

Transported PDF modeling of turbulent nonpremixed combustion

By Chong M. Cha

1. Motivation and objectives

In moment methods of predicting turbulent combustion (Klimenko & Bilger 1999), closure of the nonlinear chemical source term presents the most difficult modeling challenge. In contrast, the products of the state-space variables pose no explicit closure problem in the transport equation for the joint PDF $p_{\psi\theta}$ of the reacting scalars, ψ , and the normalized temperature, θ (Dopazo 1994):

$$\frac{\partial}{\partial t} p_{\psi\theta}(\phi; t) = \sum_j^{N_s+1} \frac{\partial}{\partial \psi_j} [\dot{s}(\phi) - \langle \mathcal{D} \nabla^2 \psi_j | \psi = \phi \rangle] p_{\psi\theta}, \quad (1.1)$$

where statistical homogeneity has been assumed for simplicity. Here, $\psi = (\psi_1, \dots, \psi_{N_s})$ is a vector representing the concentrations of the N_s number of reacting species in the system; $\phi = (\phi_1, \dots, \phi_{N_s}, \phi_{N_s+1})$ are the corresponding sample space variables for ψ and θ ; \mathcal{D} is the molecular diffusivity, assumed equal for all species; and \dot{s} is the chemical source term, a known function of the ψ and θ sample space. The notation “ $\langle A | B \rangle$ ” represents the average of A conditional on the event B . The transported PDF equation (1.1) is derived from the exact transport equations of $\psi(\mathbf{x}, t)$ and $\theta(\mathbf{x}, t)$ (O'Brien (1980) gives a good, detailed description of the derivation). Because no multi-point information exists at this single-point level, the molecular diffusion term in Eq. (1.1) must be modeled to obtain closure.

Due to the high-dimensionality of the transported PDF equation for practical engineering flows, where N_s can be large, Monte Carlo methods have been developed by Pope and co-workers (Pope 1990) to efficiently integrate Eq. (1.1). For closure, particle interaction mixing models are used to describe molecular diffusion by prescribing a mixing frequency between the notional particles of the Monte Carlo calculation. For example, in the simplest of these particle interaction models (Dopazo 1975),

$$(\mathcal{D} \nabla^2 \psi_j)^{(i)} = - \frac{\phi_j^{(i)} - \frac{1}{N_p} \sum_{i=1}^{N_p} \phi_j^{(i)}}{T_j}$$

for the i -th notional particle of the j -th species. This model is termed “linear mean square estimation” (LMSE). N_p is the total number of particles in a computational volume. The mixing frequency, $1/T_j$, is usually taken as the inverse of the integral time scale of the turbulence, T_L , to within a multiplicative constant of order unity. This introduces two assumptions concerning the various ratios of the relevant time scales:

- (a) The mixing frequency of a passive scalar, $1/T$, is proportional to the turbulence frequency, $T/T_L \sim \mathcal{O}(1)$;
- (b) The mean mixing frequency is identical for all reacting species and proportional to that of a passive scalar, $T_j/T \sim \mathcal{O}(1)$.

The constant time scale ratio for the dissipation rate of scalar and velocity fluctuations is a turbulence modeling issue. The latter assumption is a combustion modeling issue and is the focus of the present paper.

Peters (2000) has pointed out the implicit assumption made in prescribing $T_j \sim T$. To review, for the passive scalar, ξ , T is the characteristic time for the dissipation of scalar energy:

$$\frac{1}{\langle \xi^2 \rangle} \frac{d\langle \xi^2 \rangle}{dt} = - \frac{\langle 2\mathcal{D}(\nabla \xi)^2 \rangle}{\langle \xi^2 \rangle} \equiv -\frac{1}{T}$$

with no change of the passive scalar mean. Defining the dissipation rate of ξ as $\chi \equiv 2\mathcal{D}(\nabla \xi)^2$, $T \equiv \langle \xi^2 \rangle / \langle \chi \rangle$, it follows that Equilibrium of developed turbulence implies that the cascade of turbulent kinetic energy produced at the large scales is in equilibrium with its dissipation occurring at the smallest scales. Thus, T can be represented by the integral scalar time scale. From assumption (a) above, the proportionality of T and the turbulence frequency gives $T \sim T_L \sim u'/L$. For a reacting scalar,

$$\frac{1}{\langle \psi_j^2 \rangle} \frac{d\langle \psi_j^2 \rangle}{dt} - \frac{\langle 2\psi_j \dot{s}_j \rangle}{\langle \psi_j^2 \rangle} = - \frac{\langle 2\mathcal{D}(\nabla \psi_j)^2 \rangle}{\langle \psi_j^2 \rangle} \equiv -\frac{1}{T_j} .$$

Defining $\chi_j \equiv 2\mathcal{D}(\nabla \psi_j)^2$, we have $T_j \equiv \langle \psi_j^2 \rangle / \langle \chi_j \rangle$. Clearly, $T_j = T$ is strictly valid only in the infinitely-fast and frozen-chemistry limits where $\dot{s} = 0$; is a good approximation for slow chemistry where the assumption of dissipation balancing production is sufficiently accurate; but would be poor for fast (but not infinitely fast) chemistry where chemical reaction is significant enough to modify the energy budget. Variations of the equilibrium assumption, like balance of production, dissipation, and reaction, have led to insight on the influence of chemistry on the T/T_j ratio, but for linear reaction (Peters 2000). In this paper, mapping closure (Chen *et al.* 1989; Pope 1991) is used to develop a model for T/T_j for realistic chemistry.

The paper is organized as follows: In the next section, the main ideas of mapping closure are summarized. A new model to prescribe the time-scale ratio of a passive-to-reactive scalar is formulated. The model is compared to results from DNS, where the exact time-scale ratio can be calculated. Finally, future applications are outlined to treat local extinction and reignition in the framework of transported PDF and moment closure methods.

2. Results and discussion

Very little work in applying mapping closure for turbulent reacting scalars has been done since its original conception by Chen *et al.* (1989) and generalization for multiple reactive scalars by Pope (1991). Gao, Jiang, and O'Brien have made many analytical developments for single (Gao 1991*b,a*; O'Brien & Jiang 1991) and multiple passive scalars (Gao & O'Brien 1991; Jiang *et al.* 1992). Girimaji (1993) has considered mapping(s) from time-evolving reference field(s), has made comparisons with a presumed beta pdf distribution of passive scalar mixing (Girimaji 1992*b*), and has pointed out problems with mapping closure of a passive scalar at very late stages of mixing (Girimaji 1992*a*). Although Valiño and co-workers applied a Monte Carlo method (Valiño *et al.* 1991) for a reacting case (Valiño & Gao 1992), the time scale of the reacting scalar was replaced by that of the passive scalar.

2.1. Mapping closure revisited

The main ideas behind mapping closure are reviewed. The normalized temperature is used as an illustrative example, but may be replaced by any reacting scalar in the summary to follow. Mapping closure introduces a mapping

$$\theta(\mathbf{x}, t) = Y_{N_s+1}(z_0(\mathbf{z}), z_1(\mathbf{z}), \dots, z_{N_s}(\mathbf{z}), t) , \quad (2.1a)$$

where Y_{N_s+1} is a deterministic function and (z_0, \dots, z_{N_s}) a vector of random variables. Then, the gradient of θ simply follows from application of the chain rule and can be written as

$$\nabla \theta = \sum_{j=0}^{N_s} \frac{\partial Y}{\partial z_j} \nabla z_j(J(t)\mathbf{x}) , \quad (2.1b)$$

where $J(t)$ is the Jacobian of the coordinate transformation $\mathbf{z} \rightarrow \mathbf{x}$ accounting for advective stretching (Chen *et al.* 1989). For notational convenience, the sample space variable for z_j is also represented by “ z_j ”. If the random variables (z_0, \dots, z_{N_s}) are jointly Gaussian, then the transported PDF closure problem is addressed as multi-point information for z_j are known from their single-point statistics. An equally important motivation of choosing all z_j normally distributed is that it also allows conditional averages of θ to be related to its unconditional counterpart. More generally, it allows small-scale structure to be reconstructed from information at the integral scale.

Pope (1991) has derived the governing equations for the mapping functions of a general chemically reacting system. In the present notation, we have, for a reacting scalar,

$$\left[\frac{\partial}{\partial t} - \sum_{i=1}^j \langle \mathcal{D}_j (\nabla z_{i-1})^2 \rangle \left(\frac{\partial^2}{\partial z_{i-1}^2} - \frac{z_{i-1}}{\langle z_{i-1}^2 \rangle} \frac{\partial}{\partial z_{i-1}} \right) \right] Y_j = \dot{s}_j(Y_1, \dots, Y_{N_s}, Y_{N_s+1}) . \quad (2.2a)$$

For a passive scalar, $\dot{s}_j \equiv 0$, and Y_j is written as “ X_j ”. No general initial and boundary conditions exist. “External” information on the generally time-dependent evolution of the unconditional statistics of $|\nabla \psi_j|$ (or $|\nabla \xi_j|$ for X_j) must be prescribed.

Mapping closure is a self-contained turbulent combustion model. With the solution of Eq. (2.2a), the solution of Eq. (1.1) can be written directly as

$$p_{\psi\theta}(\phi_1, \dots, \phi_{N_s+1}; t) = \left(\prod_{j=1}^{N_s+1} \left| \frac{\partial Y_j}{\partial z_{j-1}} \right| \right)^{-1} \prod_{i=1}^{N_s+1} p_{z_{i-1}}(z_{i-1}) , \quad (2.2b)$$

where p_{z_i} is normally distributed and Y_j is the solution of Eq. (2.2a). However, the mapping equations without simplification would be $N_s!$ times more expensive to integrate and therefore would not be computationally tractable for practical engineering flows where the number of species is usually large. Below, we simplify and solve the mapping equations in the flamelet regime.

2.2. Dissipation rate of a passive scalar

To illustrate past work on the application of mapping closure to the turbulent mixing of a passive scalar advected by Navier-Stokes turbulence, we consider the statistics of the mixture fraction of a simple one-step, second-order, reversible reaction: $F + \nu O \rightleftharpoons (1+\nu)P$, where one mole of fuel (F) reacts with ν moles of oxidizer (O) to yield $(1+\nu)$ moles of product (P). The production rates for F, O, and P are $\dot{s}_F = -\dot{s}$, $\dot{s}_O = -\nu\dot{s}$, and

$\dot{s}_P = (1 + \nu)\dot{s}$, respectively, where

$$\dot{s}(\psi_F, \psi_O, \psi_P, \theta) = A \exp\left(-\frac{Ze}{\alpha}\right) \left(\psi_F \psi_O - \frac{1}{K} \psi_P^2\right) \exp\left[-\frac{Ze(1-\theta)}{1-\alpha(1-\theta)}\right] .$$

Here, A is the frequency factor, α is the heat release parameter, and Ze is the Zel'dovich number. The Schmidt number is 0.7 and Lewis numbers are unity. The molecular diffusivities and viscosity are independent of the temperature. The turbulent flow is incompressible, isotropic, homogeneous, and decaying (*cf.* Sripakagorn *et al.* (2000) for details of the simulation). The passive scalar for this binary mixing problem, the mixture fraction, is defined as

$$\xi = \frac{\nu \psi_F - \psi_O + 1}{\nu + 1}$$

which is then conserved under reaction.

The transport of $p_\xi(\eta, t)$, the PDF of ξ , is governed by (O'Brien 1980)

$$\frac{\partial}{\partial t} p_\xi(\eta, t) = -\frac{\partial}{\partial \eta} \langle \mathcal{D} \nabla^2 \xi | \eta \rangle p_\xi = -\frac{\partial^2}{\partial \eta^2} \langle \mathcal{D} (\nabla \xi)^2 | \eta \rangle p_\xi . \quad (2.3)$$

Spatial homogeneity has been assumed. To close Eq. (2.3), the mapping $\xi = X(z_0, t)$ is defined. Application of Eq. (2.2a), (2.1b), and (2.2b) gives

$$\frac{\partial}{\partial t} X(z_0, t) = \frac{\langle \mathcal{D} (\nabla \xi)^2 \rangle}{\langle (\partial X / \partial z_0)^2 \rangle} \left(\frac{\partial^2 X}{\partial z_0^2} - z_0 \frac{\partial X}{\partial z_0} \right) \quad (2.4a)$$

$$\langle \mathcal{D} (\nabla \xi)^2 | \xi = \eta \rangle = \langle \mathcal{D} (\nabla \xi)^2 \rangle \frac{(\partial X / \partial z_0)^2}{\langle (\partial X / \partial z_0)^2 \rangle} \quad (2.4b)$$

$$p_\xi(\eta, t) = \frac{1}{|\partial X / \partial z_0|} p_{z_0}(z_0) , \quad (2.4c)$$

respectively. The independence of z_0 and ∇z_0 (Chen *et al.* 1989) has been assumed. In Eq. (2.4a), the relation $\langle \mathcal{D} (\nabla \xi)^2 \rangle / \langle (\partial X / \partial z_0)^2 \rangle = \langle \mathcal{D} (\nabla z_0)^2 \rangle$ has been used and hence knowledge of the Jacobian can be circumvented by knowledge of the effect of the turbulent velocity field on ξ directly. (Models for $\langle \mathcal{D} (\nabla \xi)^2 \rangle \equiv \langle \chi \rangle / 2$ are well known.) For this initially segregated system, boundary conditions are $X(-\infty, t) = 0$ and $X(+\infty, t) = 1$. Initial conditions are specified using an iterative approach such that the variance from $p_{z_0} / (|\partial X / \partial z_0|) = p_\xi$ gives the exact value of the DNS. The exact average dissipation rate from the DNS is used in integrating Eq. (2.4a). Figure 1 shows good agreement with the data for $\langle \mathcal{D} (\nabla \xi)^2 | \eta \rangle$ and $p_\xi(\eta, t)$ calculated using Eq. (2.4b) and (2.4c) respectively, corroborating the previous work listed at the beginning of this section.

2.3. Mapping function for a fast reacting scalar

In the flamelet regime, ψ_j is governed by (Peters 2000)

$$\frac{\partial \psi_j}{\partial \tau} = \frac{\chi}{2} \frac{\partial^2 \psi_j}{\partial \xi^2} + \dot{s}_j . \quad (2.5)$$

Correspondingly, the mapping Y_j in Eq. (2.2a) becomes a function of (z_0, t) only for all j and the mapping equations simplify to

$$\frac{\partial Y_j}{\partial t} = \frac{\langle \mathcal{D} (\nabla \xi)^2 \rangle}{\langle (\partial X / \partial z_0)^2 \rangle} \left(\frac{\partial^2 Y_j}{\partial z_0^2} - z_0 \frac{\partial Y_j}{\partial z_0} \right) + \dot{s}_j(Y_1, \dots, Y_{N_s+1}) . \quad (2.6)$$

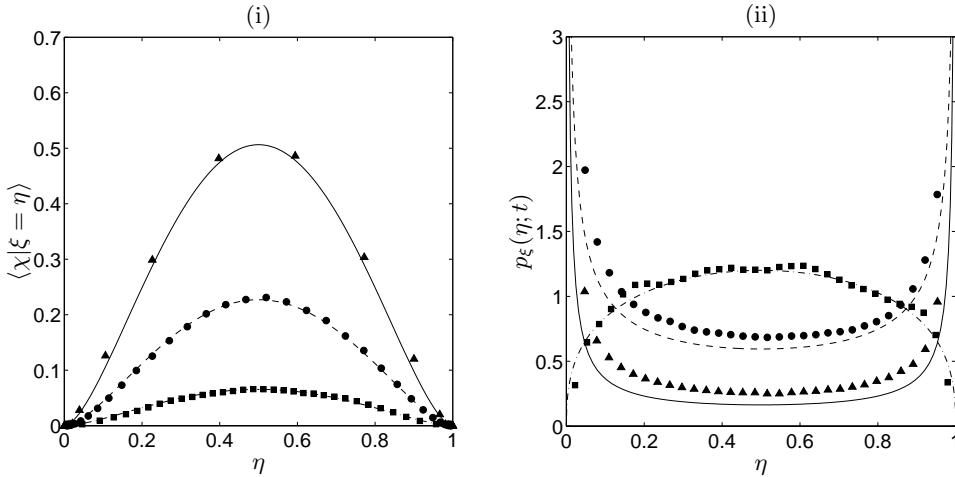


FIGURE 1. Passive scalar results. Comparison of mapping closure results with DNS data initially (triangles = DNS, solid line = mapping closure) and at times $t/\tau_{\text{eddy}} = 1$ (circles = DNS, dash-dot = mapping closure), and 2 (squares = DNS, dash-dot = mapping closure).

The mapping $\psi_j = Y_j(z_0, t)$ is not generally one-to-one. Initial conditions for Eq. (2.6) can be given by $Y_j = \psi_j(X(z_0, t_0), t_0)$, which is the steady-state solution of Eq. (2.5) with $\chi/2$ replaced by Eq. (2.4b). Boundary conditions for Eq. (2.6) are $Y_j(-\infty, t) = \psi_j(0, t)$ and $Y_j(+\infty, t) = \psi_j(1, t)$.

Given a solution for the mapping function Y_j , small scale processes for the reacting scalars can be described using the average dissipation rate of the passive scalar at the integral scale. In particular,

$$\langle \mathcal{D}(\nabla \psi_j)^2 | \psi_j = \phi \rangle = \frac{\langle \chi \rangle}{2} \frac{(\partial Y_j / \partial z_0)^2}{\langle (\partial X / \partial z_0)^2 \rangle} \quad (2.7a)$$

$$p_{\psi_j}(\phi, t) = \frac{1}{|\partial Y_j / \partial z_0|} p_{z_0}(z_0) . \quad (2.7b)$$

Using Eq. (2.7a) and Eq. (2.4b), the desired time-scale ratio for a passive-to-reactive scalar is then

$$\frac{T_j}{T} = \frac{\langle \psi_j^2 \rangle / \langle (\partial Y / \partial z_0)^2 \rangle}{\langle \xi^2 \rangle / \langle (\partial X / \partial z_0)^2 \rangle} . \quad (2.8)$$

Figure 2 shows good agreement with the DNS data for (i) $\langle 2\mathcal{D}(\nabla \psi_P)^2 | \psi_P = \phi \rangle \equiv \langle \chi_P | \psi_P = \phi \rangle$ and (ii) $p_{\psi_P}(\phi, t)$ calculated using Eq. (2.7a) and (2.7b) respectively. Figure 3 shows (i) the mean and standard deviation of ψ_P from Eq. (2.7b) and (ii) the time scale ratio calculated using Eq. (2.8). The figure shows that the relaxation time scale for a fast reacting scalar, T_j , can deviate significantly from T in the flamelet regime. Further, the mixing time scale is reduced in the presence of active chemistry ($T_j < T$).

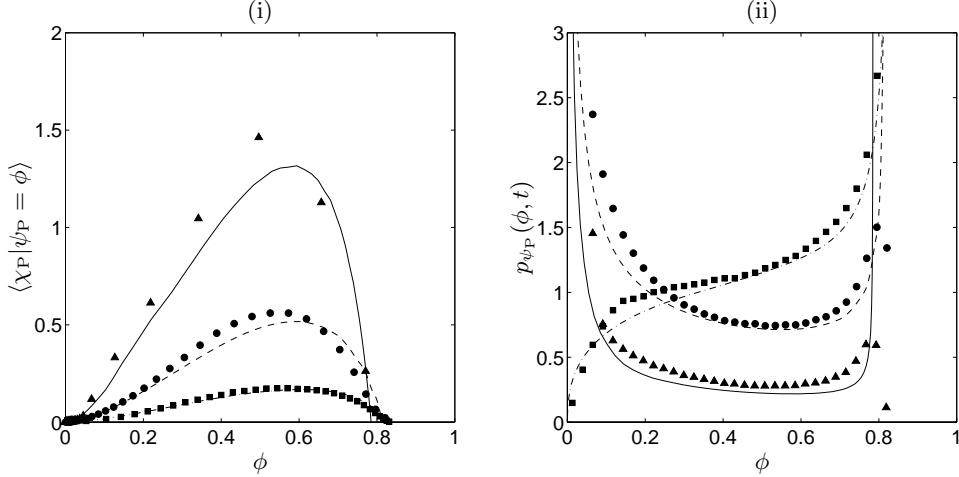


FIGURE 2. Reacting scalar results. Comparison of mapping closure results with DNS data initially (triangles = DNS, solid line = mapping closure) and at times $t/\tau_{\text{eddy}} = 1$ (circles = DNS, dash-dot = mapping closure), and 2 (squares = DNS, dash-dot = mapping closure).

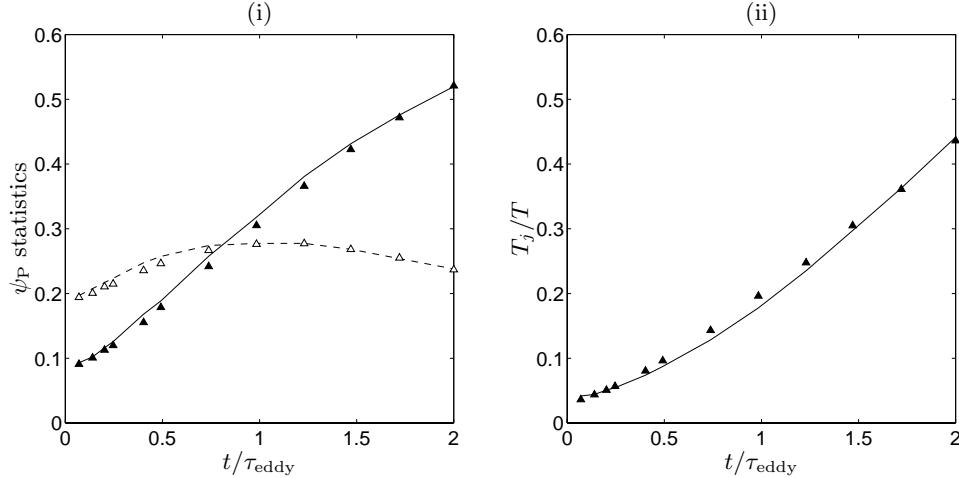


FIGURE 3. Prediction of time scale ratio by mapping closure in fast chemistry regime: (i) mean and rms and (ii) time scale ratio. Symbols are DNS data. Lines are modeling predictions.

3. Conclusions and future work

For sufficiently fast chemistry, the average time-scale ratio for a passive-to-reactive scalar was derived:

$$\begin{aligned} \frac{T_j}{T} &\equiv \frac{\langle \psi_j^2 \rangle / \langle \chi_j \rangle}{\langle \xi^2 \rangle / \langle \chi \rangle} \\ &= \min \left\{ 1, \frac{\langle \psi_j^2 \rangle}{\langle \xi^2 \rangle} \frac{\langle (\partial X / \partial z_0)^2 \rangle}{\int_{-\infty}^{+\infty} (\partial \psi_j / \partial \xi)^2 (\partial X / \partial z_0)^2 p_{z_0} dz_0} \right\}, \end{aligned} \quad (3.1)$$

where $\psi_j(\xi, t)$ is the solution of Eq. (2.5), the first or leading-order (un)steady flamelet equation. Equation (2.5) cannot describe reignition. Equation (3.1) can be directly applied to existing particle-interaction models for transported PDF closure modeling, which

can, in principle, describe global reignition. Equation (3.1) is not expected to describe the entire transition $T_j/T \rightarrow 1$ and the “min” function is required to properly bound the T_j/T ratio by the infinitely fast and frozen chemistry limits, where $T_j/T = 1$.

Ongoing/future work includes application to the extinction/reignition problem based on the following modeling approaches.

(a) Conditional moment closure modeling: Moment closure conditional on ξ represents the least computationally burdensome of turbulent combustion models. Application of Eq. (2.2a) may yield a description of the complex shapes of the conditional pdfs when extinction and reignition processes are significant. This is the subject of ongoing work (Cha & Pitsch 2001).

(b) Transported PDF modeling: To describe extinction/reignition using transported PDF modeling, more sophisticated particle interaction models are required where intermittency effects of the dissipation must be accounted for (Xu & Pope 2000). An accurate estimate of the overall mean mixing frequency is also essential in these local particle interaction models such as the extended LMSE model of Sabel'nikov & Gorokhovski (Sabel'nikov & Gorokhovski 2001).

In both these applications, a sound physical basis would be necessary to assign proper initial and boundary conditions to the more general mapping function equations, Eq. (2.2a) in this paper. Currently, the mapping closure approach is being developed for transported PDF modeling in large-eddy simulations (Cha & Trouillet 2001).

REFERENCES

- CHA, C. M. & PITSCHE, H. 2001 Higher-order conditional moment closure modeling of local extinction and reignition in turbulent combustion. *Combust. Theory Modelling* (submitted).
- CHA, C. M. & TROUILLET, P. 2001 A model for the mixing time scale of a turbulent reacting scalar. *Bull. Amer. Phys. Soc.* **46** (10), 14.
- CHEN, H., CHEN, S. & KRAICHNAN, R. H. 1989 Probability distribution of a stochastically advected scalar field. *Phys. Rev. Lett.* **63**, 2657–2660.
- DOPAZO, C. 1975 Probability density function approach for a turbulent axisymmetric heated jet. Centerline evolution. *Phys. Fluids A* **18** (4), 397–404.
- DOPAZO, C. 1994 Recent developments in PDF methods. In *Turbulent Reacting Flows* (ed. P. A. Libby & F. A. Williams), chap. 7, pp. 375–474. New York: Academic.
- GAO, F. 1991a An analytical solution for the scalar probability density function in homogeneous turbulence. *Phys. Fluids A* **3**, 511–513.
- GAO, F. 1991b Mapping closure and non-Gaussianity of the scalar probability density functions in isotropic turbulence. *Phys. Fluids A* **3**, 2438–2444.
- GAO, F. & O'BRIEN, E. E. 1991 A mapping closure for multispecies Fickian diffusion. *Phys. Fluids A* **3**, 956.
- GIRIMAJI, S. S. 1992a A mapping closure for turbulent scalar mixing using a time-evolving reference field. *Phys. Fluids A* **4**, 2875–2886.
- GIRIMAJI, S. S. 1992b On the modeling of scalar diffusion in isotropic turbulence. *Phys. Fluids A* **4**, 2529.
- GIRIMAJI, S. S. 1993 A study of multiscalar mixing. *Phys. Fluids A* **5**, 1802.
- JIANG, T.-L., GIVI, P. & GAO, F. 1992 Binary and trinary scalar mixing by Fickian diffusion—some mapping closure results. *Phys. Fluids A* **4**, 1028–1035.

- KLIMENKO, A. Y. & BILGER, R. W. 1999 Conditional moment closure for turbulent combustion. *Prog. Energy Combust. Sci.* **25**, 595–687.
- O'BRIEN, E. E. 1980 The probability density function (pdf) approach to reacting turbulent flows. In *Turbulent Reacting Flows* (ed. P. A. Libby & F. A. Williams), *Topics in Applied Physics* 44, chap. 5, pp. 185–218. Springer.
- O'BRIEN, E. E. & JIANG, T. L. 1991 The conditional dissipation rate of an initially binary scalar in homogeneous turbulence. *Phys. Fluids A* **3**, 3121–3123.
- PETERS, N. 2000 *Turbulent Combustion*. Cambridge: Cambridge University Press.
- POPE, S. B. 1990 Computations of turbulent combustion: Progress and challenges. *Proc. Combust. Inst.* **23**, 591–612.
- POPE, S. B. 1991 Mapping closures for turbulent mixing and reaction. *Theoret. Comput. Fluid Dynamics* **2**, 255–270.
- SABEL'NIKOV, V. A. & GOROKHOVSKI, M. 2001 Extended LMSE and Langevin models of the scalar mixing in the turbulent flow. In *Second International Symposium on Turbulence and Shear Flow Phenomena*. Royal Institute of Technology (KTH), Stockholm, Sweden, June 27–29.
- SRIPAKAGORN, P., KOSÁLY, G. & PITSCHEIDER, H. 2000 Local extinction-reignition in turbulent nonpremixed combustion. In *CTR Annual Research Briefs*, pp. 117–128. Stanford University / NASA Ames.
- VALIÑO, L. & GAO, F. 1992 Monte Carlo implementation of a single-scalar mapping closure for diffusion in the presence of chemical reaction. *Phys. Fluids A* **4** (9), 2062.
- VALIÑO, L., ROS, J. & DOPAZO, C. 1991 Monte Carlo implementation and analytic solution of an inert-scalar turbulent-mixing test problem using a mapping closure. *Phys. Fluids A* **3** (9), 2191.
- XU, J. & POPE, S. B. 2000 PDF calculations of turbulent nonpremixed flames with local extinction. *Combust. Flame* **123**, 281–307.