Joint-Pdf Modelling of Reactive Sprays via an Evaporation-Progress Variable

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Abstract

In this paper we present the modelling of reactive sprays via a probability density formulation. Without loss of generality the joint pdf is written as a sum of a joint pdf for the liquid and a joint pdf for the gaseous phase. Based on suitable assumptions the gasphase combustion chemistry can be reduced to a three-variable formalism, whereas the liquid phase is described in the usual manner. For low-Mach flows a special pressure-correction algorithm has been developed to ensure consistency of mean fluid density and normalized particle density. This algorithm shows its effectiveness even for laminar burner-stabilized and freely propagating flames, where the results agree well with benchmark solutions. Further computations focus on the interaction of liquid and gaseous fluid phase.

Introduction

A popular and yet sophisticated approach to modelling turbulent gasphase combustion is based on joint probability density functions, so-called joint pdf's, for which transport equations are derived, modelled and numerically solved. This methodology to describe flows was introduced in 1967 by Lundgren [1] for turbulent velocity fields and in 1970 by Hill [2] and Dopazo and O'Brien [3] in the context of turbulent reactive flows; in combustion it has become popular and more widespread through the work of Pope, see e.g. [4].

Due to the very large number of very small liquid droplets usually involved in liquid sprays, sprays too are often described in terms of a joint probability density function. An early version of joint pdf for sprays was derived by *Williams* [5] and hence sometimes it is referred to as *Williams' spray equation*.

It appears natural that for turbulent reactive flows involving sprays a joint-pdf formulation should exist that – in a sense yet to be specified – includes, say, Pope's joint gasphase pdf and, say, Williams' spray equation. A first formulation along these lines was developed by *Zhu et al* [6]. In the present paper, a similar but simpler and hence more practical spray model is developed which is based on only three scalar gasphase variables, viz., (i), a mixture-fraction variable describing the extent to which local and instantaneous mixing of gaseous fuel and ozidizer has taken place, (ii), a reaction-progress variable describing the extent to which local and instantaneous gasphase reaction has taken place, and (iii), an evaporation-progress variable describing the extent to which locally and instantaneously evaporation has taken place. A joint pdf for both phases is derived. For a laminar one-dimensional geometry, this pdf is numerically solved using a particle method which involves a special pressure-correction algorithm. Specifically, two cases are considered, viz., (i), a steady non-reactive evaporation and mixing case where a cold fuel spray is injected into a hot environment of oxidizer and, (ii), a steady laminar premixed spray flame. The numerical results clearly demonstrate both the efficiency and the accuracy of the joint-pdf method thereby underlining its usefulness not only for laminar but also for turbulent combustion simulations.

Gasphase Description

Locally and instantaneously in a two-phase flow, the gasphase is governed by the well known conservation equations for overall mass, species mass, momentum and energy which, however, contain terms describing

mass, momentum and energy transfer between the phases. For instance, the *everywhere* in the flowfield locally and instantaneously valid overall mass conservation equation for the *gasphase* can be written as

$$L(1) = g_M av{(1)}$$

where for any dependent variable ϕ – in tensor notation –

$$L(\phi) := \frac{\partial \rho \epsilon \phi}{\partial t} + \frac{\partial \rho \epsilon \phi U_i}{\partial x_i}$$
(2)

is the operator representing accumulative (or unsteady) and convective terms; ϵ is a phase function taking values of zero and one in the liquid and gaseous phase, respectively, and g_M is the mass of gasphase generated per unit volume and time by evaporation of liquid; the other symbols in Eq. (1) have their usual meaning. The evaporation term g_M differs from zero only at the interface separating the two phases; its magnitude there is proportional to the relative velocity between flow and interface.

Based on the assumption that the gasphase combustion chemistry can be described by a global one-step reaction between fuel and oxidizer leading to a single combustion product, a Shvab-Zel'dovich type of procedure to derive coupling functions between the mass fractions of individual species and between the mass fraction of product and enthalpy leads, together with suitable normalization, to three scalar variables that describe the gasphase, viz., a mixture fraction variable ζ governed by $L_W(\zeta) = 0$, a reaction-progress variable c governed by $L_W(c) = \epsilon w_c$ and an evaporation-progress variable η governed by $L_W(\eta) = w_{\eta}$. Here L_W is an operator similar to that defined in (2) but also including diffusive effects; ζ and c are defined as usual, and η is a suitably normalized fuel mass fraction; w_c and w_{η} denote the respective reaction and evaporation term.

Liquid-Phase Description

The liquid phase is described in a Lagrangian manner. To this end, groups of droplets are considered, each group being occupied by droplets with comparable properties and hence being represented by one particle $\underline{\xi}$. The Lagrangian equations of motion for a droplet group can written in the form $(\partial \underline{x}_d/\partial t)|_{\underline{\xi}} = \underline{U}_d$ with $(\partial \underline{U}_d/\partial t)|_{\underline{\xi}} = \underline{W}$, the respective mass conservation equation as $(\partial R/\partial t)|_{\underline{\xi}} = Q_M$ and the respective energy conservation equation as $(\partial e/\partial t)|_{\underline{\xi}} = Q_e$. The symbols and source terms have the usual and obvious meaning; source terms have to be specified.

Joint-Pdf for Both Phases

Without loss of generality, for the joint pdf f the additive form $f = f_I + f_{II}$ is assumed. Here f_I denotes the contribution to f of the liquid phase, f_{II} the contribution to f of the gasphase. For the sytems and flames considered herein, $f_I = f_I(\underline{\hat{U}}, \hat{e}, \hat{R}; \underline{x}, t)$ and $f_{II} = f_{II}(\underline{\hat{U}}, \hat{\zeta}, \hat{c}, \hat{\eta}; \underline{x}, t)$. Here carets are used to denote the phase variables of the respective stochastic quantities; $\underline{\hat{U}}$ is the phase-independent velocity vector (the phase being taken into account explicitly by distuiguishing between f_I and f_{II}). For f_I the transport equation

$$\frac{\partial}{\partial t} \{ \rho_l f_I \} + \hat{U}_i \frac{\partial}{\partial x_i} \{ \rho_l f_I \} + \frac{\partial}{\partial \hat{U}_i} \left\{ W_i(\underline{\hat{U}}, \hat{R}) \rho_l f_I \right\} + \frac{\partial}{\partial \hat{e}} \left\{ Q_e(\underline{\hat{U}}, \hat{e}, \hat{R}) \rho_l f_I \right\} + \frac{\partial}{\partial \hat{R}} \left\{ Q_M(\underline{\hat{U}}, \hat{e}, \hat{R}) \rho_l f_I \right\} = 0$$
(3)

can be derived, for f_{II} the transport equation

$$\frac{\partial}{\partial t} \{ \rho_g f_{II} \} + \hat{U}_i \frac{\partial}{\partial x_i} \{ \rho_g f_{II} \} + \frac{\partial}{\partial \hat{U}_j} \left\{ \left(-\frac{\partial \langle p \rangle}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle}{\partial x_i} \right) f_{II} \right\} - \frac{\partial}{\partial \hat{c}} \left\{ \frac{\partial \langle J_i^c \rangle}{\partial x_i} f_{II} \right\} + \frac{\partial}{\partial \hat{c}} \left\{ w_c(\hat{\zeta}, \hat{c}, \hat{\eta}) f_{II} \right\} - \frac{\partial}{\partial \hat{\zeta}} \left\{ \frac{\partial \langle J_i^{\zeta} \rangle}{\partial x_i} f_{II} \right\} - \frac{\partial}{\partial \hat{\eta}} \left\{ \frac{\partial \langle J_i^{\eta} \rangle}{\partial x_i} f_{II} \right\} = - \frac{\partial}{\partial \hat{U}_i} \left\{ \gamma \left(\left\langle -\frac{\partial p'}{\partial x_i} \right\rangle_g + \left\langle \frac{\partial \tau'_{ij}}{\partial x_j} \right\rangle_g \right) f_{II} \right\}$$

$$(4)$$

$$+ \frac{\partial}{\partial\hat{\zeta}} \left\{ \gamma \left\langle \frac{\partial J_{i}^{\zeta'}}{\partial x_{i}} \right\rangle_{g} f_{II} \right\} + \frac{\partial}{\partial\hat{c}} \left\{ \gamma \left\langle \frac{\partial J_{i}^{c'}}{\partial x_{i}} \right\rangle_{g} f_{II} \right\} + \frac{\partial}{\partial\hat{\eta}} \left\{ \gamma \left\langle \frac{\partial J_{i}^{\eta'}}{\partial x_{i}} \right\rangle_{g} f_{II} \right\}$$
$$+ \left\langle \rho B | \underline{\hat{U}}, \hat{\zeta}, \hat{c}, \hat{\eta}, \hat{\beta}^{I} \right\rangle f(\underline{\hat{U}}, \hat{\zeta}, \hat{c}, \hat{\eta}, \hat{\beta}^{I}; \underline{x}, t) .$$

In Eqs. (3) and (4) it is understood that $\rho_l = \rho_l(e)$ and $\rho_g = \rho_g(\zeta, c, \eta)$, respectively. Integration of (3) shows that, if the temperature dependence of the ρ_l is neglected, then Williams' spray equation is obtained for the marginal distribution $f_s := \int_{-\infty}^{\infty} f_I d\hat{e}$.

Numerical Method and Results

Equations (3) and (4) are solved using a particle method. The usefulness of a particle method for the simulation of flow problems heavily relies on the consistency between fluid density and particle density, which requires that both are proportional to each other. Given an initial density field, at any instant of time and at any location, this proportionality has to be ensured by a proper pressure gradient.



Figure 1: Profiles of fluid density (solid line) and normalized particle density (symbols) through a laminar premixed burner-stabilized flame. Evaporation has been completed.

To this end an effective pressure-correction algorithm has been developed and implemented into a particle method, which is valid for laminar and turbulent flows with steep gradients in density and velocity like those encountered in thermal expansion. Since laminar flames represent more stringent test cases for numerics than turbulent ones, the method has been applied to various laminar non-reactive and reactive flows.

Figure 1 demonstrates that the pressure algorithm developed herein indeed ensures consistency, here shown for a laminar premixed burner-stabilized flame for fully evaporized liquid. The solid line represents the mean or fluid density, the circles represent the normalized particle density. The latter is randomly distributed about the fluid density due to statistical error, which is seen to increase with decreasing particle numbers per cell downstream of the flame.

Further calculations have been carried out for burner-stabilized and freely propagating premixed laminar flames, where analytical results are known from large-activation energy asymptotics [7]. The computed results agree very well with the benchmark solutions. They clearly demonstrate both the efficiency and the accuracy of the method thereby underlining its usefulness for laminar and turbulent combustion simulations.

In Fig. 2 we study a non-evaporating case, where the interaction of liquid and gaseous fluid phase is reduced to the exchange of momentum. The equations are solved for a laminar, one-dimensional and mono-disperse spray.



Figure 2: Exchange of momentum for mono-disperse spray in laminar flow; $\rho_l/\rho_q = 100$.

Figure 2 displays in its left column the mass-weighted joint pdfs of the liquid phase $\rho_l f_I(\hat{U}, x; t)$ and the gasphase $\rho_g f_{II}(\hat{U}, x; t)$, respectively. Mean profiles for all liquid-phase and gasphase variables of interest are derived by integration, like those shown in the right column, which are for the velocities of liquid and gas respectively and for the mean pressure distribution and its gradient. The recovery of static pressure due to the exchange of momentum is clearly seen.

The simulations currently under way focus on (i) a steady non-reactive evaporation and mixing case, where a cold fuel spray is injected into a hot environment of oxidizer and (ii) a steady laminar spray flame.

References

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