Monte-Carlo implementation of mapping closures: application to chemical reacting flows

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1. Motivation and objectives

1.1 Motivation

A promising approach for solving chemical reacting turbulent flows is to use the one-point probability density function (PDF) of the fields of interest (Lundgren, 1969). The main advantage of the PDF methods lies in the chemical terms being closed (Dopazo & O'Brien, 1974; Pope, 1985). The PDF gives as much information as the statistical moments of every order, but the price paid is a much more complicated equation. In every point of space and time, we have to know a function of several variables, the PDF, instead of a handful of numbers representing the statistical moments. In order to solve numerically such an equation with so many variables, Monte-Carlo methods are most suitable and have allowed the solution of flows of industrial interest (Pope, 1985; Haworth *et al.*, 1990).

The major stumbling block in the PDF formulation is to close the diffusion term. A new family of models, the mapping closures (Chen *et al.*, 1989), seems to be very promising overcoming this difficulty. Notice, however, that an external characteristic dissipation time has to be provided. Monte-Carlo methods have been suggested to implement the one-scalar mapping closure for diffusion in homogeneous turbulence. But they have not been able to properly treat complex chemical reactions because the mapping affects the whole equation and greatly complicates the chemical terms, a defect shared by any other scheme in the multispecies case (Pope, 1991). A fractional step technique (Yanenko, 1971) is used to solve this problem.

1.2 Objectives

The first objective of this research is to solve the PDF equation of one reacting scalar in a constant density homogeneous turbulent field with a Monte-Carlo technique, using a mapping closure for the diffusion term. The second objective is to solve a similar problem for the multispecies case. The choice of a suitable method to calculate the needed characteristic time-scale should follow the accomplishment of these two objectives. Further extensions to more complex flows are also the aim of this research.

2. Accomplishments

The single-scalar case has been solved and is explained in the rest of this section. The multispecies case is still under development. Although there are some preliminary results for the latter case, more work is required before it can be published.

2.1 Background

Let $c(\mathbf{x}, t)$ be a reacting scalar field that obeys the equation (for constant density)

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \kappa \nabla^2 c + S(c), \tag{1}$$

where $\mathbf{u}$ is the turbulent velocity field, κ is the molecular diffusivity coefficient, $S(c)$ is a unimolecular chemical source term, and $\mathbf{x}$ and t denote the space and time variables respectively. Both c and $\mathbf{u}$ are statistically homogeneous.

The equation for the scalar PDF $P_c(\psi; t)$ is (Dopazo & O'Brien, 1974)

$$\frac{\partial P_c}{\partial t} = -\frac{\partial}{\partial \psi} \left[\langle \kappa \nabla^2 c \mid c = \psi \rangle P_c \right] - \frac{\partial}{\partial \psi} \left[S(\psi) P_c \right], \tag{2}$$

where ψ stands for c in the probability space and $\langle \mid c = \psi \rangle$ means expected value conditioned on $c = \psi$. Notice that the chemical term is closed in this formulation, while the mixing one remains open.

A monotonically increasing mapping X can be defined between a time independent zero-mean one-variance isotropic multivariate Gaussian reference field $c_0(\mathbf{x})$ and a surrogate scalar field $c^s(\mathbf{x}, t)$:

$$c^s(\mathbf{x}, t) = X\left(c_0(\mathbf{x}); t\right). \tag{3}$$

The mapping closure assumption identifies all the statistics of the surrogate and real fields (Pope, 1991), i.e. $\left\langle |\nabla c^s|^2 \right\rangle$ would be equal to $\left\langle |\nabla c|^2 \right\rangle$.

It is straightforward to show that X obeys the equation (Chen *et al.*, 1989)

$$\frac{\partial X}{\partial t} = \kappa \left\langle |\nabla c_0|^2 \right\rangle \left[-\frac{\psi_0}{\langle c_0^2 \rangle} \frac{\partial X}{\partial \psi_0} + \frac{\partial^2 X}{\partial \psi_0^2} \right] + S(X), \tag{4}$$

where $\left\langle |\nabla c_0|^2 \right\rangle$ can be related to $\left\langle |\nabla c|^2 \right\rangle$ using the chain rule on equation(3) (Chen *et al.*, 1989)

$$\left\langle |\nabla c|^2 \right\rangle = \left\langle \left(\frac{\partial X}{\partial c_0} \right)^2 \right\rangle \left\langle |\nabla c_0|^2 \right\rangle. \tag{5}$$

It should be noted that the scalar dissipation rate, $\varepsilon_c \equiv \left\langle \kappa |\nabla c_0|^2 \right\rangle$ or some related quantity, as a characteristic variance dissipation time, has to be provided by some other means, for example, using the standard k-ε equations.

The relation between the PDF of the reference field $P_{c_0}(\psi_0)$ and that of the real one is (Chen *et al.*, 1989)

$$P_c(\psi; t) = P_{c_0}(\psi_0) \left(\frac{\partial X}{\partial \psi_0} \right)^{-1}. \tag{6}$$

We need to solve the mapping equation (4), and equation (6) will provide us with the solution for P_c. Gao has solved the mapping equation analytically for

non-reacting flows (Gao, 1991), but an analytical solution is not possible for the general reacting case.

2.2 Monte-Carlo implementation

A Monte-Carlo method which numerically solves equations (2) and (4) is described next. The approach for obtaining P_c is slightly different from that employed in the previous section. The fractional step method is applied to equation (2), solving first the chemical term, which is closed, and then the mixing one using an inert scalar mapping closure. Equation (6) will not be employed.

2.2.1 Chemical fractional step

The real scalar PDF $P_c(\psi; t)$ is represented by N stochastic particles with scalar values $c^{(i)}(t)$,

$$P_c(\psi; t) = \frac{1}{N} \sum_{i=1}^{N} \delta\left(\psi - c^{(i)}(t)\right). \tag{7}$$

The chemical term in equation (2) yields for $c^{(i)}$ the evolution equation (Pope, 1985)

$$c_{(1)}^{(i)}(t + \Delta t) = c_{(1)}^{(i)}(t) + S\left(c_{(1)}^{(i)}(t)\right)\Delta t, \tag{8}$$

where the scalar subindex indicates the current fractional step, '1' in this case. The new values obtained for the stochastic particles from the previous equation will be the initial values for the next fractional step, i.e., in the next subsection we take $c_{(2)}^{(i)}(t) \equiv c_{(1)}^{(i)}(t + \Delta t)$.

2.2.2 Mixing fractional step

In this fractional step the mixing term, closed by the mapping equations of the section 1 (with the chemical term removed), is considered. First, $X(\psi_0; t)$, the mapping at the beginning of this fractional step, has to be set. To do so, a static Gaussian reference field is represented. This is done by N sorted particles $c_0^{(j)}$ obtained at the very beginning by a normalized Gaussian number generator. After sorting the N particles $c_{(2)}^{(j)}$ representing the real PDF (or surrogate PDF, both fields have the same one-point probability density function), X is set as a discretized function

$$cmin = X(-\infty; t),$$
$$c^{(j)}(t) = X\left(c_0^{(j)}; t\right), \quad j = 1, \ldots, N, \tag{9}$$
$$cmax = X(\infty; t),$$

where the '2' subindex is dropped for easier reading, $cmax$ and $cmin$ are the upper and lower bounds respectively for the real scalar field, and j indexes are (and will be) used to indicate that particles are sorted.

We want to obtain $X(\psi_0; t + \Delta t)$, the mapping at the end of this fractional step, that will allow us to obtain the new real field, by means of the equation (9) applied at $t + \Delta t$.

Using the same idea of Valiño *et al.*(1991), we define a distribution function $F(\psi_0;t)$ as

$$F(\psi_0;t) = \frac{X(\psi_0;t) - cmin}{cmax - cmin}.$$ (10)

Its ψ_0 derivative, $f(\psi_0;t)$, is a PDF, and from the previous equation,

$$f(\psi_0;t) = \frac{\partial X(\psi_0;t)}{\partial \psi_0}\left(cmax - cmin\right)^{-1}.$$ (11)

The PDF $f(\psi_0;t)$ can be represented (see equation (7)) by N particles $c_f^{(j)}(t)$ that are obtained from N uniform distributed random particles $v^{(j)}$ by (Abramowitz, 1965)

$$c_f^{(j)}(t) = F^{-1}(v^{(j)};t), \quad j = 1,\ldots,N,$$ (12)

where discretized F is known at t from equations (9) and (10), and linear interpolation can be used when needed.

We want to know $c_f^{(j)}(t + \Delta t)$, the representation of $f(\psi_0;t + \Delta t)$. From their value, we will be able to determine X at $t + \Delta t$.

Taking ψ_0 derivatives in equation (4) (with the chemical term removed), yields (Valiño *et al.*, 1991)

$$\frac{\partial f}{\partial t} = \kappa \left\langle |\nabla c_0|^2 \right\rangle \left[-\frac{1}{\langle c_0^2 \rangle} \frac{\partial}{\partial \psi_0}(\psi_0\, f) + \frac{\partial^2 f}{\partial \psi_0^2} \right].$$ (13)

Equation (13) is the transport equation for a Langevin diffusion process. Notice that keeping the chemical term in the equation would yield an impracticable nonlinear integro-differential equation.

The values of $c_f^{(j)}(t + \Delta t)$ can be deduced now from the previous equation (Valiño & Dopazo, 1991):

$$c_f^{(i)}(t + \Delta t) = c_f^{(i)}(t) + \frac{\kappa \left\langle |\nabla c_0|^2 \right\rangle}{\langle c_0^2 \rangle} c_f^{(i)}(t)\, \Delta t + \left(2\,\kappa \left\langle |\nabla c_0|^2 \right\rangle \Delta t\right)^{1/2} \xi^{(i)}(t),$$ (14)

where $\xi^{(i)}$ is a normalized Gaussian variable, chosen independently at every time step. The value of $\left\langle |\nabla c_0|^2 \right\rangle$ is deduced from the provided external characteristic time and equation (5), smoothing the mapping derivative obtained from the discretized mapping by central differences.

Notice that $F(\psi_0;t + \Delta t)$ is the integral of $f(\psi_0;t + \Delta t)$, so it can be represented as

$$F(\psi_0;t + \Delta t) = \frac{1}{N}\sum_{i=1}^{N} H\left(\psi_0 - c_f(t + \Delta t)^{(i)}\right),$$ (15)

where H stands for the Heaviside function,

$$H(x) = \left\{ \begin{array}{ll} 0 & x < 0 \\ 1 & x \geq 0 \end{array} \right\}.$$

From equations (10) and (15), we can get a set of discretized values of X at $t + \Delta t$

$$cmin = X(-\infty; t + \Delta t),$$
$$cmin + (cmax - cmin)v^{(j)} = X\left(c_f^{(j)}(t + \Delta t); t + \Delta t\right), \quad j = 1, \ldots, N, \quad (16)$$
$$cmax = X(\infty; t + \Delta t).$$

Finally, using equation (9),

$$c^{(j)}(t + \Delta t) = X\left(c_0^{(j)}; t + \Delta t\right), \quad j = 1, \ldots, N, \quad (17)$$

we get the new values representing $P_c(\psi; t + \Delta t)$. Linear interpolation for X can be used when needed.

2.3 Numerical results

A Monte-Carlo code has been developed following the previous ideas. Its results have been tested against different set of DNS data, for inert, linear reacting, and second order reacting scalars and for different Damkhöler numbers (Da). Details about the DNS can be found in the work by Valiño & Gao (1991).

In all cases, 10^5 sample points have been taken, although 10^4 are enough to grasp the low order moment statistics. Every time-step takes 1.5 seconds CPU time on a Cray Y-MP, running on one processor. A two eddy-turnover time run requires about 1200 time-steps of size $[100 \max{(\omega_q, \omega_c)}]^{-1}$, where ω_c and ω_q are characteristic frequencies for scalar dissipation and reaction, respectively. The definitions of these quantities are

$$Da = \omega_q/\omega_c,$$
$$\omega_c = \frac{\varepsilon}{\langle c'^2 \rangle / 2},$$
$$\omega_q = -k_c \, c^{n-1},$$

where n equals to 1 (linear reaction) or 2 (second order reaction), k_c is the reaction constant and c' denotes the fluctuating part of the scalar. The definition and values of the eddy-turnover time, l/u, used to non-dimensionalize the time, can be found in the cited article by Valiño & Gao (1991).

To empirically prove the convergence of this numerical method, several runs of the code have been made, randomly choosing in every time step the order of the fractional steps, and the results compared to those obtained when prescribing this order. The results were indistinguishable. It should also be remarked that Monte-Carlo methods converge as $1/N^{(1/2)}$ and that the CPU time requirement for the

present implementation varies practically linearly with the number of stochastic particles. For most practical purposes, 10^4 particles are enough, and the CPU time required per time-step in this case is 0.15 seconds.

Figures 1 to 10 show the comparisons between Monte-Carlo and DNS results. Although the height of the PDF's peaks are slightly underpredicted when the mixing is dominant (and hence the effects of the mapping closure), the agreement is remarkable. The means and variances predicted reproduce the DNS results. It is remembered that the characteristic frequency was chosen to fit the data of the inert scalar run, and it has the same value in all cases.

In the inert scalar case, the skewness and flatness predicted by the mapping clearly tend to the Gaussian values, but the DNS data flatness overshoots the corresponding Gaussian value of 3. Eswaran and Pope (1988) observed the same behavior in their simulations, and they claimed that the flatness returns to 3 after a few more eddy-turnover times. This overshooting cannot be reproduced by the mapping closure in its current form (and, logically, by its Monte-Carlo implementation), which implies an asymptotic relaxation without crossing the Gaussian values. A similar kind of behavior can be observed in the reacting case. The Monte-Carlo calculation of skewness shown in figure 9 indicates a slightly greater tendency to recover the zero values than indicated by DNS data. The flatness evolutions predicted by the Monte-Carlo simulations in figure 10 show a more steady path towards Gaussianity without any kind of oscillation. A new mapping closure model now under development is supposed to overcome this difficulty (Gao & Kraichnan, 1991).
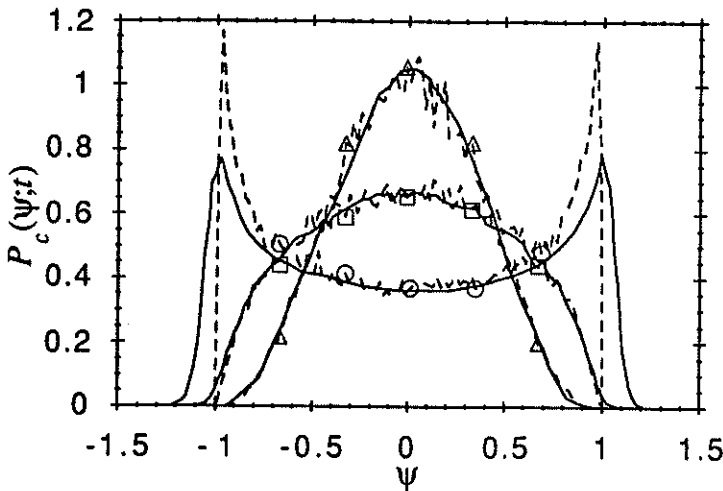

FIGURE 1.   Comparison of the PDF's predicted by the Monte-Carlo mapping closure ($-\!\!\circ\!\!-$ $tu/l = 0.22$; $-\!\!\Box\!\!-$ $tu/l = 0.42$; $-\!\!\triangle\!\!-$ $tu/l = 0.62$) with those obtained by Eswaran and Pope's DNS ($-\!\!\!-\!\!\!-$ $tu/l = 0.22$; 0.42; 0.62).
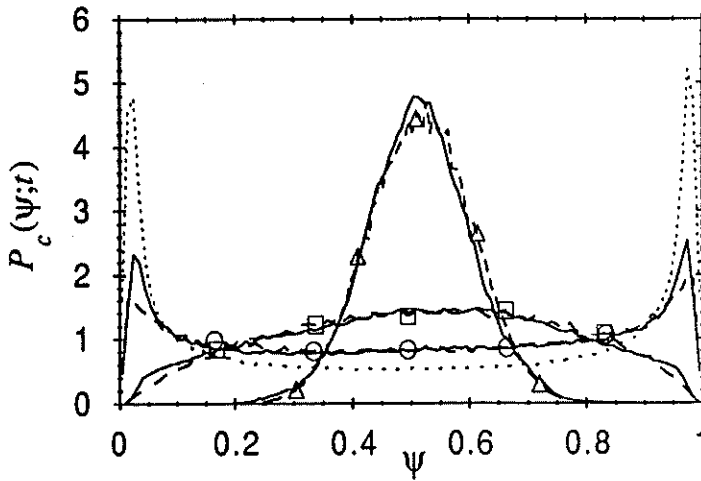
FIGURE 2.   Comparison of the PDF's predicted by the Monte-Carlo mapping closure $(-\!\!\circ\!\!-\ tu/l\ =\ 0.24\ ;\ -\!\!\circ\!\!-\ tu/l\ =\ 0.71\ ;\ -\!\!\triangle\!\!-\ tu/l\ =\ 2.08)$ with those obtained by DNS data $(\cdots\cdots tu/l\ =\ 0.00\ ;\ \rule{1cm}{0.4pt}\ tu/l\ =\ 0.24;0.71;2.08)$. Inert scalar.
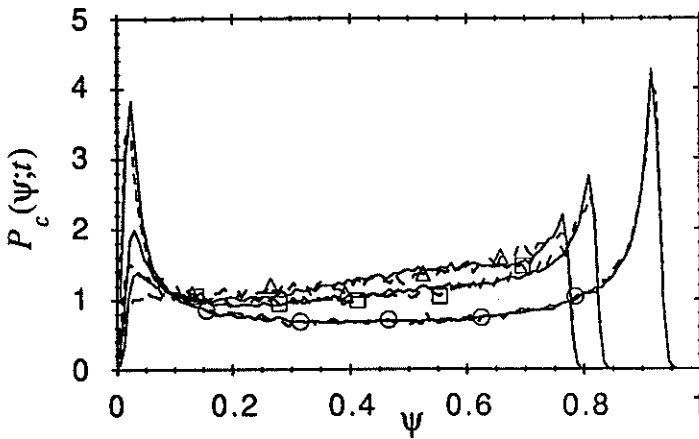

FIGURE 3.   Comparison of PDF's predicted by the Monte-Carlo mapping closure for three early times $(-\!\!\circ\!\!-\ tu/l\ =\ 0.06\ ;\ -\!\!\circ\!\!-\ tu/l\ =\ 0.19\ ;\ -\!\!\triangle\!\!-\ tu/l\ =\ 0.25)$ with those obtained by DNS $(\rule{1cm}{0.4pt}\ tu/l\ =\ 0.06;\ 0.19;\ 0.25)$. Da $=\ 0.275$.
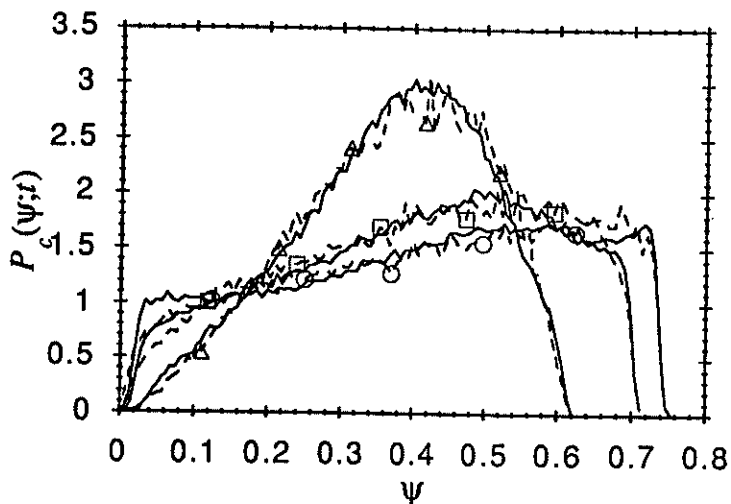
FIGURE 4.   Comparison of PDF's predicted by the Monte-Carlo mapping closure for three later times ($-\text{o}-$ $tu/l = 0.31$; $-\text{e}-$ $tu/l = 0.37$; $-\text{a}-$ $tu/l = 0.55$) with those obtained by DNS ($\underline{\qquad}$ $tu/l = 0.31$; 0.37 ; 0.55). $Da = 0.275$.
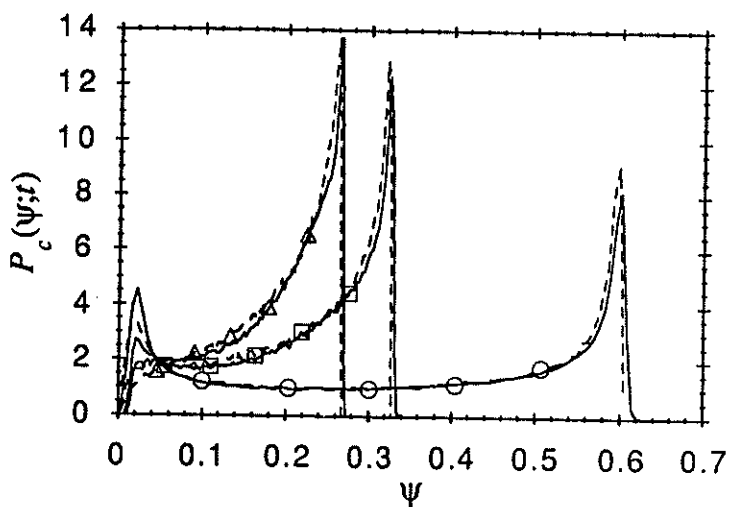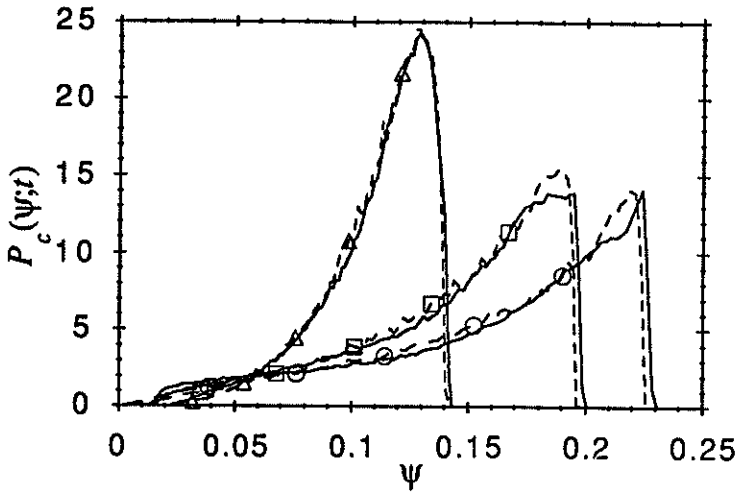

FIGURE 5.   Comparison of PDF's predicted by the Monte-Carlo mapping closure for three early times ($-\text{o}-$ $tu/l = 0.06$; $-\text{e}-$ $tu/l = 0.19$; $-\text{a}-$ $tu/l = 0.25$) with those obtained by DNS ($\underline{\qquad}$ $tu/l = 0.06$; 0.19 ; 0.25). $Da = 2.75$.

FIGURE 6. Comparison of PDF's predicted by the Monte-Carlo mapping closure for three later times ($-\!\circ\!-$ $tu/l = 0.31$; $-\!\circ\!-$ $tu/l = 0.37$; $-\!\triangle\!-$ $tu/l = 0.55$) with those obtained by DNS (——— $tu/l = 0.31$; 0.37 ; 0.55). Da = 2.75.
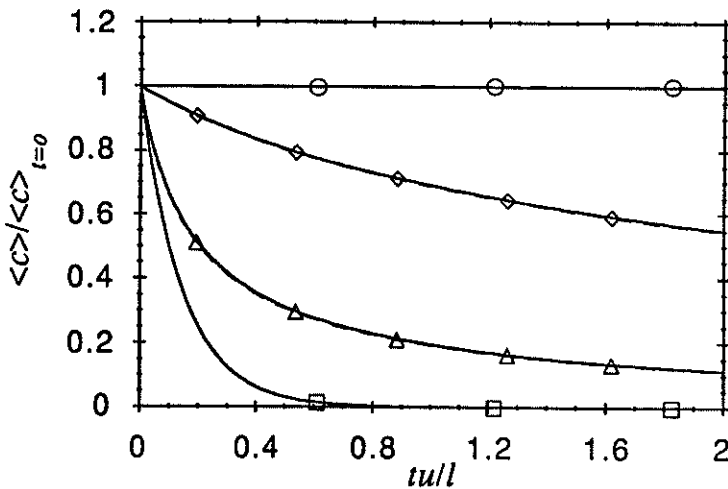

FIGURE 7. Comparison of the scalar mean evolutions predicted by the Monte-Carlo mapping closure for different reactions ($-\!\circ\!-$ none ; $-\!\circ\!-$ linear Da=5.5 ; $-\!\diamond\!-$ second order Da=0.275 ; $-\!\triangle\!-$ second order Da=2.75) and those obtained by DNS data (——— all cases).
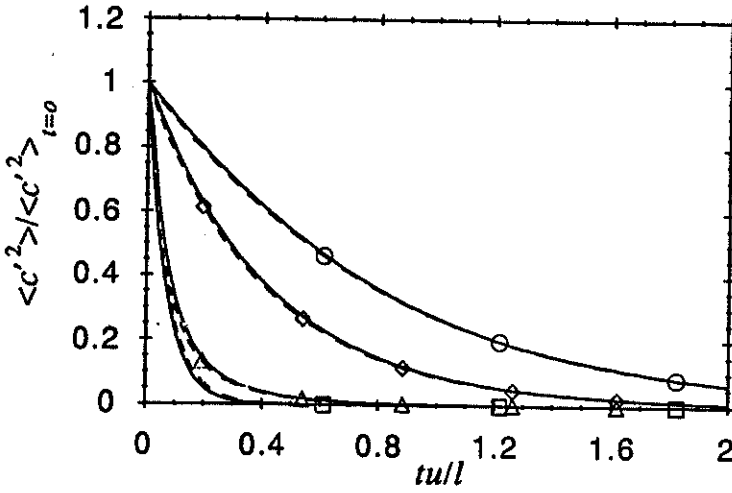
FIGURE 8.   Comparison of the scalar variance evolutions predicted by the Monte-Carlo mapping closure and those obtained by DNS. Same cases as figure 7.
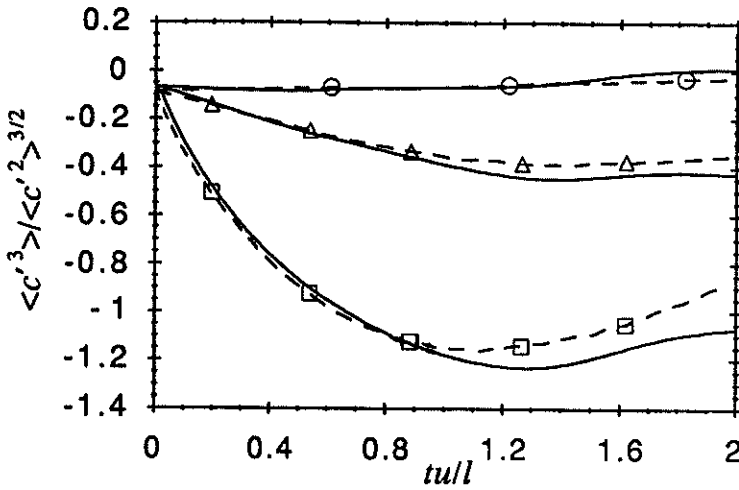

FIGURE 9.   Comparison of the scalar skewness evolutions predicted by the Monte-Carlo mapping closure for different reactions ($-\!-\!\circ\!-$ none ; $-\!-\!\triangle\!-$ second order Da=0.275 ; $-\!-\!\square\!-$ second order Da=2.75) and those obtained by DNS (———— all cases).
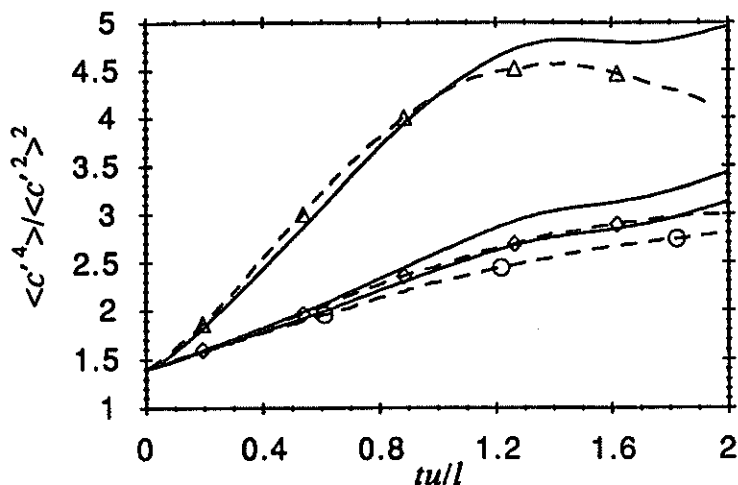
FIGURE 10. Comparison of the scalar flatness evolutions predicted by the Monte-Carlo mapping closure and those obtained by DNS. Same cases as figure 9.

2.4 Summary

A fractional-step Monte-Carlo technique has been used to predict the evolution of a single-scalar PDF with chemical reaction, using a mapping closure for single inert scalar diffusion to solve the fractional-step corresponding to the mixing term. A code has been developed and its numerical results (mean, variance, skewness, flatness, and PDF) have been tested against DNS data obtained using modified versions of Rogallo's code (Eswaran & Pope, 1988; Gao, 1990). The needed characteristic time was chosen to fit the variance of the non-reacting case. Comparisons have been done for the double delta initial PDF case and different Damkhöler numbers in forced homogeneous turbulence. The agreement is remarkable. An interesting point is the difference between the steady tendency to Gaussianity shown by the mapping predictions and the more erratic shown by the DNS. The CPU times needed have been high, but still reasonable, showing the computational feasibility of this technique.

3. Future plans

The extension of this methodology to several scalar PDF might be possible, although the increasing dimensionality of the mappings with the number of scalars (Pope, 1991; Gao & O'Brien, 1991) will greatly complicate the implementation. A simpler multispecies diffusion closure based on the single-scalar mapping closure is under development. This closure will make the problem much easier. The next step will be the extension to homogeneous cases allowing mean gradients. Finally, a $k - \epsilon$

model or the two particles Durbin's Lagrangian model may provide the characteristic time or, alternatively, the new mapping by Gao and Kraichnan (1991) may be considered.

Acknowledgements

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