A multiple-inlet mixture fraction model for nonpremixed combustion

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ABSTRACT

The conserved scalar or mixture fraction approach was originally derived for two-feed systems with one oxidizer stream and one fuel stream. Under the assumptions of unity Lewis number for all chemical species and sufficiently large values of the Damköhler number, it is known to provide a widely used and very efficient basis for the calculation of turbulent diffusion flames, which may be handled through the single knowledge of the mixture fraction statistics. The mixture fraction variable is also central to steady laminar flamelet representations, which provide a common building block to a variety of modelling proposals for turbulent combustion in nonpremixed and partially premixed situations. However, as soon as dilution by a third inlet stream comes into play, the corresponding formalisms, which rely on the mixture fraction concept, should be revisited. This restriction occurs, for instance, when an additional stream of oxygen-enriched air is introduced with the purpose of either achieving high temperature levels or favoring flame stabilization. Such a situation clearly exceeds the scope of the standard conserved scalar framework. The present study is aimed at extending the two-inlet mixture fraction basis to the consideration of such multiple-inlet injections. For this purpose, we introduce the notion of a *fictive* (or notional) injector, whose characteristics are reconstructed from the transport of either (i) inlet tracers or (ii) associated compositions of each inlet. The performance of the proposed approach is illustrated through its application to moderate and intense low-oxygen dilution (MILD) combustion of a jet in a hot coflow (JHC) burner. Comparisons performed between measurements and numerical simulations confirm that the proposed framework is able to render the third inlet influence, as well as the effects induced by variations of oxygen concentration in the hot coflowing stream. The proposed approach thus offers a simple way to extend the use of a wide variety of available turbulent combustion closures, which are based on the mixture fraction, to practical conditions featuring more than two feeding streams.

1. Introduction

Nonpremixed combustion is often considered on the basis of the diffusion flame limit, which is related to the rate-controlling step: molecular diffusion. For such conditions, which rely on the fast chemistry assumption, the problem may be solved from an equivalent nonreactive mixing description with the reaction zone or flame location identified as the surface where the injected reactants (fuel and oxidizer) are mixed in stoichiometric proportions [1]. The standard approach to deal with such nonpremixed flames therefore consists in describing the mixture through a chemistry-independent conserved scalar. Many definitions of this conserved scalar have been provided in the literature. The Shvab–Zel'dovich functions have been used in conjunction with a global (single-step) chemistry representation. Once made nondimensional to vary between zero, in the oxidizer inlet stream, and unity, in the fuel inlet stream, these Shvab–Zel'dovich variables make it possible to recover the standard mixture fraction (SMF) definition. The conserved scalar can also be defined by considering the total mass fractions of a given set of chemical elements (conservation of atoms), as early proposed by Bilger [2], or as the local ratio of the mass flux originating from the fuel feeding stream to the sum of oxidizer and fuel mass fluxes [3,4]. These different definitions share the same physical grounds and the conserved scalar, or mixture fraction ξ, attempts to express nothing else but the conservation of chemical elements (atoms). In practice, Lewis number effects are often ignored, and the form of the transport equation considered for the mixture fraction finally remains the same whatever the definition used for ξ. As long as no chemical reaction takes place, the

Nomenclature

Latin letters

C_p	heat capacity (J kg^{-1} K^{-1})
D	inner diameter coflow (m)
Da	Damköhler number
d_j	inner diameter central jet (m)
$\mathcal{D}$	molecular diffusion coefficient (m^2 s^{-1})
h	enthalpy of the mixture $h = h(Y_i, T)$ (J kg^{-1})
k	turbulent kinetic energy (TKE) (m^2 s^{-2})
$\dot{m}$	mass flow rate (kg s^{-1})
N_ξ	scalar dissipation rate (SDR), $N_\xi = \mathcal{D}(\partial \xi/\partial x_\alpha)(\partial \xi/\partial x_\alpha)$ (s^{-1})
$\widetilde{P}$	Favre probability density function (PDF)
Re_T	turbulence Reynolds number
r_{st}	stoichiometric mass ratio
T	temperature (K)
u_i	ith Cartesian component of the velocity (m s^{-1})
Q	specific heat of reaction (J kg^{-1})
x_i	ith coordinates in Cartesian reference (m)
Y	species mass fraction

Subscripts and superscripts

ad	related to adiabatic conditions
D	related to diluent or chemically inert species
eq	related to thermodynamic equilibrium
F	related to fuel species
$fuel$	related to fuel inlet stream
j	related to the jth inlet
O	related to oxidizer species
ox	related to oxidizer inlet stream
P	related to combustion products
st	related to stoichiometric conditions
tot	related to total quantity (summed over all inlets)
u	related to unburnt conditions
∞	related to injection conditions

Greek letters

$\delta(.)$	Dirac distribution function
ϵ	turbulent dissipation rate (m^2 s^{-3})
ζ_j	tracer of the jth inlet, $\zeta_j = \dot{m}_j/\dot{m}_{tot}$
v_t	turbulent viscosity (m^2 s^{-1})
ξ	mixture fraction
ρ	density (kg m^{-3})
τ_ξ	scalar mixing time scale (s), $\tau_\xi = \widetilde{\xi''^2}/\widetilde{\chi}_\xi$
τ_t	turbulence integral time scale (s), $\tau_t = k/\epsilon$
ϕ	composition vector $\phi = (Y_i, h)$
Φ	equivalence ratio, $\Phi = r_{st} Y_{F,fuel}^\infty / Y_{O,ox}^\infty$
χ_ξ	turbulent scalar dissipation rate, $\chi_\xi = \mathcal{D}(\partial \xi''/\partial x_\alpha)(\partial \xi''/\partial x_\alpha)$ (s^{-1})
ω_Y	chemical species production rate (kg^2 m^{-3} s^{-1})

Acronyms

BC	boundary conditions
FI	fictive injector
HM3%	hydrogen methane 3%
HM9%	hydrogen methane 9%
JPDF	joint probability density function
LES	large eddy simulation
MILD	moderate and intense low-oxygen dilution
PDF	probability density function
RANS	Reynolds-averaged Navier–Stokes
SDR	scalar dissipation rate
SLFA	steady laminar flamelet approximation
SLFM	steady laminar flamelet models
SMF	standard mixture fraction

Operators

$\bar{q}$	Reynolds average of quantity q
$\tilde{q}$	Favre average, $\tilde{q} = \overline{\rho q}/\bar{\rho}$
q''	Favre fluctuation, $q'' = q - \tilde{q}$

transport equation for the mass fraction Y_i of any chemical species is thus similar to the one considered for the mixture fraction ξ. As a consequence, the mass fractions of any chemical species present in the fresh (unburned) mixture, denoted by $Y_{i,u}$, as well as the mixture fraction, ξ, are all linearly interrelated. These quantities will differ only from their boundary conditions. For instance, fuel and oxidizer mass fractions in the unburned mixture, $Y_{F,u}$ and $Y_{O,u}$, are coupled through the relationship $Y_{O,u} = Y_{O,ox}^\infty + (Y_{O,fuel}^\infty - Y_{O,ox}^\infty) \cdot (Y_{F,u} - Y_{F,ox}^\infty)/(Y_{F,fuel}^\infty - Y_{F,ox}^\infty)$, which explicitly involves the boundary condition values of the oxidizer mass fraction (resp. fuel mass fraction) in the fuel and oxidizer inlet streams $Y_{O,fuel}^\infty$ and $Y_{O,ox}^\infty$ (resp. $Y_{F,fuel}^\infty$ and $Y_{F,ox}^\infty$). In practice, the mass fraction of any chemical species, including both fuel and oxidizer mass fractions, may also be expressed from the knowledge of the mixture fraction according to $Y_{i,u} = \xi Y_{i,fuel}^\infty + (1 - \xi)Y_{i,ox}^\infty$.[1] From such a representation, the underlying two-inlet assumption (fuel and oxidizer with respective weights ξ and $1 - \xi$) becomes obvious. However, practical devices often feature more than two inlets and, in such cases, the standard mixture fraction (SMF) framework is no longer suited to capture the local variations of mixture composition. The principal objective of the present study is to introduce a simple strategy able to

extend the use of existing mixture-fraction-based turbulent combustion closures, which were initially put forward for two-feeding-stream conditions, to practical situations featuring more than two inlets.

It is noteworthy that, based on the conservation of atomic elements and on the reaction coefficient matrix, the case of multiple inlets and arbitrary finite-rate chemistry has been already covered for constant-density reactive flows in the chemical engineering literature; see Fox [5]. The composition can readily be decomposed into a mixture-fraction vector and a reaction-progress vector. A precise definition of the mixture-fraction vector can be derived and the derivation is very instructive: for example, it is shown how the length of this vector will depend on the number of inlets and the number of chemical elements. Application to turbulent flows requires determination of the multivariate mixture-fraction PDF [5]. The difficulties associated with the representation of such a joint PDF have been illustrated for the case of two passive scalars (ternary mixing) by Juneja and Pope [6], who conducted a detailed investigation of the effects of the initial length scales and the molecular diffusivity of the scalars on the evolution of this PDF and the corresponding conditional diffusion terms. These DNS data have been used, for instance, in Ref. [7] to analyze the performance of the Lagrangian Fokker–Planck (LFP) model of Fox [8]. Even in nonreacting flows, the presence of multiple inlets combined with partial premixing and recirculating flow makes the a priori specification of such a joint scalar PDF challenging. However, this

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[1] In the absence of any partial premixing between fuel and oxidizer, we have $Y_{F,ox}^\infty = 0$ and $Y_{O,fuel}^\infty = 0$, in such a manner that the classical pure mixing formulae, i.e., $Y_{O,u} = (1 - \xi)Y_{O,ox}^\infty$ and $Y_{F,u} = \xi Y_{F,fuel}^\infty$, may be deduced from these expressions.