Modelling of Premixed Counterflow Flames Using the Flamelet-Generated Manifold Method

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Abstract

The recently introduced reduction technique called flamelet-generated manifold (FGM) method is used to compute premixed methane/air counterflow flames. In the FGM method the ideas of the manifold and the flamelet approach are combined: a manifold is constructed using one-dimensional flamelets. In this paper the effect of flame stretch on the accuracy of the FGM method is investigated. In the case of unit Lewis numbers a one-dimensional manifold is able to model the main effects of flame stretch. A manifold with two progress variables reproduces the results computed using detailed kinetics almost exactly. When non-unit Lewis numbers are used, the enthalpy and element composition of the burnt mixture change, which influences the mass burning rate significantly. If these composition changes are included in the manifold using an additional controlling variable, the results agree well with detailed computations.

Introduction

Although the power of computers has increased a lot during the last decade, the computation time of realistic flame simulations using detailed reaction kinetics remains extremely high. To reduce the computational cost of these simulations, several methods have been developed to simplify the description of the chemical kinetics. One of the most promising reduction techniques is the one proposed by Maas and Pope [1], called Intrinsic Low-Dimensional Manifold (ILDM) method. This technique is based on a time scale analysis of the chemical source term. Recently, another manifold technique called Flamelet-Generated Manifold (FGM) method has been introduced [2], in which steady-state assumptions are not only based on 'chemical' assumptions but also on the most important transport processes. This method shares the idea with flamelet approaches that a more-dimensional flame can be considered as an ensemble of one-dimensional (1D) flamelets. In the FGM method 1D laminar flamelets are used to create a manifold, which can be used for subsequent flame simulations in the same way as an ILDM. A similar technique called Flame Prolongation of ILDM (FPI) has been proposed recently by Gicquel *et al.* [3].

In this paper we will study the effect of flame stretch on the accuracy of the FGM method. Flame stretch is one of the most important multi-dimensional effects, which is neglected while constructing a FGM. However, we will demonstrate that this does not mean that flame stretch effects (possibly in combination with preferential diffusion) cannot be taken into account using FGM. Moreover, we will show that a FGM can be extended with extra progress variables in order to reach a higher accuracy.

Stationary premixed counterflow flames are modelled using both detailed reaction kinetics

and FGM. These flames are very suitable to investigate flame stretch, because other effects such as flame curvature and instationary effects are not present.

Flamelet-generated manifold

In this section we review the FGM method shortly; for more details the reader is referred to [2]. Consider a curve $\mathbf{x}(s)$ through a premixed flame, locally perpendicular to isosurfaces of a certain species mass fraction Y_j, and parametrized by the arclength s. The 3D instationary conservation equations for the species mass fraction can be rewritten into a 1D equivalent along this curve:

$$\frac{\partial m Y_i}{\partial s} - \frac{\partial}{\partial s}\left(\frac{\lambda}{Le_i\, c_p}\frac{\partial Y_i}{\partial s}\right) - \dot{\rho}_i = P_i, \tag{1}$$

with λ the thermal conductivity, c_p the specific heat, Le_i the Lewis number, $\dot{\rho}_i$ the chemical source term, and m the mass flow rate. All multi-dimensional and instationary effects are gathered in the perturbation term P_i. Since it is expected that in most situations in premixed flames P_i is small compared to the other terms in Eq. (1), the perturbation P_i is neglected. The remaining steady-state balance between reaction, convection and diffusion is called a flamelet equation. Note that the diffusion and convection terms are also neglected in the ILDM method. The set of flamelet equations for all species together with a similar equation for the enthalpy can be solved treating the system as a 1D adiabatic premixed flame. Its solution is called a flamelet and forms a 1D curve in composition space, which can be considered as a 1D manifold.

The accuracy of the FGM method can be increased by increasing the number of progress variables. When the perturbation P is not small, an extra dimension can be added to the manifold. In this way an extra degree of freedom is added to the system and the magnitude of the component of the vector P perpendicular to the manifold is reduced.

A FGM with two progress variables can be constructed from a set of flamelets with inlet boundary conditions at different points on a 1D curve in composition space with constant enthalpy h and element mass fractions Z_j. This set of 1D flamelets can be used to form a 2D surface in composition space: a 2D FGM. This method to generate multi-dimensional manifolds can be extended to the general case of d dimensions by choosing a $(d-1)$-dimensional starting plane.

Similar to the ILDM method, the FGM can be extended with additional controlling variables to account for variations in the conserved variables h and Z_j as well. If, for instance, changes in the enthalpy are expected, a series of manifolds is created for different values of the enthalpy and h is added to the manifold as extra controlling variable.

Once a manifold is constructed, it is used in the same way as an ILDM. The manifold is parametrized as a function of the controlling variables and is stored in a database. This database can be linked to a flame-solver, which solves conservation equations for the controlling variables.

Premixed methane/air counterflow flames

To investigate the influence of flame stretch premixed stoichiometric methane/air flames in a planar stagnation flow are modelled. It is well known that these flames can be described by a set

of 1D equations [4]:

$$\frac{\partial m}{\partial x} = -\rho K, \tag{2}$$

$$\frac{\partial mK}{\partial x} - \frac{\partial}{\partial x}\left(\eta\frac{\partial K}{\partial x}\right) = \rho_u a^2 - 2\rho K^2, \tag{3}$$

$$\frac{\partial mY_i}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\lambda}{Le_i\, c_p}\frac{\partial Y_i}{\partial x}\right) - \dot{\rho}_i = -\rho K Y_i, \tag{4}$$

$$\frac{\partial mh}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial x}\right) = -\rho K h + \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\sum_i^{N_s} h_i\left(\frac{1}{Le_i}-1\right)\frac{\partial Y_i}{\partial x}\right), \tag{5}$$

with K the local stretch rate, a the applied strain rate, η the viscosity, and N_s the number of species. If we compare Eq. (4) with Eq. (1), we see that in these flames the perturbation P_i is given by a stretch term $-\rho K Y_i$ and that there are no curvature and instationary effects.

Conservation equations for the element mass fractions Z_j can be derived by taking the proper linear combinations of Eq. (4):

$$\frac{\partial mZ_j}{\partial x} - \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\frac{\partial Z_j}{\partial x}\right) = -\rho K Z_j + \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\sum_i^{N_s} w_{ji}\left(\frac{1}{Le_i}-1\right)\frac{\partial Y_i}{\partial x}\right), \tag{6}$$

where w_{ji} denotes the mass fraction of element j in species i. Note the resemblance between equation (6) and the conservation equation for the enthalpy (5). When unit Lewis numbers are applied for all species, one can easily show that the enthalpy and the element mass fractions are constant $Z_j = Z_{j,u}$ and $h = h_u$. In general, however, these variables are changing in stretched flames. Integrating Eq. (6) from unburnt ($x = -\infty$) to burnt ($x = x_b$) and substracting the integral of the unstretched case, gives us a relation for the variations in the element mass fractions in the burnt mixture due to flame stretch and preferential diffusion [5]

$$Z_{j,b} - Z^o_{j,b} \approx \frac{-1}{m_b}\int_{-\infty}^{x_b} \rho K (Z_j - Z_{j,u})\, dx, \tag{7}$$

where the changes in diffusive fluxes at x_b are neglected. The superscript o denotes stretchless variables. For weak stretch the stretch rate may be assumed constant $K = a$, and the other variables may be replaced by their stretchless values, resulting in a linear relation between the variations and the applied strain a. The enthalpy h_b and the element mass fractions $Z_{j,b}$ of the burnt mixture determine the equilibrium composition. Variations in this composition influence the mass burning rateon their turn, because the reaction layer, which determines the mass burning rate to a large extend, lies close to the burnt mixture.

The mass burning rate of these stretched flames can be derived following the ideas of De Goey and Ten Thije Boonkkamp [5]. They introduced the Karlovitz integral *Ka*

$$Ka = \frac{1}{m^o_b}\int_{-\infty}^{x_b} \rho K \tilde{Y}\, dx, \tag{8}$$

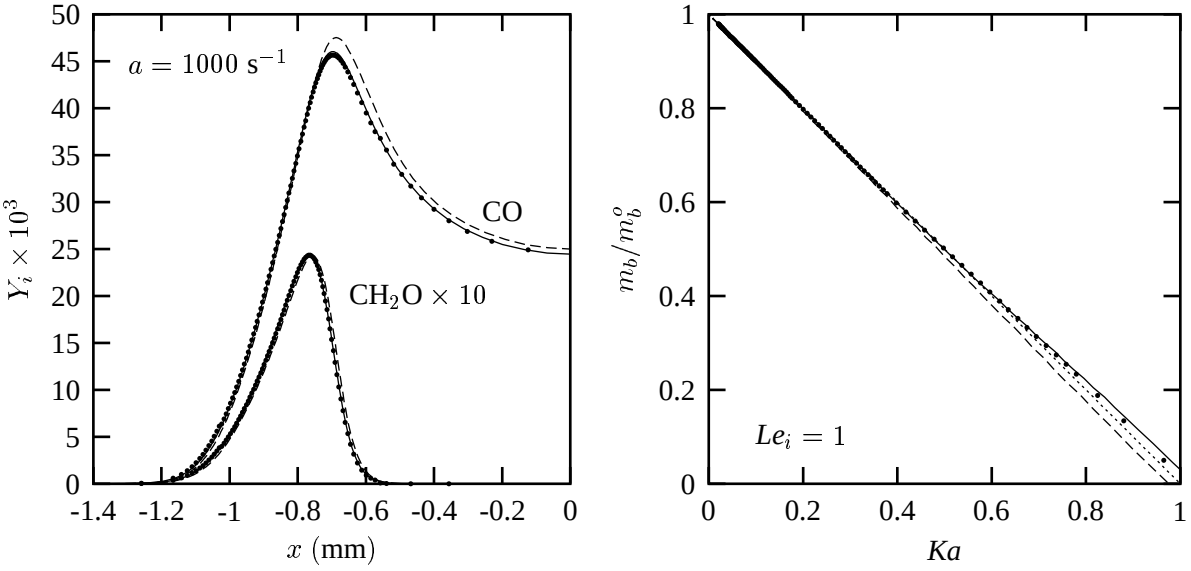

Figure 1: Results for $Le_i = 1$. (Left) Profiles of Y_{CO} and $Y_{\mathrm{CH_2O}}$. (Right) Scaled mass burning rate as function of *Ka*. (Both) solid line: full kinetics; dashed line: manifold with one progress variable; dots: manifold with two progress variables; dotted line: theory according to Eq. (9).

where $\tilde{Y}$ is a normalized progress variable, which is zero in the unburnt mixture and 1 in the burnt mixture. The boundary x_b is taken at the point where the chemical source term of the progress variable has been decreased by a factor of 10 from its maximum value. Using integral analysis De Goey *et al.* showed that the scaled mass burning rate decreases linearly with *Ka*:

$$m_b/m_b^o = 1 - Ka \tag{9}$$

The computations are performed for the case of unit Lewis numbers ($Le_i = 1$) as well as for non-unit Lewis numbers ($Le_i \neq 1$). Some results for $Le_i = 1$ are shown in Fig. 1. The profiles of the mass fractions of the species CO and CH_2O computed using a 1D FGM are in good agreement with the detailed computations. When a manifold with two progress variables is used, the results are even better. A similar observation can be made for the results of the mass burning rate. Using FGM the correct mass burning rate can be obtained for almost stretchless flames up to flames near extinction ($Ka = 1$).

When non-unit Lewis numbers are applied, variations in element mass fractions and enthalpy occur, due to differential diffusion effects. These variations and the mass burning rate of these flames are shown in Fig. 2. The variations in element mass fractions are well described by Eq. (7). The enthalpy variation, however, is not correctly predicted, because the diffusive fluxes for the enthalpy cannot be assumed constant at the position x_b. The enthalpy and element variations result in a significant extra decrease of the mass burning rate as function of *Ka* compared to Eq. (9). A 1D FGM is not able to represent this effect, because Z_j and h are conserved in this manifold. Results of computations using a 2D FGM, where the variations in Z_j and h are included using one additional controlling variable, are much closer to the detailed computations (See Fig. 2).

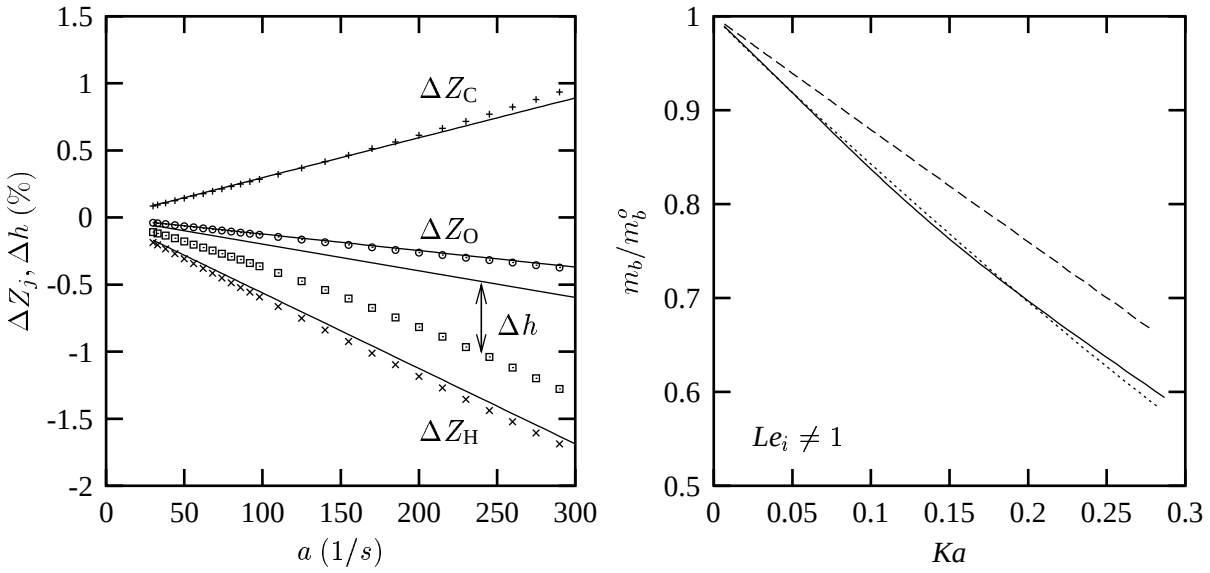

Figure 2: Results for $Le_i \neq 1$. (Left) Relative variation in element mass fraction $\Delta Z_j = Z_{j,b} - Z^o_{j,b}$ and enthalpy Δh as function of the applied strain a. Symbols: computed; solid line: theory according to Eq. (7) using stretchless variables. (Right) Scaled mass burning rate as function of *Ka*. Solid line: full kinetics; dashed line: 1D FGM; dotted line: 2D FGM.

Conclusions

More insight in the effect of flame stretch on the accuracy of the FGM method is obtained by modelling premixed methane/air counterflow flames. A manifold with only one progress variable is sufficient to model the main effect of flame stretch on the mass burning rate. If a higher accuracy is desired, a second progress variable can be added to the manifold.

When non-unit Lewis numbers are used, the element composition and enthalpy of the burnt mixture change, which results in an extra decrease of the mass burning rate. These differential diffusion effects can be modelled by FGM when the variations in $Z_{j,b}$ and h_b are taken into account using an additional controlling variable.

References

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