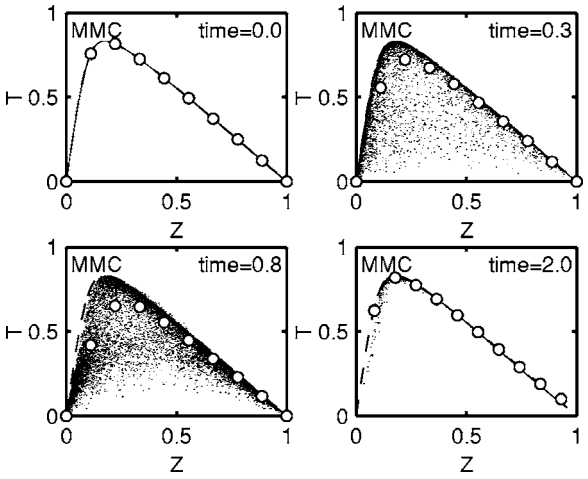

FIG. 3. Scatter plots of $T(Z)$ for $\tau_{min}/\tau_{maj}=1/8$ (showing 16384 particles). Conditional averages, ○; equilibrium temperature, --.

the mean temperature well[2]—as did MMC at $\tau_{min}/\tau_{maj}=1/8$—but MMC performed somewhat better in predicting the stoichiometric temperature by reproducing the correct shape. All other models [first-order CMC, IEM, Curl's, and fast chemistry limit (FCL)] cannot adequately predict the DNS results for this difficult case. The main source of difference between the models is the different levels of simulated conditional fluctuations T‴, which is nonexistent in first-order CMC and is overpredicted by Curl's model. The other models (IEM and FCL) are too simple to predict the complex phenomena occurring. The capability of MMC may be seen from observation of the scatter plots (Fig. 3) which are very similar to those produced by the DNS.[3] Those generated by EMST indicate strange behavior since the scalars are not treated independently, causing mixing between particles along preferential lines.[2] Different realizations of the mean temperature, which seem to be typical, are shown in Fig. 4 for varying numbers of particles. The convergence of the method for large n_p is clear.

Localness is one of the major advantages of MMC over the conventional mixing models (IEM and Curl's). MMC

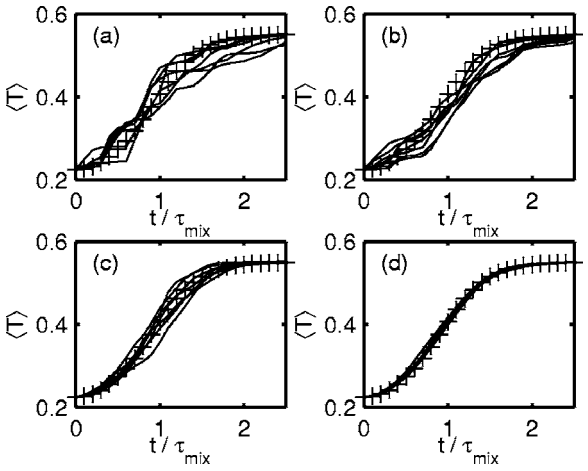

FIG. 4. Sample realizations of mean temperature. $n_p=172800$, +; (a) $n_p=8$; (b) 20; (c) 100; (d) 1000.

defines locality in terms of the reference variables in a way that preserves independence of the simulated scalars. The minor fluctuations are treated in MMC by conventional mixing models that are not local in their usual formulations. The EMST model has a more strict definition of locality using the scalar values themselves but this makes mixing of different scalars dependent on each other. In general, MMC is expected to work well under conditions when localness is not grossly violated by the approximate treatment of the simulated problem. While no model can be implemented without compromising localness due to the discrete nature of nodes or stochastic particles, MMC's compromise in its treatment of localness does not allow any completely nonlocal interactions to occur.

The problem considered in the present work involves a rapid initial change of Z in the reference space that can allow two particles with quite different values of Z (but similar values of ξ) to be mixed. The initial singularity disappears as the simulations advance in time. Thus, the localness is compromised to a larger extent at the initial stages (compared to the final stages) even if the value of τ_{min}/τ_{maj} remains constant. The less local treatment of mixing in MMC skews the results towards Curl's model and overpredicts the level of the conditional fluctuations T‴ while the more local treatment shifts the curves towards CMC and underpredicts the level of T‴. This behavior can be noticed in Fig. 1 and, after careful comparison of the scatter plots with the DNS,[3] in Fig. 3. A more accurate evaluation of the ratio τ_{min}/τ_{maj}, which may change in time and should be selected to match the level of conditional fluctuations,[5,6] will remove the bias. The physical behavior of the conditional fluctuations [such as T‴] in reacting systems needs further examination. Another difficulty can appear due to dependence of the conditional generation on reaction rates, with fast reactions suppressing the generation and reducing the effective generation time.[5,6,11] According to analysis,[11] universal modeling of the conditional generation may need explicit and accurate emulation of the Lagrangian behavior of the scalar dissipation.

The MMC model has been shown to perform well (provided the ratio τ_{min}/τ_{maj} is properly selected) for a combustion case that is close to extinction, with no unusual behavior observed in its scatter plots. In determining the appropriate ratio τ_{min}/τ_{maj}, the rate of generation of conditional variance is important. The correct selection of this ratio will be important depending on the relative importance of the chemical processes to the mixing processes—it is especially important in cases such as that simulated here, where partial extinction occurs. Effectively, MMC unites most major turbulent combustion models (CMC, Curl's, and IECM) into a combined, consistent approach.

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