



Composition-space premixed flamelet solution with differential diffusion for in situ flamelet-generated manifolds

G. Lodier^{a,b}, L. Vervisch^{a,*}, V. Moureau^a, P. Domingo^a

^a CORIA – CNRS and INSA de Rouen, Technopole du Madrillet, BP 8, 76801 Saint-Etienne-du-Rouvray, France

^b RENAULT – Technocentre 1, Avenue du Golf, 78288 Guyancourt cedex, France

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ABSTRACT

Canonical flame problems have been widely used in the combustion literature to tabulate detailed chemistry. Prior to three-dimensional flame simulations, reference laminar premixed flames are usually solved in physical-space, and, diffusion flames in either physical, or, mixture fraction space. Composition-space solutions would be convenient for premixed flame also, because all the points are relevant for chemistry, as a result of the zoom inside the flame zone; however, differential diffusion is not always easy to introduce with accuracy in these moving-frame coordinate systems, parameterized by their physical-space gradients (or scalar dissipation rates). A projection is discussed in this paper that ensures that differential diffusion is properly accounted for, in any composition-space coordinates, thus allowing for perfect matching between physical- and composition-space solutions, even for premixed flames. Both a diffusion velocity correction, which is necessary to properly conserve mass with Fick's law, and a differential diffusion effect between the composition-space moving with the flow and fast diffusing species, are introduced. A procedure for rapidly building converged composition-space solutions for premixed flamelets is then proposed and tested. It provides the framework for an efficient in situ calculation of complex chemistry with differential diffusion, to be applied to three-dimensional unsteady flame simulations. The objective is to avoid building *a priori* look-up tables, whose range of validity is strongly limited by their boundary conditions, which are fixed once for all, therefore lacking of generic character, specifically when pressure, composition and enthalpy of fresh gases are varying in space and time.

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1. Introduction

Numerous techniques have been discussed in the literature to reduce and parameterize the complexity of combustion detailed chemistry, the main objective is to facilitate the introduction of this latter in numerical simulations [1–9]. Some of these approaches make use of pre-tabulated flame responses obtained from canonical combustion problems, as premixed or diffusion flamelets. To build tabulations, the physical-space flame solution is projected in an appropriate composition-space of reduced dimension; burning rate and species are then read from their composition-space trajectories, after transporting with the flow only their controlling parameters (*i.e.* the composition-space coordinates values).

Recently, using a systematic projection of the full set of species balance equations into a given composition-space, a Multi-dimensional Flamelet-generated Manifolds (MFM) was derived [10]. The species and temperature equations were solved directly

in composition-space instead of physical-space, the solution was validated for unity Lewis number premixed flames and explored for partially premixed flames, as triple-flame, in a two-dimensional composition-space (mixture fraction and progress of reaction). In the latter, both fluxes of mass and heat occurring across equivalence ratio surfaces and across the main reaction zones were coupled in a natural manner, to reproduce partially-premixed combustion properties. The solution procedure was time dependent, accordingly the computational effort to reach a steady-state solution was non-negligible; moreover, only the unity Lewis test case was validated and the differential diffusion drift-terms between composition-space and species were neglected, as usually done in flamelet composition-space solution. The first objective of this paper is to investigate the exact contribution of these additional terms, to propose a methodology to introduce them in the composition-space solution, and finally to derive a fast solution procedure for premixed flamelets.

The composition-space projection is very convenient for building canonical-flame solutions, mainly for two reasons. First, the composition-space is a frame attached to the flame acting as a zoom inside the diffusive and reactive layers, so that less mesh

* Corresponding author.

E-mail address: vervisch@coria.fr (L. Vervisch).

points are needed compared to physical-space solutions. Second, asymptotic solutions exist in composition-space in the limit of large mixing rate, even for intermediate radicals. These asymptotic solutions are very helpful to initialize flame solving and reduce convergence time versus physical-space solutions, where the unavoidable departure between the first guess of intermediate species profiles and their converged distribution, may lead to quite time consuming runs.

However, some important issues still need to be discussed concerning such chemistry tabulation directly obtained from composition-space premixed flame solution. The determination of the proper composition-space coordinates for complex hydrocarbon fuels may not be trivial, this point is not addressed in this paper, only methane vitiated-air combustion is considered for which proper coordinates have been previously derived [4]. Differential diffusion is another major point, it is an essential ingredient to reproduce the proper flame propagation speed and the exact intermediate species profiles.

Differential diffusion appears in composition-space in two terms. The first is a relative diffusion term between the composition-space coordinates and the chemical species that is solved. This differential-diffusion drift is usually neglected and it is discussed thereafter how to include it, along with a diffusive velocity correction, to ensure mass conservation with diffusion coefficients obtained with Curtiss and Hirschfelder's law [11]. The other differential-diffusion contribution is usually cast as a correction to the scalar dissipation rate of the composition-space coordinate, expressed via a Lewis number. It is shown that this is not enough to avoid an additional drift between the reference physical-space solution and the composition-space one. An alternative formalism is proposed where the composition-space solution perfectly matches the physical-space distribution. In the light of this result, a specific numerical treatment is discussed that allows for fast building of chemical solutions for premixed flamelets in composition-space directly.

Another major drawback of canonical-flame based chemistry tabulations is the need to highly reduce the complexity of the reference diffusive-reactive problem, specifically to fix the boundary conditions. Fresh and burnt gases conditions are usually chosen once for all, and an in situ flame solution, with boundary conditions evolving according to the local flow properties, as already done in some advanced simulations [12], would tremendously improve the chemical modeling; in principle allowing for dilution by burnt products, heat loss due to wall or radiative transfer coupled with soot, and pressure variations, to be included with precision. This point is addressed with the description of a modeled, or canonical, flame solution fast procedure for an in situ flamelet-generated manifolds (IFM). The wording modeled is here essential; indeed the physical-space gradient of the composition-space coordinate is needed as an input in this approach and composition-space solutions cannot fully supplement standalone physical-space solutions with detailed chemistry, but are rather a modeling tool for getting fast approximate solutions in turbulent flames. It is also important to note that this solution is only valid for the flame mode retained (here premixed) and cannot be considered as fully generic.

2. Composition-space canonical-flame solution with differential diffusion

2.1. Budget equations

The balance equation verified by the N species mass fractions Y_i and temperature T , in the case of a low Mach-number steady flame at constant pressure, may be written [13]:

$$\nabla \cdot (\rho(\mathbf{u} + \mathbf{V}_i + \mathbf{V}_a)Y_i) = \dot{\omega}_i \quad (1)$$

$$\begin{aligned} \nabla \cdot (\rho \mathbf{u} T) &= \frac{1}{C_p} \nabla \cdot (\lambda \nabla T) - \frac{1}{C_p} \sum_{i=1}^N h_i \dot{\omega}_i \\ &\quad - \frac{1}{C_p} \sum_{i=1}^N \rho C_{p_i} Y_i (\mathbf{V}_i + \mathbf{V}_a) \cdot \nabla T \end{aligned} \quad (2)$$

where \mathbf{u} is the velocity vector; ρ is the density; D_i , C_{p_i} , h_i are the molecular diffusion coefficient, the calorific capacity at constant pressure and the enthalpy of the i th species, respectively; λ is the thermal conductivity and C_p is the calorific capacity of the mixture. The diffusive velocity is written:

$$\mathbf{V}_i = -D_i \frac{1}{X_i} \nabla X_i \quad (3)$$

D_i is the diffusion coefficient obtained from the Hirschfelder and Curtiss approximation [11], X_i is the molar fraction of the i th species, $X_i/W = Y_i/W_i$ with W_i and $W = 1/\sum_{k=1}^N (Y_k/W_k)$ the molar weights of the i -th species and of the mixture, respectively. (W_i is a constant and W varies with space.) The diffusive flux of mass thus reads:

$$\rho \mathbf{V}_i Y_i = -\rho D_i \frac{W_i}{W} \nabla X_i = -\rho D_i \left(\nabla Y_i + Y_i \frac{\nabla W}{W} \right) \quad (4)$$

\mathbf{V}_a is an additional correction velocity ensuring global mass conservation (i.e. $\nabla \cdot (\rho \mathbf{u}) = 0$ summing up Eq. (1) over all species):

$$\mathbf{V}_a = - \sum_{k=1}^N \mathbf{V}_k Y_k = \sum_{k=1}^N D_k \left(\nabla Y_k + Y_k \frac{\nabla W}{W} \right) \quad (5)$$

These species and temperature equations are projected into a frame attached to the flame. This projection is applied in this paper to a one-dimensional composition-space Y_c , which may be a reactive coordinate. The physical-space derivative may be written:

$$\nabla \bullet = \nabla Y_c \frac{d\bullet}{dY_c} \quad (6)$$

Denoting $\nabla Y_c = G_c(Y_c)$, one may introduce A_i and B_i so that the diffusive flux becomes $-\rho V_i Y_i = \rho G_c A_i$, with

$$A_i = D_i \frac{dY_i}{dY_c} + B_i \quad (7)$$

$$B_i = D_i Y_i \frac{d \ln(W)}{dY_c} \quad (8)$$

The equation for Y_c takes a form similar to Eq. (1) and may be organized in:

$$\rho(\mathbf{u} + \mathbf{V}_a) \cdot \nabla Y_c = \dot{\omega}_c - \nabla Y_c \cdot \left[\frac{d}{dY_c} (\rho \mathbf{V}_c Y_c) + Y_c \frac{d}{dY_c} (\rho \mathbf{V}_a) \right] \quad (9)$$

Using Eq. (6) in Eq. (1), the term $\rho(\mathbf{u} + \mathbf{V}_a) \cdot \nabla Y_c$ appears in Eq. (1) and is replaced by the RHS of Eq. (9). The same is done in the equation for T in which $\rho \mathbf{u} \cdot \nabla Y_c$ is made explicit with Eq. (6), to be expressed from Eq. (9). After some additional manipulations making also use of Eq. (6), the governing equations become:

$$\begin{aligned} &\left[\underbrace{\dot{\omega}_c - Y_c G_c \frac{d}{dY_c} \left(\rho G_c \sum_{k=1}^N A_k \right)}_{(ii)} + \underbrace{G_c \frac{d}{dY_c} (\rho G_c (D_c - D_i + B_c))}_{(iii)} \right] \frac{dY_i}{dY_c} \\ &\quad - \underbrace{\rho D_i G_c^2 \frac{d^2 Y_i}{dY_c^2} - G_c \frac{d}{dY_c} (\rho G_c B_i)}_{(iv)} + \underbrace{Y_i G_c \frac{d}{dY_c} \left(\rho G_c \sum_{k=1}^N A_k \right)}_{(v)} - \underbrace{\dot{\omega}_i}_{(vi)} = 0 \end{aligned} \quad (10)$$

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