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First and second order lagrangian conditional moment closure method in turbulent nonpremixed flames

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Abstract

The Lagrangian CMC method is developed by conditionally averaging the quantities associated with Lagrangian particles originating from the nozzle exit. It involves multiple flame groups of sequentially injected fuel, each of which shares the same conditional flame structure under the same residence time. The probability, p_k, to find the kth group is assumed proportional to the partial mean mixture fraction, ξ^k, to obtain the local conditional flame structure as a weighted average by p_k. The Lagrangian CMC method allows flexibility of flamelet based methods and requires less computational load than Eulerian CMC. It is implemented in OpenFOAM and applied with first and second order closure to the piloted jet diffusion flames near extinction, Sandia Flame D and E. Results show good agreement for all conditional profiles and noticeable improvement by second order correction of four rate limiting steps in the GRI 3.0 mechanism. Good agreement is achieved for conditional variances and covariances among temperature and species involved in the rate limiting reaction steps.

Keywords: Conditional moment closure; Second order CMC; Lagrangian; Turbulent nonpremixed combustion; Flamelet

1. Introduction

The conditional moment closure (CMC) method is based on conditional averaging in terms of the sampling variable for mixture fraction without a priori assumption on flame structures or combustion regimes in turbulent nonpremixed combustion. Nonlinear reaction rates were modeled by first and second order closure in terms of conditional means, variances and covariances of species mass fractions and temperature [1–3]. Eulerian CMC is appropriate for complicated recirculating flow, while it suffers from an additional dimension of the sampling variable and uncertainties in the closure models [4]. Conditional equations were often discretized with homogeneity assumed in the cross-stream direction or in the whole domain as an incompletely stirred reactor to reduce the dimension in Eulerian

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Nomenclature

A	pre-exponential factor
b	exponent for temperature
D	turbulent diffusivity
erf	error function
G	conditional variance or covariance
k	turbulent kinetic energy
N	scalar dissipation rate
N_{st}	conditional SDR at stoichiometry
N^*_{st}	N_{st} of each flame group
P	probability density function
p_k	probability to find kth flame group
Q	conditional mean scalar
$Sc_{\tilde{\xi}}$	turbulent Schmidt number
T	temperature
T_a	activation temperature
T_1, T_2	second order correction terms
V	volume
W	molecular weight
$\dot{w}_\Phi$	reaction rate
$\mathbf{Y}$	species mass fraction

Greek symbols

δ	delta function
ε	turbulent dissipation rate
η	sampling variable
μ_t	turbulent viscosity
ξ	mixture fraction
ξ^k	partial mixture fraction of kth group
ξ_p	mixture fraction in pilot stream
ρ	density
Φ	reacting scalar

Subscript symbols

i, j	species index
L	Lagrangian quantity

Superscript symbols

k	kth flame group
$'$	fluctuation about conditional mean scalar

CMC [5]. Dual meshes were employed to reduce computational burden in three dimensional CMC and Reynolds Averaged Navier Stokes (RANS) fields of furnaces [6], diesel engines [7], and compartment fires [8].

Steady and unsteady flamelet models have been employed in a wide range of practical problems due to their simpler structure and computational efficiency [9–11]. They require less computational load than Eulerian CMC for a limited number of Lagrangian flamelets coupled with mean flow field or in the postprocessing mode. Lagrangian CMC [12] was proposed in terms of multiple Lagrangian fuel groups according to injection sequence or residence time to resolve some of the difficulties in Eulerian CMC. The same conditional profile was assumed for each fuel group with no convection and diffusion terms, therefore, no model required for conditional velocity nor the gradient diffusion assumption. Lagrangian CMC has some similarity with the Eulerian Particle Flamelet Model (EPFM) [13,14] which tracks the mass weighted fraction of particles for multiple Lagrangian flamelets. The CMC method has its strength in general validity of the conditional equations derived through rigorous mathematical procedure and flexibility to allow higher order closure of conditional reaction rates. Flame group interaction was taken into account by the eddy breakup model as premixed combustion along constant mixture fraction contours for a lifted flame [15] or to avoid abrupt ignition and heat release of sequential groups in a diesel engine [16]. In this paper Lagrangian CMC is established through the generalized function procedure together with a transport equation for the associated probability density function (PDF). Governing equations and conditional submodels are introduced for first and second order closure of the reaction rates and applied to Sandia Flame D and E in the Turbulent Nonpremixed Flame Workshop website [17].

2. Derivation of the Lagrangian CMC equation

Consider a Lagrangian particle originating from $\mathbf{x}_0$ at the nozzle exit at time t_0 so that $\mathbf{x}_L(t_0) = \mathbf{x}_0$ and $\xi_L(t_0) = 1$. Any Lagrangian quantity associated with the particle may be represented as $\Phi_L(t) = \Phi(\mathbf{x}_L(t), t)$ implying $Q_{\eta L}(\eta, t) = Q_\eta(\eta, \mathbf{x}_L(t), t)$. $Q_\eta(\eta, \mathrm{x}, t)$ is the conditional mean of Φ defined as $\langle \Phi(\mathbf{x}, \mathbf{t}) | \xi = \eta \rangle$ [4]. ξ is the mixture fraction and η is the sampling variable for fluctuating ξ. The subscript, L, represents a Lagrangian quantity. It holds that

$$\frac{\partial \mathbf{x}_L(t)}{\partial t} = \mathbf{v}(\mathbf{x}_L(t), t) \tag{1}$$

$$\frac{\partial \xi_L(t)}{\partial t} = \left[\frac{D}{Dt}\xi(\mathbf{x}, t)\right]_{\mathbf{x}=\mathbf{x}_L(t)} \tag{2}$$