# Numerical simulations of flat laminar premixed $CH_4$/Air flames at elevated pressure

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**Abstract**

Numerical simulation of stoichiometric methane/air flames stabilized on flat burners at elevated pressure is reported in the present work. Such flames, in practice, are experimentally obtained using the Heat flux method for measurement of laminar burning velocity of fuel/oxidizer mixtures. The method makes use of a burner with a perforated brass burner plate. The dimensions of such a plate play an important role in creating flat flames. The present investigation is focused on studying laminar premixed flame structure numerically at elevated pressure up to 15 bar using different burner plate dimensions. It was observed that flame surface decreases with decrease in hole diameter and increase in porosity of the plate.

## 1 Introduction

The laminar burning velocity defines the rate at which the unburnt mixture is consumed in a propagating laminar flame. This parameter is considered one of the most important properties in assessing flame stability and flashback in practical systems like burners and combustors. Apart from its importance in designing combustors, this parameter also holds key responsibility in validating chemical reaction mechanisms. The heat flux method (HFM) is an experimental method through which this property can be determined and has proven to be accurate in its measurements [1].

In heat flux method, heat loss from the flame is compensated by adding heat to the unburnt gas mixture. The method requires a balance in the heat that is lost from the flame to the burner. A perforated plate is fitted on a burner head. The burner head is maintained at a temperature higher than the unburnt gas temperature. This gives a heat transport from the head to the burner plate and finally to the unburnt gas mixture. A more detailed description of the concept and principle is discussed by Bosschaart and de Goey [1]. In order to assess how a flat (heat flux method) flame behaves in a high pressure environment numerical simulations have been performed. The present study focuses on the question if the flatness of the flame depends on the plate hole diameter and distance between successive holes.

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# 2 Axisymmetric simulations

The simulations are performed with a stoichiometric methane/air mixture with an unburnt gas temperature of 25 °C. Three different burner plates as summarized in Table 1 are modeled. Steady state axysymmetric simulations with an incompressible flow with a one step mechanism are performed up to 7 bar, to find the influence of the hole diameter and porosity on the amount of flame curvature. Detailed simulations with the DRM19 mechanism [2] are performed up to 15 bar, with model 3 that resembles the burner plate from the experimental setup in Fluent [3]. In the following section, two methods are presented to determine the amount of surface area increase of a curved flame compared to a flat flame. The influence of the burner plate geometry on the amount of flame curvature are compared. The combustion of gases is governed by a set of equations describing the conservation of mass, momentum, energy and species. The solver utilizes a control volume based technique and second order upwind scheme is used for spatial discretization of all the governing equations.

Table 1: Dimensions of the burner plate models

| Model | Hole diameter (mm) | Porosity $\chi$ (-) | Pitch s' |
|---|---|---|---|
| 1 | 0.5 | 0.63 | 0.6 |
| 2 | 0.3 | 0.63 | 0.36 |
| 3 | 0.3 | 0.51 | 0.4 |

## Computational domain

The burner plate used in experiments is a round perforated plate with a diameter of 30 mm and a thickness of 1 mm. The holes have a diameter of $d$ = 0.3 mm and a pitch of $s'$ = 0.4 mm. They are placed in a hexagonal pattern in order to stabilize a flat flame above the burner plate. The actual plate has over 5000 holes, but a schematic representation is shown in Fig. 1 (top). The presence of symmetry planes can be used to isolate a small hexagonal unit cell, this unit cell is approximated by an axisymmetrical cell. The red rectangle represents the plane that needs to be modeled, with the axis of rotation through the center of a hole. The round edge of the cell is modeled as a symmetry boundary. The right side of Fig. 2 shows that when the actual pitch, $s'$, is used in the model, there will be parts of the burner plate that are not taken into account. This will lead to a different porosity than the actual plate. To compensate for this, the pitch, $s$ is now chosen such that the porosity of the axisymmetrical cell (axi) is equal to the porosity of the hexagonal unit cell (hex).

$$\chi_{axi} = \left(\frac{d}{s}\right)^2 ; \chi_{hex} = \left(\frac{\pi}{2\sqrt{3}}\right)\left(\frac{d}{s'}\right)^2 \tag{1}$$

The axisymmetric axis is defined along the x-axis and goes through the center of a hole. The round edge of the domain is modeled as a symmetry boundary and the burner plate as a wall. The in-flow of the premixed gases is defined as a velocity inlet, where the velocity magnitude and the species mass fractions are defined. The blue line in Fig. 1 (bottom) represents the approximate position of the flat flame. The exhaust gases leave through the pressure outlet, which is placed sufficiently far from the flame. The length of the computational domain is determined by: the length of the in-flow area $L_{in}$, the thickness of the burner plate $L_{hole}$ and the length of the flame/outflow area $L_{out}$.

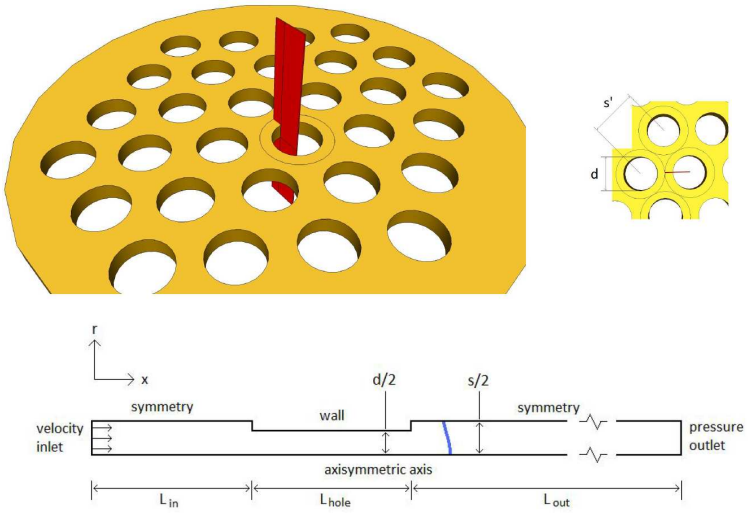


Figure 1: (Top) Axisymmetric domain (Bottom) Computational domain

## Surface area increase

To determine the curvature and surface area increase of the flame, an indicator for the flame stand-off distance is introduced. The parameter $\delta T_{iso}$ gives the distance from the burner plate outlet to a certain isotherm with value $T_{iso}$, along the center and the side boundary, as indicated in Fig. 2 (left). The center boundary is the axisymmetric axis that is defined through the center of the hole and the side boundary is the symmetry boundary condition that is located above the burner plate. In previous studies, the 900 K isotherm has been chosen to determine the curvature, because this is the approximate temperature above which chemical reactions become important [4].

The isotherms for the pressures 1, 5 and 10 bar are illustrated in Fig. 2 (left). The corresponding laminar burning velocities of the three adiabatic cases are used as the inlet velocity. This shows that the flame is flat, when the stand-off distance of the 900 K isotherm is equal along the two boundaries. This is the case at 1 bar and the flame exhibits curvature as the pressure increases. The difference between the stand-off distances along the two boundaries ($\delta_{900}$) is used to calculate the surface area increase of the curved flame compared to an ideal flat flame. The surface area increase according to the 900 K isotherm, is calculated for all the simulations performed with the one-step mechanism and the DRM19 mechanism.

Instead of using the 900 K isotherm to determine the flame curvature, it is also possible to define a different parameter. One of the post-processing options is to present the net reaction rate of methane, $R_{CH_4}$. This is shown for the simulations at 10 bar in Fig. 2 (right). The curvature of the layer where the reactions take place can also be regarded as a suitable indicator for the flame curvature.

The net reaction rate is plotted along the center and the side boundary (Fig. 2 (right)). The shift that occurs between the two plots is essentially the same principle as the parameter $\delta_{900}$, used to determine the curvature of the 900 K isotherm. When the flame is entirely flat, the plots are exactly the same and on top of each other. The shift can be measured by determining the distance between the peaks of the plots, which will be referred to as the parameter $\delta_{CH_4}$.

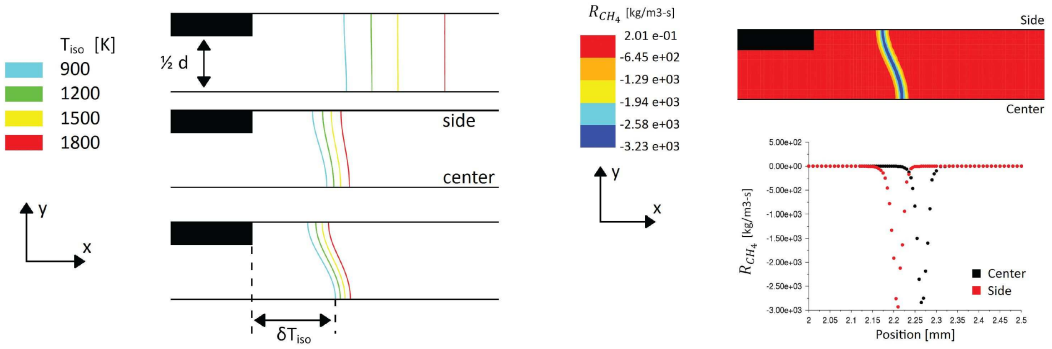


Figure 2: (Left) $\delta T_{iso}$ for 1, 5 and 10 bar (top to bottom) (Right) Net reaction rate of methane at 10 bar

## 3 Results and Discussion

The surface area increase, $S_{incr}$ has been calculated according to both the 900 K isotherm and the net reaction rate of methane. The results, using the one-step mechanism and 900-K isotherm ranging from p = 1 to 7 bar, are presented in Fig. 3 (left). The experimentally determined burning velocities [5] were used as the inlet velocity in the models. The results suggest a non-linear increase of $S_{incr}$ with elevating pressure. The results in Fig. 3 show that the amount of surface area increase strongly depends on the geometry of the burner plate. The results for burner plate (2) are plotted with the blue diamonds. Compared to burner plate (1) with $d$ = 0.5 mm, $\chi$ = 0.63, represented by the red squares, the amount of $S_{incr}$ is reduced by a factor of 3. This reduction is achieved by decreasing the hole diameter from 0.5 to 0.3 mm, while the porosity remains constant. The results from burner plate (3) with $d$ = 0.3 mm, $\chi$ = 0.51, plotted with the green triangles, are compared to burner plate (2) with $d$ = 0.3 mm, $\chi$ = 0.63 to find the influence of the porosity. The amount of $S_{incr}$ is reduced by a factor of 2, when the porosity is increased from $\chi$ = 0.51 to $\chi$ = 0.63. The significant increase in porosity is achieved by decreasing the pitch of the burner plate by only 0.04 mm.

The detailed simulations using DRM19 mechanism were performed up to 15 bar and show this increase more clearly in Fig. 3 (right). For 1 and 5 bar, the results from the one-step mechanism are included. This shows the influence of using the detailed reaction mechanism. The difference is small between the DRM19 mechanism and the one-step mechanism. At 5 bar, the surface area increases are 1.7 % and 2.2 % respectively. The simulations at 1 bar show a negligible increase for both cases. This suggests that for further simulations, the one-step mechanism is sufficient to determine the approximate surface area increase. The results at 10 and 15 bar clearly show a non-linear increase of the $S_{incr}$ with elevating pressure. The surface area increase determined from the maximum reaction rate of $CH_4$ shows the same non-linear increase. However, the values are smaller compared to the 900 K isotherm criterion. At 5 bar the $S_{incr}$ is only 0.45 % but it rises quickly to 3.4 % and 11.8 % for 10 and 15 bar respectively.

The detailed species structure of the flat flame is presented Fig. 4. The profiles of the major species mass fraction along the center and side boundary are compared for the cases at 1 and 10 bar. This shows the influence of the flame curvature and increase in pressure. The dotted vertical blue line represents the location of the burner plate. The case at 10 bar shows the largest difference between both boundaries. This is caused by the large curvature that was already shown in Fig. 3, for the temperature isotherms and the reaction rate of methane. The profiles along the side boundary are shifted towards the burner plate compared to the center boundary. They coincide after the reaction layer, where the flow becomes uniform again and the mixture reaches chemical equilibrium.

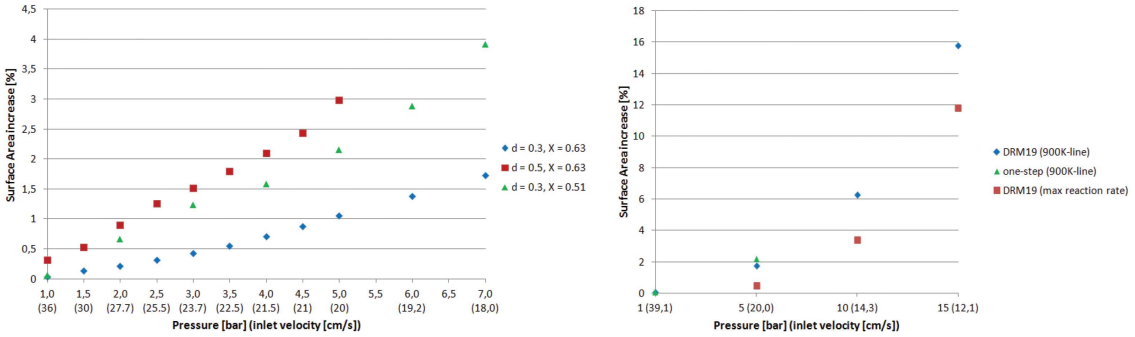


Figure 3: Surface increase of the flame

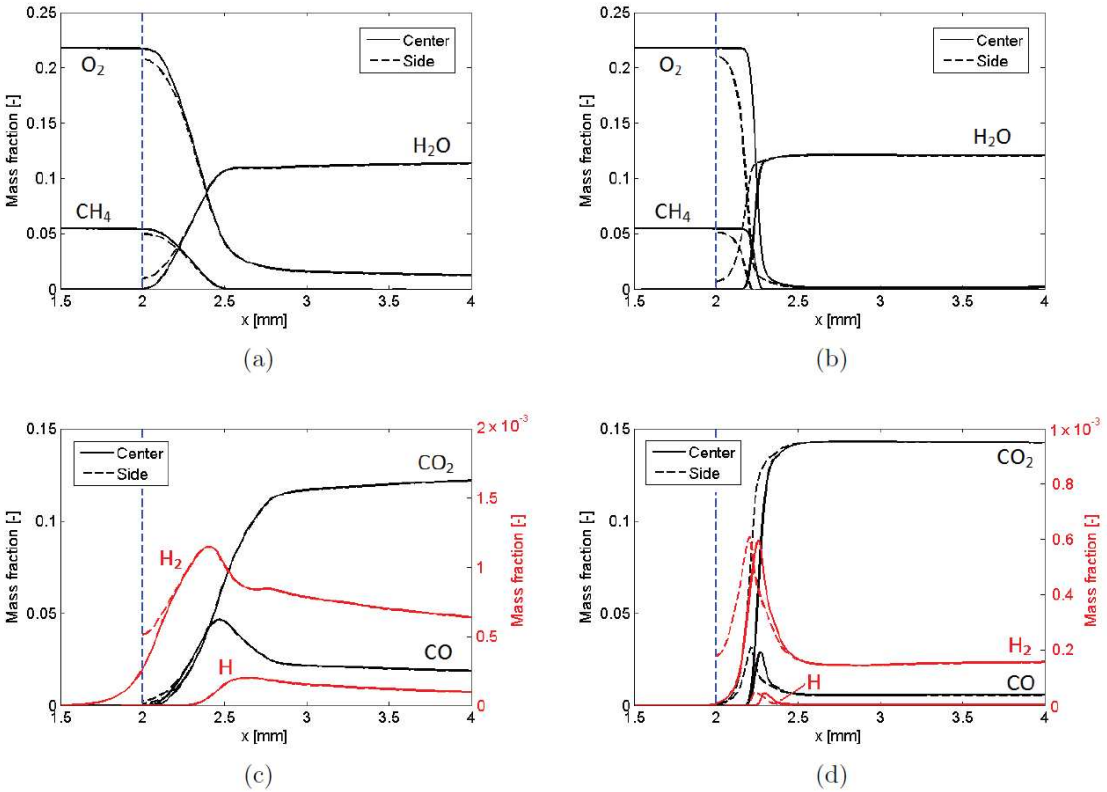


Figure 4: Species profiles at (left) 1 bar (right) 10 bar

The influence of the pressure becomes clear when comparing the two cases. At elevated pressure, the collision rates of molecules increase, which cause the reactions to take place at a higher rate. This decreases the thickness of the reaction layer, which is shown by the steeper mass fraction profiles and the mixture becomes uniform very fast. The maximum mass fractions of $H$, $H_2$ and $CO$ are approximately two times lower at 10 bar, which is a result of the high reaction rate. Simulations showed that the maximum reaction rate of methane is approximately 15 times higher at 10 bar compared to atmospheric pressure. Highly mobile hydrogen radicals promote the burning rate of the mixture. To minimize the flame curvature effects, the hole diameter must be reduced and the porosity must be increased. Presently, the holes are drilled in the brass plate and a hole diameter of $d$ = 0.25 mm should be considered as the lower limit. Somers [6] recommended to use porosities higher than $\chi$= 0.67. It was found that the porosity of $\chi$= 0.8 can be considered as an upper limit to avoid corrosion of the burner plate material. The burner plate that is expected to show the least amount of surface area increase, will therefore have a hole diameter of $d$ = 0.25 mm and a pitch of $s$ = 0.29 mm. This corresponds to a porosity of $\chi$= 0.67.

# 4 Conclusions

The surface area increase of the curved flames, compared to a perfectly flat flame is calculated according to the 900 K isotherm and the reaction rate of methane. Both show the same trend in surface area increase with elevating pressure. Three burner plates have been modeled for pressures up to 7 bar with a one-step mechanism. The comparison of these models shows that the surface area increase can significantly be reduced by choosing a smaller hole diameter and larger porosity. The results of the detailed simulations up to 15 bar show a non-linear increase of the flame curvature with elevating pressure. The surface area increase of the methane/air flame is around 16 % at 15 bar with the burner plate that is used in the current setup. This must be reduced by manufacturing a new burner plate with a smaller hole diameter and a larger porosity.

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