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Influence of evaporation on spray flamelet structures

Hernan Olguin, Eva Gutheil *

Interdisciplinary Center for Scientific Computing, University of Heidelberg, Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

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A B S T R A C T

The structure of laminar spray flames considerably differs from their gaseous counterpart. However, most often flamelet models employed in the simulation of turbulent spray combustion are based on laminar gas flame structures neglecting the influence of spray evaporation in the laminar spray flamelets. In this work, a combined theoretical and numerical study of the impact of spray evaporation on the structure of laminar spray flames is presented. Spray flamelet equations are derived, which explicitly take into account evaporation effects – the classical gas flamelet equations are recovered for non-evaporating conditions. Two new terms accounting for evaporation and for combined mixing and evaporation, respectively, are identified, and their relative importance is evaluated by means of numerical simulations of an axisymmetric laminar mono-disperse ethanol/air counterflow spray flame. The results show that the distribution of the spray evaporation rate plays a key role in the characterization of the spray flame structure. The new source terms overweigh the dissipation term of the gas phase in most situations even for non-evaporating species. Therefore, spray evaporation should always be considered. The relevance of the present formulation for turbulent spray modeling is evaluated and discussed, and a novel spray flamelet formulation is suggested.

1. Introduction

Spray combustion under turbulent conditions occurs in many practical combustion systems such as internal combustion engines, industrial furnaces, household burners, turbines and liquid-fueled rockets. Therefore, a proper prediction of the characteristics of turbulent spray flames is of vital importance for the design of these combustion devices in view of combustion efficiency and pollutant reduction, where the latter requires consideration of detailed chemical reaction mechanisms in numerical simulations. Unfortunately, a direct inclusion of detailed chemical reactions dramatically increases the computational cost of the numerical simulations of technical combustion processes, and it is prohibitive in practical situations. Therefore, flamelet models have been established to include detailed chemical schemes into turbulent (spray) flame computations.

Several flamelet formulations have been derived in the last decades [1–4]. The flamelet concept for turbulent combustion considers the turbulent flame as an ensemble of laminar flames [1], and it is valid for high Damköhler numbers, which is fulfilled in many technical combustion applications. The success of flamelet based models in the simulation of turbulent gas flames has motivated their application in the simulation of turbulent spray flames [5–9]. In classical flamelet models for gas flames, strict assumptions regarding the different combustion regimes that may occur in turbulent flames are made. In general, either non-premixed or premixed combustion is considered, whereas partially premixed regimes are discarded.

The multi-regime nature of turbulent flames must be taken into account in order to overcome the limitations of classical flamelet models. Recently, several multi-regime flamelet models have been developed [10–12] using gas flamelets. In this context, Franzelli et al. [12] proposed the use of partially-premixed pure gas flame libraries for the simulation of spray flames. However, spray flames exhibit combustion regimes which are strongly dominated by evaporation effects. These regimes are not found in pure gas flames and, therefore, libraries based on gas flame structures are not suitable to properly describe the flame structure in spray combustion. A separation of the regimes with pure gas combustion, i.e. all droplets have vaporized, and the regimes where both evaporation and combustion occur simultaneously [13], allows the implementation of multi-regime gas flamelet models in the pure gas combustion regimes, but it does not solve the question of how to model the regimes, where both evaporation and chemical reactions occur.

Hollmann and Gutheil [14] and Gutheil [13] proposed an extension of the classical non-premixed flamelet model [1] for spray flames, which consistently uses a library based on laminar spray structures. It is found that the structure of spray flamelets is not only determined by the mixture fraction and its scalar dissipation rate (associated with the strain rate) as in counterflowing laminar gas diffusion flames [1], but they also depend on the initial droplet

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* Corresponding author.
E-mail address: gutheil@iwr.uni-heidelberg.de (E. Gutheil).

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size and velocity and the equivalence ratio on the spray side of the configuration [15,16,13,14]. The inclusion of these additional parameters is required in order to characterize laminar spray flamelets. This has been successfully achieved for turbulent methanol/air [14,17] and ethanol/air [18] spray flames. However, this approach includes a high-dimensional flamelet library of the order five for the mixture fraction, its scalar dissipation rate, the equivalence ratio, and the initial droplet size and velocity.

Currently, most studies of turbulent spray flames use laminar gas flamelet structures [9,6,8,7], even though it is known that evaporation may greatly influence the spray flamelet [19–21,13,14,22–24]. Recent studies [25–28] in the framework of conditional moment closure (CMC) models for turbulent spray combustion also highlighted the need for including the spray evaporation source term into spray flame modeling.

The scope of the present study is the reconsideration of flamelet equations for use in spray combustion with emphasis on the evaporation and its effect on the spray combustion process. For this purpose, the spray flamelet equations are derived and the different contributions in the new equations are analyzed for laminar ethanol/air spray flames. The new flamelet equations and their evaluation lead to a revised formulation of the flamelet model for spray combustion.

2. Mathematical model

A Eulerian–Lagrangian formulation of a dilute, reactive spray flow in the counterflow configuration is employed. An axi-symmetric two-dimensional ethanol/air spray flame is considered. The mono-disperse spray is characterized through equations accounting for droplet heating, evaporation, and motion. A single component, spherically symmetric, unsteady droplet model is employed, even though the formulation, in general, is not restricted to single component and mono-disperse sprays [29]. Similarity [15,16] is assumed, which transfers the two-dimensional problem into a one-dimensional formulation. This transformation and its application to viscous flows allow for the inclusion of detailed chemical reaction mechanisms [16,29,13]. A chemical reaction mechanism consisting of 38 species and 337 elementary reactions for ethanol/air [30,29] is implemented. In view of the derivation of the spray flamelet formulation, the general equations to describe the problem are summarized.

2.1. Governing equations

The general governing equations for the gas and liquid phase are presented, which then are used for the derivation of novel spray flamelet equations.

2.1.1. Gas phase

The conservation equations of the mass, momentum, mass fractions of chemical species and energy can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = S_v, \tag{1}$$

$$\rho\frac{\partial u_j}{\partial t} + \rho u_i \frac{\partial u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_i} - u_j S_v + S_{m,j}, \tag{2}$$

$$\rho\frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} + \frac{\partial V_{k,i}}{\partial x_i} = \dot{\omega}_k + (\delta_{lk} - Y_k)S_v, \quad k = 1,\ldots,N, \tag{3}$$

$$\begin{aligned}\rho C_p\frac{\partial T}{\partial t} + \rho u_i C_p \frac{\partial T}{\partial x_i} = {} & -\sum_{k=1}^{N} h_k\dot{\omega}_k + \frac{\partial p}{\partial t} + u_i\frac{\partial p}{\partial x_i} - \tau_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x_i}\right) \\ & - \frac{\partial T}{\partial x_i}\sum_{k=1}^{N} C_{p,k}V_{k,i} - S_v\int_{T_0}^{T} C_{p,l}\,\mathrm{d}T + S_e,\end{aligned} \tag{4}$$

where u_i is the gas velocity in i direction, ρ is the gas density, Y_k is the mass fraction of species k, C_p and $C_{p,\,k}$ are the specific heat capacity at constant pressure of the mixture and of species k, respectively, p is the static pressure, h_k is the enthalpy of species k, and λ denotes heat conductivity. S_v, $\mathbf{S}_m$, and S_e are sources of mass, momentum and energy, respectively, and they will be given in sub-Section 2.1.2. δ is the Kronecker symbol, l denotes the evaporating liquid component and $\dot{\omega}_k$ is the specific chemical reaction rate of species k for $k = 1, \ldots, N$. $V_{k,\,i}$ is the diffusion velocity of species k in i direction into the mixture, which is given as

$$V_{k,i} = -\rho D_k \frac{Y_k}{X_k}\frac{\partial X_k}{\partial x_i} - \frac{D_T}{T}\frac{\partial T}{\partial x_i}, \tag{5}$$

where D_k is the diffusion coefficient of species k in the mixture and D_T is the thermal diffusion coefficient. The viscous tensor τ_{ij} is defined by

$$\tau_{ij} = -\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij} \tag{6}$$

neglecting the bulk viscosity, and μ is the dynamic gas viscosity.

The terms including the spray mass source, S_v, appearing in Eqs. (2)–(4) are introduced through use of the continuity Eq. (1) in these equations.

The formulation of the spray flamelet equations requires the definition of the mixture fraction. In gas combustion processes including hydrocarbons or alcohols, most often the mixture fraction definition is based on the chemical element C, because this formulation fulfills the requirements of monotonicity and boundedness of the mixture fraction between zero and unity [31]. In general, the definition of the mixture fraction based on a chemical element, A, yields

$$\xi_{\mathrm{A}} = \frac{Z_{\mathrm{A}} - Z_{\mathrm{A,min}}}{Z_{\mathrm{A,max}} - Z_{\mathrm{A,min}}}, \tag{7}$$

where Z_{A} is the mass fraction of element A and N is the total number of chemical species in the system. Z_{A} can be expressed as

$$Z_{\mathrm{A}} = \sum_{k=1}^{N}\left(\frac{a_{k\mathrm{A}}M_{\mathrm{A}}}{M_k}\right)Y_k, \tag{8}$$

where $a_{k\mathrm{A}}$ denotes the number of moles of element A in species k, and M_{A} and M_k denote the molecular weights of element A and of species k, respectively. In the remainder of the present work, the mixture fraction is noted as ξ.

With the definition of Y_k and the product law, Eq. (5) can be rewritten as

$$V_{k,i} = -\frac{\partial}{\partial x_i}\left(\rho D_k\frac{\partial Y_k}{\partial x_i}\right) - \frac{\partial}{\partial x_i}\left(\rho\frac{D_k Y_k}{\overline{M}}\frac{\partial \overline{M}}{\partial x_i}\right) - \frac{D_T}{T}\frac{\partial T}{\partial x_i}, \tag{9}$$

where $\overline{M}$ is the mean molecular weight of the mixture. If the contribution of the last two terms on the right hand side is small, Eq. (9) reduces to Fick's diffusion law, and Eq. (3) yields

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_i Y_k)}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_k\frac{\partial Y_k}{\partial x_i}\right) = \dot{\omega}_k + \delta_{lk}S_v. \tag{10}$$

In the numerical computations, thermal diffusion is considered only for the light species H and H_2. Analysis of the pertinence of the negligence of the term containing the variable mean molecular weight $\overline{M}$ in the derivation of the mixture fraction, cf. Eq. (9), will be presented in the results' section.

Multiplication of Eq. (10) by $a_{k\mathrm{A}}M_{\mathrm{A}}/M_k$ and summation over all species N yields the transport equation of the mass fraction of element A, Z_{A}, and with the assumption of equal diffusion coefficients, $D_k = D$, $k = 1, \ldots, N$ for all species k, and following Eq. (7), the transport equation of the mixture fraction, ξ, is obtained as