Measurements and Experimental Database Review for Laminar Flame Speed Premixed Ch4/Air Flames

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Abstract. Laminar flame speed \( S_L \) of CH4 was determined at atmospheric pressure and initial gas temperatures in range from 298 to 358 K. The heat flux method was employed to measure the flame speed in non-stretched flames. The kinetic mechanism GRI 3.0 [1] were used to simulate \( S_L \). The measurements were compared with available literature results. The data determined with the heat flux method agree with some previous burner measurements and disagree with the data from some vessel closed method and counterflow method. The GRI 3.0 mechanism was able to reproduce the present experiments. Laminar flame speed was determined at pressures range from 1 to 20 atmospheres through mechanism GRI 3.0. Based on experimental data and calculations was obtained \( S_L \) dependence on pressure and temperature. The resulting of dependence recommended use during the numerical simulation of methane combustion.

1. Introduction

Development of new gas-turbine engines for power plants is very challenging task. The combustion chamber is one of the main components of any gas turbine engine. Design and working of the combustion chamber process of determining the essential characteristics of the engine. Currently in the design of the combustion chambers using Computational Fluid Dynamics (CFD) methods. CFD can quickly and accurately determine the basic characteristics of the designed (or modified) combustion chamber, such as the complete loss of pressure, air distribution laws, as well as emission characteristics and others. However, a qualitative prediction of pollutant formation processes is impossible without the use of detailed chemical kinetics, as well as a qualitative description of combustion processes. One of the main parameters influencing the physics of combustion of fuel-air mixture is \( S_L \) [2]:

\[
S_L = S_{L0} \left( \frac{T_{uo}}{T_0} \right)^\alpha \left( \frac{P_{uo}}{P_0} \right)^\beta ,
\]

where \( T_{uo} \) – the initial temperature of the unburned mixture,
\( P_{uo} \) – the initial pressure of the unburned mixture
\( S_{L0} = C_1 + C_2 (\varphi - C_3)^2 \)
where \( \varphi \) - the equivalence ratio
\( C_1, C_2 \) and \( C_3 \) - constants depending on the type of fuel
The exponents \( \alpha \) and \( \beta \) are calculated as:
\( \alpha = 2.18 - 0.8(\varphi - 1) \).
\[ \beta = -0.16 + 0.22(\phi - 1). \]

As can be seen from the equation (1) \( S_L \) depends on the coefficient \( \alpha \) and \( \beta \). The CFD software mainly uses one of two equations to determine \( S_L \). One of them is (1) and another one is from [3]:

\[
S_L = FY_{F,a} \cdot \exp(-G / T^0) \left( \frac{T_u}{T^0} - \frac{T_b}{T^0} \right)^n,
\]

where \( Y_{F,a} \) – the mass fraction of the fuel in the fuel-air mixture,
\( T^0 \) – the temperature of the inner layer of the laminar flame,
\( T_b \) – adiabatic equilibrium temperature of combustion products,
\( B, E, F, G, m, n \) – coefficients (presented in [3]).

As shown below, the calculation of the results of these two equations do not accurately superimposed on the experimental results, taken from open sources. Therefore, as proposed a process for preparing solutions according to the refined \( S_L = f(\phi, T_b, P_{atm}) \).

Aims of this paper are to investigate different data on methane+air laminar flame speed and to determine the dependence of \( S_L \) on pressure and temperature.

2. Details of experiment

The measurements of CH4 and air mixtures flame speed were performed by experimental facility to determine the speed of the flame by the heat flux method. The heat flux method allows stabilization of flat adiabatic flames on a perforated burner due to possibility of balancing heat transfer between the flame and the burner plate. The edge of the burner plate is kept preheated to 368 K by a water circuit in the burner head, controlled by a water bath. The temperature difference between the burner plate and the unburned mixture forces negative heat flux from the plate to the gas, which is balanced by the positive heat flux from the flame back to the plate. The unburned gas temperature \( T_{atm} \) was set in range from 298 to 358 K. The unburned gas pressure \( P_{atm} \) was set to values of 1 atm. The range of equivalence ratios was limited to \( \phi = 0.6-1.6 \). The experimental facility shown in the figure 1.

![Figure 1 - Test rig to measure \( S_L \).](a) general view, (b) burner device.)

3. Simulation

Simulation of adiabatic premixed one-dimensional flames was performed using Chemkin 4 code [4]. Grid-independent solutions were obtained for high-temperature mechanism GRI 3.0, which contains 325 reactions, 56 chemical species and were made by M. Frenklach et al [1]. The calculation was performed under the following initial conditions: \( P_{atm} = 1 \ldots 20 \text{ bar}, T_{atm} = 298 \ldots 800 \text{ K, } \phi = 0.6 \ldots 1.6 \).

4. Approximation equation

Based on the simulation results several three-dimensional graphics were built. Two of them you can see in the figure 2: \( S_L = f(\phi, P_{atm}) \) and \( S_L = f(\phi, T_{atm}) \).
Figure 2 – Calculated $S_L$ dependence on $\phi$ and $P_u$ with $T_u=800$ K (a) and dependence on $\phi$ and $T_u$ with $P_u=1$ bar (b).

The data obtained from the calculation can be described by the equation presented below:

$$S_L = (145\phi^3 - 850\phi^2 + 1265\phi - 325)(\frac{T_u}{800})^{5.1\phi^2 - 10.8\phi + 7.6}(\frac{P_u}{101325})^{-0.4715\phi^2 + 1.1\phi - 0.966} \quad (3)$$

It should be noted that the use of this dependence is limited by the equivalence ratio range as $\phi=0.33…1.9$.

5. Results and discussion

5.1 Temperature dependence

Figures 3 - 4 show values of $S_L$ experimentally obtained, calculated by (1), (2), (3) and the mechanism GRI 3.0 in comparison with data of other authors [5-36].

Figure 3 – Laminar speed $S_L$ (a) $T_u = 298$ K and (b) $T_u = 318$ K

(more details about the chart legend can be seen in Appendix).
Figure 4 – Laminar flame speed $S_L$ (a) $T_u = 338$ K, (b) $T_u = 358$ K

(more details about the chart legend can be seen in Appendix).

Figures 3-4 show for this temperature range all data are in a good agreement, except equation (1) which shows higher values for rich equivalence ratio. Equation (2) shows a good prediction for all provided initial conditions. The experimental data of this work are in a good agreement with data of other authors [5-35] and with the data obtained in the works [1-4]. This indicates that used method is valid. Based on these graphs, it is clear that the kinetic mechanisms of chemical reactions GRI 3.0 is in good agreement with experiments and is suitable for further use in order to obtain the calculated values. This is necessary due to the lack of available experimental data for large pressures and temperatures. Equation (3) shows a bit of lower values according to results of GRI 3.0 simulations.

5.2 Pressure dependence

Figures 5 - 6 show values of $S_L$ calculated by the equations (1), (2), (3) and the mechanism GRI 3.0 for initially temperature equal to 500 and 700K, and pressure equal to 10 and 20 bar.

As the presented graphs show, equation (2) significantly overestimates the value of $S_L$ at high values of $P_u$ in comparison with the experimental data. In turn, the calculation from equation (1) shows slightly understated $S_L$ values with respect to the experimental data. Calculation by formula (3) allows obtaining $S_L$ values, which agree satisfactorily with both experimental and kinetic calculations of the GRI 3.0 mechanism.
Figure 7 presents a comparison of the $\alpha$ and $\beta$ values obtained in this paper with the data of other authors [37-39]. As can be seen from the presented graphs, the value of the degrees used in equation (2) is linear and does not correspond to the experimental data. Whereas the proposed values of $\alpha$ and $\beta$ have extrema in the range $1 < \phi < 1.2$, which corresponds to the experimental data and the calculations of other authors.

![Figure 7](image)

**Figure 7** – Power exponents $\alpha$ (a) and $\beta$ (b) as a function of $\phi$

### 6. Conclusions

During this work $S_l$ was determined experimentally at atmospheric pressure and initial gas temperature in the range 298-358 K by heat flux method. $S_l$ was also was determined by simulation with GRI 3.0 kinetic mechanism for initial temperature up to 800 K and pressure up to 20 bar. Based on results of simulations was developed equation (3). The presented experimental data and calculation using equation (3) are in good agreement with results of other authors and calculations using the kinetic mechanism GRI 3.0. The equation (3) can be used for modeling in the software packages.

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### Appendix

| Reference | Method                        | Symbol | Reference | Method                        | Symbol |
|-----------|-------------------------------|--------|-----------|-------------------------------|--------|
| 5         | Counterflow                   |        | 20        | Counterflow                   |        |
| 6         | Closed vessel                 |        | 21        | Counterflow                   |        |
| 5         | Counterflow                   |        | 22        | Bunsen flame                  |        |
| 7         | Flat flame, heat flux         |        | 23        | Closed vessel                 |        |
| 8         | Closed vessel                 |        | 24        | Closed vessel                 |        |
| 5         | Counterflow                   |        | 25        | Closed vessel                 |        |
| 9         | Closed vessel                 |        | 26        | Closed vessel                 |        |
| 10        | Closed vessel                 |        | 27        | Closed vessel                 |        |
| 11        | Closed vessel                 |        | 28        | -                              |        |
| 12        | Flat flame, heat flux         |        | 29        | -                              |        |
| 13        | Closed vessel                 |        | 30        | -                              |        |
| 14        | Closed vessel                 |        | 31        | -                              |        |
| 15        | Bunsen flame                  |        | 32        | -                              |        |
| 16        | Flat flame, heat flux         |        | 33        | -                              |        |
| 17        | Flat flame, heat flux         |        | 34        | -                              |        |
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