# Modelling of Premixed Laminar Flames Using Flame-Generated Low-Dimensional Manifolds

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#### Abstract

In order to reduce the computational cost of premixed laminar flame simulations, a new method has been developed to simplify chemical kinetics. In this technique a low-dimensional manifold is constructed using one-dimensional premixed flamelets. The manifold is stored in a look-up table and can be used in subsequent flame calculations. Since this flame-generated manifold is more accurate in the 'colder' zones of a premixed flame than existing techniques, the number of controlling variables can be kept low. Results show that two controlling variables (one progress variable and the enthalpy) are sufficient to reproduce detailed computations of premixed laminar flames very well.

### Introduction

Recently, detailed numerical simulations of more-dimensional time-dependent flames have become within reach (see, e.g. [1, 2, 3, 4, 5]). However, computing times of these simulations prohibit an extensive study on the effect of different combustion parameters. In order to improve the computational efficiency several methods have been developed which reduce the chemical reaction mechanism [6, 7, 8, 9]. The conventional reduction method, introduced by Peters [6], is based on the assumption that some intermediate species are in a so-called steady state. This implies that the left hand side of the conservation equation

$$\rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{v} \cdot \nabla Y_i - \nabla \cdot (\rho D_{im} \nabla Y_i) = \dot{\rho_i}^+ - \dot{\rho_i}^-, \qquad (1)$$

can be neglected for some species, remaining a balance between chemical production  $\dot{\rho_i}^+$  and consumption  $\dot{\rho_i}^-$ . A more accurate approach to find the steady-state relations has been developed by Maas and Pope [8] and is referred to as the ILDM method. In this method the steady-state processes are identified using an eigenvalue analysis of the Jacobian of the chemical source term. In both methods differential equations are replaced by algebraic equations, effectively restricting the chemical state to a low-dimensional subspace of the composition space; the *manifold*. In the ILDM method the steady-state relations are solved for given values of controlling variables and these results are stored in a database. The dimension of this database is determined by the number of controlling variables which is needed to represent the slow chemical processes. The dimension increases with the complexity of the fuel. Even for atmospheric methane-air flames Eggels [9] has shown that, apart from the controlling variables needed for the element mass fractions and the enthalpy, at least three controlling variables are needed. This causes the ILDM method to be unsuitable for higher hydrocarbon fuels.

#### Flame-generated manifolds for premixed flames

In this paper a new method is presented to create a manifold. The resulting manifold, to which we will refer as Flame-Generated Low-Dimensional Manifold (FGLDM), will be a better approximation of the chemical state in the 'colder' zones of premixed flames than the ILDM. The FGLDM can be derived by rewriting Eq. (1) as follows:

$$\dot{m}\frac{\partial Y_i}{\partial s} - \frac{\partial}{\partial s}\rho D_{im}\frac{\partial Y_i}{\partial s} = \dot{\rho_i}^+ - \dot{\rho_i}^- + P_i(s), \qquad (2)$$

where s parameterises a curve locally perpendicular to the flame front. The transient term and more-dimensional effects related to flame stretch and curvature are represented by  $P_i(s)$ , which depends on the



Figure 1: Projection of the one-dimensional ILDM and FGLDM onto the H–H<sub>2</sub>O plane for a stoichiometric hydrogen–air mixture. The dots represent the chemical state at different positions in a 2D hydrogen–air flame.

exact choice of s. We now assume that  $P_i(s)$  is negligible compared to the other terms. The resulting balance between convection, diffusion and reaction can be considered as a steady-state relation. Note that conventional reduction techniques neglect not only  $P_i(s)$ , but also the left hand side of Eq. (2). The remaining set of equations is solved treating the system as a 1D adiabatic premixed flame. The solution  $Y_i(s)$  represents a line in composition space, which can be considered as a 1D manifold. In Fig. 1 the onedimensional ILDM and FGLDM for a stoichiometric hydrogen-air mixture are shown together with a scatter plot of the chemical state at different positions in a 2D stationary flame computed using detailed kinetics. In the high temperature range  $(Y_{H_{2O}} > 0.2, T > 1750 \text{ K})$  the composition is determined by chemical processes and the results are therefore equivalent. However, in the 'colder' zones ( $Y_{\rm H_2O} < 0.2$ ) convection and diffusion play an important role, which causes the FGLDM to lie much closer to the detailed computation than the ILDM. The small deviations between the FGLDM and the 2D flame are mainly caused by non-adiabatic effects in the latter. To account for these enthalpy-losses the FGLDM is extended with an extra controlling variable, i.e. the enthalpy h. Therefore, Eq. (2) is solved for mixtures with varying enthalpy. This set of 1D solutions then forms a 2D manifold in composition space, which is stored in a database as function of the controlling variables  $(Y_{H_2O} \text{ and } h)$ , similar to the ILDM method. Note that variations in element mass fractions due to non-unit Lewis-number effects, are accounted for by the FGLDM. This attracting feature prevents that extra dimensions have to be added to the database for the varying element mass fractions, which would be the case for the ILDM method.

#### Application to a 2D methane-air flame

The use of two-dimensional FGLDM's is implemented in a CFD-code in the same way as ILDM's. Together with the Navier-Stokes equations, the equations for the controlling variables are solved:

$$\rho \mathbf{v} \cdot \nabla h - \nabla \cdot \left(\frac{\lambda}{c_p} \nabla h\right) = S_h,\tag{3}$$

$$\rho \mathbf{v} \cdot \nabla Y_{\mathrm{H}_{2}\mathrm{O}} - \nabla \cdot (\rho D_{\mathrm{H}_{2}\mathrm{O}} \nabla Y_{\mathrm{H}_{2}\mathrm{O}}) = S_{\mathrm{H}_{2}\mathrm{O}}.$$
(4)

The variables needed to solve these equations  $(\rho, \lambda, c_p, S_h, S_{H_2O}, \text{ etc.})$  are stored in the FGLDM database. Note that, since the perturbations  $P_i$  are neglected, there is no need to project equations (3–4) onto the manifold.

A 2D stoichiometric methane-air flame is simulated using both a detailed reaction mechanism and a flame-generated manifold with two controlling variables  $(Y_{H_2O} \text{ and } h)$ . In Fig. 2 the resulting temperature fields are shown. A good agreement between the detailed and reduced computations is found. By applying a FGLDM the computation time has been reduced from a few weeks to a few hours.



Figure 2: Temperature field for methane-air flame computed with (left) a detailed chemical mechanism and (right) a flame-generated manifold.

#### Conclusions

In this paper a new method is presented to create low-dimensional manifolds. In this method a manifold is constructed by solving 1D flame equations. In the colder zones of a premixed flame, the resulting FGLDM is more accurate than methods based on local chemical equilibria. Therefore, the number of controlling variables can be kept low, resulting in a much smaller dimension of the manifold. The results of the simulations show that, apart from the enthalpy, one controlling variable is sufficient for premixed methane-air flames to reproduce detailed calculations reasonably well. In order to increase the accuracy, the method can easily be extended to more progress variables. The enormous reduction of computation time allows us to perform more extensive studies of realistic flames.

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