Two-dimensional methane/air flame

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SHORT COMMUNICATION

Two-dimensional Methane/Air Flame

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ABSTRACT—First results are presented of a new flame code for modeling transport processes in two-dimensional flames using a one-step reaction model. The code is applied to a study on the flame shape of methane/air flames on a triple-slit burner. The results compare reasonably well with experimental data. We expect further improvement when more accurate measurements become available. These measurements are necessary to come to a more definite conclusion on the reliability of the model.

Key Words: Modeling, two-dimensional, flame shape, laminar

1 INTRODUCTION

Numerical tools for studying the behavior of more-dimensional flames are often needed in engineering studies of burners and combustion appliances. Therefore, a code has been developed especially suited for modeling flow and transport processes in two-dimensional (2D) laminar flames [Lange, 1992]. Numerical models of more-dimensional flames containing complex reaction mechanisms, are scarce and are at present not applicable for engineering purposes, due to the enormous computing times required [Smooke, 1989]. A one-step irreversible reaction scheme is therefore applied to reduce the computing effort to an acceptable level (of about 1 hour on a SUN Sparc1 workstation).

First results, obtained with this flame code, are compared with experimental results. In this study, we concentrate on the global flame structure of 2D premixed CH_4 /air flames on a triple-slit burner. The results presented, show that the applied reaction model is appropriate to describe the global flame shape of premixed flames. As [Lange, 1992] shows, the code also proves to be useful for studying flash-back and quenching phenomena in premixed flames.

Some important features of the numerical and the chemical model are presented in section 2. A more detailed description is given in refs. [Lange, 1992, Lange, 1992a]. The code will be used to model the center flame on a triple-slit burner. The experimental burner and the related boundary conditions used in the numerical model are presented in section 3. Numerically obtained flame front positions and flame lengths will be compared with experiments in section 4.

2 NUMERICAL AND CHEMICAL MODEL

The 2D flow field is calculated using a vorticity-stream function formulation. The flow and convection-diffusion equations, describing the mass and heat transport in the flame, are discretized using finite-differences on adaptive locally-refined grids and are solved using the ADI method [Lange, 1992, Lange, 1992a]. We further use a one-step irreversible reaction *fuel + oxygen* $\rightarrow$ *products*, in terms of the following fuel-mass production rate:

$$\dot{\rho}_{fu}(T, \rho, Y_{fu}, Y_{ox}) = -A\rho^{\alpha+\beta}(Y_{fu})^{\alpha}(Y_{ox})^{\beta}e^{-T_a/T}. \quad (1)$$

Here, A , α , β and T_a are reaction rate parameters and ρ , T and Y_i are the local mass density, temperature and mass fractions, respectively.

The essential point of the reaction mechanism is that the rate equation and rate parameters are chosen in such a way that the numerical temperature dependence of the burning velocity is fitted to experimental results in a range of equivalence ratios. The idea of this method is similar to that of Coffee et al. [Coffee, 1984], who determined ϕ -dependent one-step reaction parameters, using detailed numerical chemistry data on the temperature dependence of the burning velocity. The method ensures that differences in the burning velocity, due to local temperature and concentration variations near the flame front are taken into account by the rate equation. This method is chosen, because the local value of the burning velocity seems to be the key parameter in the prediction of the flame shape and stability behavior. The parameters for methane/air flames ($\alpha = 2.8$, $\beta = 1.2$, $A = 4.2 \cdot 10^{15} [kg\,m^{-3}]^{-3}s^{-1}$ and $T_a = 16900K$) [Lange, 1992] are determined from experimental burning velocities of [Andrews, 1972, Kaskan, 1956], within a temperature range of $1500 < T < 2300$, for equivalence ratios $0.8 < \phi < 1.2$. A numerical study on flat (1D) burner-stabilized flames, using this chemical model, has shown that numerical values for the burning velocity in this range of temperatures and equivalence ratios, deviate no more than roughly 15% from the results, obtained with the Sandia package [Kee, 1985] and from the experimental values of [Andrews, 1972, Kaskan, 1956].

It is important that the total temperature increase, induced by the reaction, is accurately calculated, because of the sensitivity of the flame properties, through (1), to small differences in the temperature. Specification of the total combustion enthalpy and the total specific heat as a function of ϕ is therefore very delicate. In addition, a number of transport properties of the mixture has to be introduced. The thermal conductivity, viscosity and density are assumed to be dominated by the abundant nitrogen part, whereas the diffusion coefficients are determined by means of the kinetic theory of binary gasses.

3 BURNER GEOMETRY

The burner, used in the experiments, consists of three identical parallel slits, with a length of 40 mm, an inner width of $4mm (= 2L_y)$ and a wall thickness of 0.4 mm. Visual observations and measurements with Laser-Doppler Velocimetry (LDV) indicate that variations of flame shape in the direction of the length may be neglected. The center flame on the triple-slit burner will be studied here, since it has the advantage of being contained between two similar flames, which restricts the influence of the surrounding atmosphere. The center flame is modelled numerically as if it is confined between two symmetry boundaries, which is exact when the enclosure is ideal.

All burner walls are cooled with water, to make it possible to define the wall boundary conditions accurately. We have chosen for slightly diverging burner mouths, to minimize the thickness between the flames at the outflow. A disadvantage of this construction is that the velocity profile at the outflow has a non-parabolic form. The velocity profile at the outflow has been measured using LDV and has been used in the numerical model in the form of a fourth-order polynomial fitted through the data points.

Note that all mentioned boundary conditions in the numerical model are well defined. This is the main reason for using this burner.

4 FLAME STRUCTURE

Numerical results of the global flame structure are presented in this section for several values of ϕ and the velocity u_{max} in the center of the slit. An example of a converged

Figure 1a: Results for a stoichiometric CH_4/air flames for $u_{\max} = 1.21$ m/s: the 2-layer locally refined grid

adaptive locally-refined grid of one flame with $\phi = 1.0$ and $u_{\max} = 1.21$ m/s is shown in fig. 1a. The 2-layer refined grid consists of about 3500 grid points and is based on a uniform background grid of 50×20 points. Results of the other flames look similar.

The position of the "flame front" is compared with experimental and theoretical results in fig. 1b for the same flame. We choose the isotherm of $T = 1200$ K as the numerical "flame front". The experimental values are obtained with LDV and indicate the positions in the flame, where the local gas speed suddenly increases. The theoretical model [Lewis, 1961] is based on the balance between the adiabatic burning velocity and the component of the local gas speed, perpendicular to the flame. This model does not predict the rate of wall cooling, which leaves the height of the stabilization point unknown. The flame is assumed to extinguish in the area close to the wall, where the gas speed is smaller than the adiabatic burning velocity (indicated by a horizontal line in fig. 1b). Since the definitions of the flame front position are not fully in agreement, errors of the order of the thickness of the flame (about 0.3 mm) may be expected.

The resemblance between the experimental, theoretical and numerical results is clear. However, it is also clear that the experimental flame front appears to be somewhat more expanded. This is caused by an outward expansion of the center flame, observed visually

Figure 1b: results for a stoichiometric CH_4/air flames for $u_{\max} = 1.21$ m/s: a comparison of:

- the numerical result: $T = 1200$ K isotherm (continuous line)
- the theoretical result (dashed line)
- the experimentally found shape of the flame (x marked points).

during the experiments: the outer flames are pushed sideways quite strongly. We hope to be able to reduce this effect in future experiments.

For further comparison of the numerical, theoretical and experimental results, we consider the “length” of the flame (the distance between the tip of the flame and the burner outlet). For the height of the flames, we use the same definition as for the “flame front” position. The thus found flame lengths are presented in table 1 for three equivalence ratios and five velocities. Qualitative resemblance between the numerical, theoretical and experimental results is found. The occurring errors of about 20% are caused by experimental errors (0.3mm), differences between the “length” definitions and errors in reaction rate parameters. Note that largest numerical inaccuracies are found for $\phi=0.8$ and $\phi=1.2$. This is probably caused by the chosen reaction scheme and parameters, which reproduce the burning velocity at $\phi = 1.0$ more accurately as compared to those for $\phi=0.8$ and $\phi=1.2$.

Experimentally, we observed flash-back for stoichiometric flames with flow rates below 0.94 m/s, whereas the numerical results show flash-back at a flow rate of 0.83 m/s. This

TABLE I

The experimental, numerical and theoretical flame length (mm) at varying gas flow rates for $\phi=0.8$, $\phi=1.0$ and $\phi=1.2$. The dashes denote flash-back.

$u_{\max}$ m/s	$\phi = 0.8$			$\phi = 1.0$			$\phi = 1.2$		
	exp	num.	theo.	exp.	num.	theo.	exp.	num.	theo.
0.83	2.6	3.9	3.0	—	—	1.7	2.6	2.4	2.1
0.94	3.0	4.5	3.5	—	2.1	2.1	3.1	2.8	2.5
1.07	3.4	5.1	4.0	2.3	2.5	2.4	3.5	3.4	2.9
1.13	3.7	5.4	4.3	2.4	2.8	2.6	3.9	3.6	3.1
1.21	3.9	5.6	4.5	2.6	3.0	2.8	4.5	3.9	3.3

indicates that flash-back is reproduced within about 10%.

5 CONCLUDING REMARKS

The qualitative resemblance between numerical, experimental and theoretical results, presented in this paper, clearly shows that both the numerical method and the reaction scheme used, are valid for engineering studies of premixed laminar flames. As for now, it is not clear whether these results may still be improved by a better choice of transport coefficients, boundary conditions and rate parameters (derived from experimental burning velocities). Improvement of the boundary conditions and the data for the rate parameters is one of the goals of future research.

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