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Joint probability density function models for multiscalar turbulent mixing

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Modeling multicomponent turbulent mixing is essential for simulations of turbulent combustion, which is controlled by mixing of fuel, oxidizer, combustion products, and intermediate species. One challenge is to find functions that can reproduce the joint probability density function (PDF) of scalar mixing states using only a small number of parameters. Even for mixing with only two independent scalars, several statistical distributions, including the Dirichlet, Connor–Mosimann (CM), five-parameter bivariate beta (BVB5), and statistically-most-likely distributions, have previously been proposed for this purpose, with minimal physical justification. This work uses the concept of statistical neutrality to relate these distributions to each other, relate the distributions to physical mixing configurations, and develop a systematic approach to model selection. This approach is validated by comparing the ability of these distributions to reproduce the evolution of the scalar PDF from Direct Numerical Simulations of three-component passive scalar mixing in isotropic turbulence with 11 different initial conditions that are representative of a wide range of mixing conditions of interest. The approach correctly identifies whether the Dirichlet, CM, and BVB5 distributions, which are increasingly complex bivariate generalizations of the beta distribution, can accurately model the joint PDFs, but knowledge of the mixing configuration is required to select the appropriate distribution. The statistically-most-likely distribution is generally less accurate than the appropriate bivariate beta distribution but still gives reasonable predictions and does not require knowledge of the mixing configuration, so it is a suitable model when no single mixing configuration can be identified.

1. Introduction

Turbulent mixing of multiple distinct components is a critical factor affecting the operation of practical combustion devices. The rate of heat release is controlled in premixed flames by mixing of combustion products and intermediates into the unreacted mixture and in nonpremixed flames by the rate at which fuel and oxidizer mix. The mass fractions of a mixture corresponding to each inlet stream or chemical species, called the mixture fractions, are scalars transported by the turbulent flow field. Consequently, the systems of interest involve multiscalar turbulent mixing subject to the constraint that the sum of the scalars is unity, so only $N-1$ independent scalars need to be considered for mixing between N components. While turbulent mixing of a single scalar has been studied extensively [1–4], multiscalar mixing involving three or more components has not been studied as thoroughly despite its broad importance [5,6].

The present work, although more generally applicable to phenomena involving multiscalar turbulent mixing, is motivated by modeling needs for turbulent combustion. In Reynolds-averaged Navier–Stokes (RANS) and Large Eddy Simulation (LES) models for turbulent combustion, closure of the averaged or filtered nonlinear chemical reaction source term ($\overline{\dot{m}}_k$) in the species transport equation necessarily involves modeling turbulent mixing because it depends on the instantaneous, fully-resolved chemical composition. Typically, this term is closed by convolution with the ensemble (RANS) or subfilter (LES) joint probability density function (PDF) $\widetilde{P}$ of the controlling thermochemical state variables ξ_i,

$$\overline{\dot{m}}_k = \bar{\rho}\int \frac{1}{\rho(\xi_i)}\dot{m}_k(\xi_i)\widetilde{P}(\xi_i)d\xi_i\,, \tag{1}$$

where ρ is the density. Models for turbulent mixing are required to specify $\widetilde{P}$. Because modeling approaches are similar for RANS and LES, $\widetilde{P}$ will subsequently be referred to simply as the joint PDF, referring to the appropriate PDF for either approach.

Turbulent mixing can be modeled either by directly specifying a model form for the PDF (the presumed PDF approach) [4,7] or by solving a transport equation for the PDF, which has unclosed

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Table 1
Implementations of flamelet-like models using more than one mixture fraction.

Ref.	Framework	Application	Presumed PDF form
[11–13]	RANS	Split-Injection Diesel Engines	Dirichlet
[14]	RANS	Split-Injection Diesel Engines	5 Parameter Bivariate Beta (BVB5)
[15,16]	LES	Jet-In-Hot-Coflow Burner [20]	Connor–Mosimann (CM)
[17]	RANS	Jet-In-Hot-Coflow Burner [20]	Beta-Delta Limit of CM
[18]	LES	Piloted Premixed Jet Burner [21]	Dirichlet
[19]	LES	Sydney Inhomogeneous Inlet Burner [22]	Beta-Delta Limit of CM

mixing terms that must be modeled (the transported PDF approach) [8]. In the presumed PDF approach, the model form of the joint PDF is parameterized by the mean values for the relevant scalars and typically at least one variance or other moment, for which transport equations are solved. In the transported PDF approach, the standard method is to solve the PDF transport equation utilizing an ensemble of Lagrangian particles, resulting in an a substantial increase in computational cost relative to the presumed PDF approach. Turbulent transport is modeled by adding a stochastic term to the particle position equation. Molecular mixing must also be modeled to close the conditional diffusion term in the particle composition equation; several models have been developed for this purpose [9].

In general, the thermochemical state vector ξ_i includes all species mass fractions, temperature, and pressure (for compressible or closed systems). Hydrocarbon combustion can involve $O(10^2)$ or more species, resulting in a high-dimensional thermochemical state space. Reduced-order models, such as the widely used nonpremixed flamelet/progress variable approach [10], have been developed that instead parameterize the thermochemical state by only a few controlling variables, typically a reaction progress variable (C) and a single mixture fraction (Z) characterizing mixing between fuel and air inlets. While developing a presumed form for the high-dimensional joint PDF of all species mass fractions is an extremely challenging, perhaps intractable, problem [7], the presumed PDF approach is well suited to reduced-order models where the joint PDF that must modeled is low-dimensional.

In standard reduced-order modeling approaches, the joint PDF of the controlling scalars is decomposed into a marginal PDF of mixing variables and a conditional PDF of the progress variable, which are modeled separately. The focus of the current work is model development for the turbulent mixing portion of the PDF, which, because the mixture fraction is a nonreacting scalar, is fundamentally related to the problem of passive, nonreacting turbulent mixing. For two-component mixing, it is well-established that the beta distribution is an accurate model for the marginal mixture fraction PDF [3,4,7].

Flamelet-like reduced-order models coupled with the presumed PDF approach have recently been extended to apply to partially premixed systems and multiple inlet stream systems by including an additional mixture fraction in the low-order parameterization of the thermochemical state [11–19], as shown in Table 1. The systems where these models have been applied include split-injection diesel engines, where air and fuel from the first injection partially mix prior to the second injection event; the Jet-In-Hot-Coflow [20] Burner (JHCB) and Piloted Premixed Jet Burner [21] (PPJB), which involve a pipe and annulus flow that forms a jet into a third fluid; and the Sydney Inhomogeneous Inlet Burner [22], which is similar to the other jet burners but with the contents of the pipe and annulus allowed to partially premix upstream of the jet nozzle. All of these systems involve three-component mixing, characterized by two mixture fractions (Z_1 and Z_2), and present a challenge for presumed PDF closure as the joint PDF $\widetilde{P}(Z_1, Z_2)$ must be modeled.

Given the evidence showing that the marginal PDF of a single mixture fraction is well-described by a beta distribution, a bivariate generalization of the beta distribution may be desired to model $\widetilde{P}(Z_1, Z_2)$. However, many bivariate generalizations of the beta distribution with differing properties are possible [23,24]. Table 1 shows that several different bivariate beta distributions have been applied in combustion simulations, including instances where different distributions are applied in simulations of the same configuration. Models have frequently been selected with little to no physical justification and not validated. The statistically-most-likely distribution (SMLD) has also been proposed as a plausible PDF model for multiscalar mixing [25], although it does not have marginal beta distributions.

Further study of three-component mixing and, in particular, the evolution of the joint scalar PDF resulting from three-component mixing is needed to better motivate selection of appropriate models. Only one study has attempted to evaluate candidate PDF models for multiscalar mixing: Doran performed a Direct Numerical Simulation (DNS) of three-component mixing in isotropic turbulence for various initial scalar fields and assessed the ability of candidate models to recreate the distributions from the DNS [14]. That study showed that the form of the PDF depends strongly on the initial distribution of scalars but did not provide a general method to select a model and examined only a limited subset of bivariate generalizations of the beta distribution.

Other works have examined the multiscalar mixing problem from a transported PDF perspective, with a focus on testing molecular mixing models, but the qualitative variation in the form of the joint PDF based on initial conditions is still evident in their results. Juneja and Pope [5] observed large differences in the evolution of the multiscalar PDF for three-component mixing in isotropic turbulence based on whether all components had equal or unequal initial length scales. Sawford et al. [26] tested a similar configuration but with a layered initial condition where two components were initially separated by the third and saw qualitatively different PDF forms than those seen by Juneja and Pope. Cai et al. [6] also observed different PDF forms than Juneja and Pope in experimental measurements moving downstream in a nonreacting pipe and annulus jet similar to the JHCB and PPJB.

The observed dependence of the evolution of the shape of the joint scalar PDF on initial and boundary conditions occurs because the initial scalar distribution affects the rate of two-component mixing in temporally evolving flows [27], and the inlet boundary conditions have a similar effect in spatially evolving flows [28,29]. Therefore, the relative rates of mixing for three components should also be determined by initial or boundary conditions. The relative mixing rates affect the trajectories in composition space from the unmixed states to the fully mixed state and, as a result, the probability of passing through any particular location in composition space during the mixing process.

Given that the initial and boundary conditions affect the evolution of the joint scalar PDF for three-component passive mixing, the objective of this work is to develop a systematic framework for selecting an appropriate presumed form for this PDF based on the physical mixing conditions of a particular system. First, several