

Parameterization of laminar flame speed dependence on pressure and temperature in hydrogen-air mixtures

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1 Introduction

The laminar flame speed is one of the main characteristics of combustible gases. Its determination is based either on the direct experimental data or on the combustion simulation using detailed reaction mechanism. Several mechanisms describing the combustion of hydrogen in air have been proposed by different research groups [1], [2], [3].

In many applications, and for practical reasons, it is necessary to assume that chemical reactivity is described by a single one-step overall reaction. In such case, instead of looking for explicit experimental data or performing detailed simulations, it is usually feasible to rely on the approximation of the existent verified data. The laminar flame speed in this case will depend on initial conditions (mixture composition and initial pressure and temperature) and several variables characterizing the mixture, e.g. heat conductivity, reaction order, activation energy, etc. [4].

The laminar flame speed dependence on pressure, temperature and fuel composition in hydrogen-air mixtures is often characterized by the power function,

$$S_L(\varphi, T) = S_{L,0}(\varphi) \cdot (T / T_0)^\alpha (p / p_0)^\beta. \quad (1)$$

Several groups have studied the dependences of α and proposed several equations for it [5], [6]. Koroll et al. [7] extended the equation (1) to include the change of the thermal conductivity λ , obtaining,

$$S_L(\varphi, T) = S_{L,0}(\varphi) \sqrt{\frac{\lambda(T)}{\lambda(298K)}} \left(\frac{T}{298K} \right)^\alpha, \quad (2)$$

and utilized the expression for the exponent α by Liu and MacFarlane [8]. The variation of the pressure has a more complex influence on the laminar flame speed than temperature [9]. A dependence of the pressure exponent on pressure itself and species concentrations was suggested in the papers [10], [11]. Based either on measurements or numerical experiments, several expressions for the pressure exponent have been proposed by different authors [5], [6], [12], [13]. The formulas discussed in those references consider the pressure exponent either as a function of the equivalence ratio or pressure, disregarding the complex dependencies of β on equivalence ratio, temperature and pressure.

The objective of our work is to create a correlation for laminar flame speed that describes the simultaneous influence of the equivalence ratio, temperature, and pressure in ranges as large as possible. In the presented study the initial mixture parameters were varied from 200 K to the autoignition temperature and from 0.1 to 31 bar for the pressure. Since experimental data are available only in a very restricted area inside the parameter domain under consideration, we have used results of the numerical simulations with the view to build a laminar flame speed database for the whole parameter space and then to create a required correlation.

2 Creation of a database of laminar flame speeds

The speed of a laminar, flat and steadily propagating flame was calculated for different mixture compositions, temperatures and pressures with the detailed reaction mechanism of Warnatz and Maas [1] implemented in the computer code INSFLA [1], [14]. 2049 hydrogen-air mixtures were analyzed with hydrogen compositions between 3% and 75%, temperatures between 200K and the autoignition limit and pressures between 0.1 and 31 bar. The suitability of Warnatz and Maas methodology under the selected conditions for high pressures was studied in [15]. Figure 1 shows the comparison of the data obtained with the INSFLA code with the results of different experiments. A significant spread exists in the different experimental results. The dispersion is accentuated in the area of lean mixtures where large relative differences can be observed. The dispersion is especially important in the area of lean mixtures where, in spite of the virtual coincidence of the values (see Figure 1, equivalence ratio approaching 0), large relative differences, of up to 100%, can be observed. Chaumeix [16] performed a similar analysis with different detailed reaction mechanisms and showed a similar scatter in their results. The laminar flame speed obtained utilizing the INSFLA code resulted to be inside the accuracy range obtained from the different experiments.

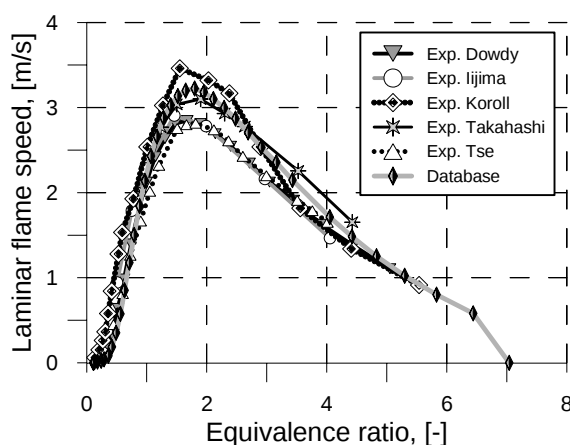


Figure 1: Laminar flame speed vs. equivalence ratio at 300 K and 1 bar. Comparison of INSFLA data with experimental results by Iijima and Takeno [5], Koroll et al. [7], Dowdy et al. [17], Takahashi et al. [18], Tse et al. [19].

3 Model describing the laminar flame speed

Using the data from the created database a search for the suitable form of an approximation of the laminar flame speed for steam diluted hydrogen-air mixtures was carried out. A key requirement for the correlation expression is self-competitive: it has to fit the original data as accurately as possible remaining meanwhile as simple as possible. The strategy followed implies the determination of the laminar flame speed at the pressure and temperature of reference. Then, a correction was implemented to take into account the effect of temperature and pressure. The dependence of the laminar flame speed on the equivalence ratio at reference conditions, $T_0=300\text{K}$ and $p_0=1\text{bar}$, was approximated by a cubic spline interpolation between the data points calculated with INSFLA and the flammability limits [13].

3.1 Dependence on temperature

The temperature dependence of the laminar flame velocity is based on the correlation (2) which was evaluated for a wide range of mixture compositions and conditions at one bar. The results obtained $S_{L,C}(\phi, T)$ were correlated with the database values $S_{L,I}(\phi, T)$ at different temperatures Figure 2 (left). In the Figure 2 left, for a perfect agreement every single point would have been located on the straight line $S_{L,C}(\phi, T) = S_{L,I}(\phi, T)$. The points positioned above this line represent an overestimation of the real values and vice versa. For temperatures sufficiently elevated, considerable systematic differences occur, revealing the limitations of equation (2).

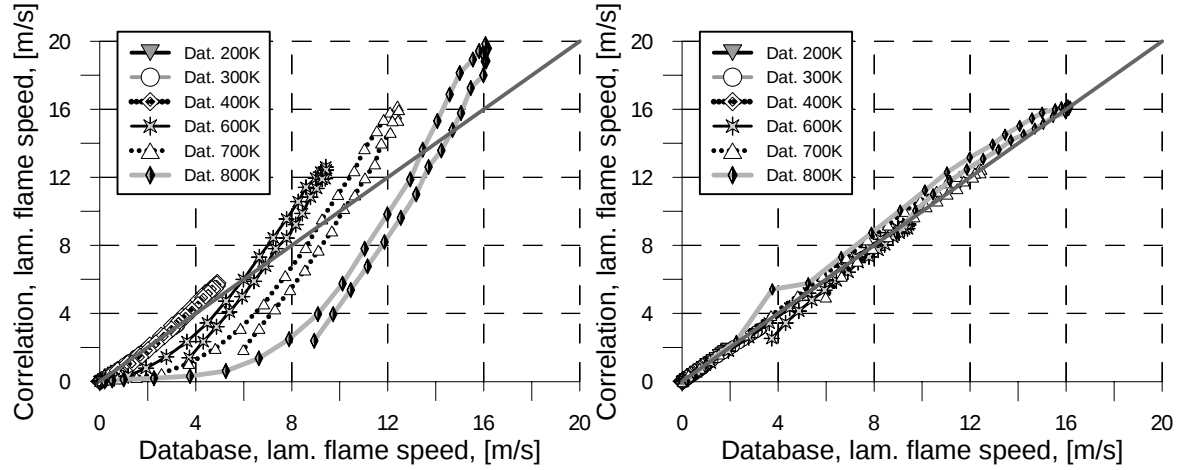


Figure 2: Left, comparison of the results of eq. (2) and INSFLA data at different temperatures and 1 bar. Right, same after new corrections were applied. Each point represents a single composition characterized by ϕ and T .

A correction function can be determined by describing the curves in Figure 2 by a temperature dependent function F . Its inverse F^{-1} converts them on the straight line $S_{L,C} = S_{L,I}$ in the following way,

$$S_{L,I} = S_{L,C}^* = F^{-1}(S_{L,C}, T) \quad (3)$$

The results represented in Figure 2 (left) can be approximated by the power function,

$$S_{L,C} = F(S_{L,I}, T) = a_2(T) S_{L,I}^{a_1(T)} \Rightarrow S_{L,C}^* = \left(\frac{1}{a_2(T)} S_{L,C} \right)^{\frac{1}{a_1(T)}}, \quad (4)$$

that may deliver a good approximation with two sets of values for a_1 , a_2 depending on ϕ and T . With the data available the corresponding expressions were derived and resulted to be,

$$a_1(T) = \begin{cases} -7.82 \cdot 10^{-4} T + 1.23 & \phi \leq 0.3 \\ 1.95 \cdot 10^{-8} T^3 - 2.08 \cdot 10^{-5} T^2 - 8.62 \cdot 10^{-3} T - 0.20 & \phi > 0.3 \end{cases} \quad (5)$$

$$a_2(T) = \begin{cases} \exp(-4.56 \cdot 10^{-3} T + 1.40) & \phi \leq 0.3 \\ 2.08 \cdot 10^{-8} T^3 - 3.34 \cdot 10^{-5} T^2 + 1.45 \cdot 10^{-2} T - 0.90 & \phi > 0.3 \end{cases} \quad (6)$$

Due to inaccuracies at high temperatures, this enhanced correlation was corrected again for temperatures above 600 K in the way,

$$S_{L,C}^T(\phi, T) = [S_{L,C}^*(\phi, T)]^{C(T)}, \quad (7)$$

in which

$$C(T) = \begin{cases} 1 & T \leq 600K \\ -1.5 \cdot 10^{-4} \cdot T + 1.09 & T > 600K \end{cases} \quad (8)$$

The results contained in Figure 2 (right) show an excellent agreement between the values obtained utilizing the equation (7) and the database. A quantitative evaluation of the correctness of the results was performed using three statistic magnitudes, the correlation coefficient, the mean absolute error and the standard deviation. The very high value obtained for the correlation coefficient, and the small values for the standard and absolute deviation assure a good approximation.

3.2 Dependence on pressure

The laminar flame speed dependency on pressure has been formulated independently for pressures smaller and bigger than 1 bar. Each curve in the $S_{L,C}$ - $S_{L,I}$ plane can be transformed into two intersecting straight lines by raising the former correlation $S_{L,C}$ by the power of a temperature dependant coefficient d_2 . These lines can be corrected on the identity $S_{L,C}=S_{L,I}$ using the coefficients d_1 and d_3 in the following way,

$$S_{L,C}^{T,p}(\varphi, T, p) = \frac{1}{d_1} [S_{L,C}^T(\varphi, T)]^{d_2} - d_3 \quad (9)$$

3.2.1 Pressures lower than 1 bar

The parameters d_1 and d_2 only depend on pressure and are approximated by

$$d_1(p) = \begin{cases} 0.7 \cdot p / p_0 + 0.3 & \varphi \leq 0.3 \\ 1 & \varphi > 0.3 \end{cases} \quad (10)$$

$$d_2(p) = 0.13 \cdot \ln(p / p_0) + 1 \quad (11)$$

d_3 depends on temperature and pressure and is calculated using

$$d_3(p, T) = \begin{cases} 0 & \varphi \leq 0.3 \\ Q & \varphi > 0.3 \end{cases} \quad (12)$$

where the value of $Q(p, T)$ is given by the linear interpolation between the following formulas

$$Q(p, T) = \begin{cases} -2.26 \cdot 10^{-6} T^2 - 4.78 \cdot 10^{-4} T + 0.11 & p = 0.1 \text{ bar} \\ -4.99 \cdot 10^{-6} T^2 + 2.58 \cdot 10^{-3} T - 0.36 & p = 0.3 \text{ bar} \\ 0 & p = 1 \text{ bar} \end{cases} \quad (13)$$

3.2.2 Pressures higher than 1 bar

The coefficient d_1 is obtained from the linear interpolation between the formulas

$$d_1(p, T) = \begin{cases} 4.71 \cdot 10^{-6} T^2 + 2.50 \cdot 10^{-4} T + 1.04 & p = 3.1 \text{ bar} \\ 2.52 \cdot 10^{-5} T^2 - 1.52 \cdot 10^{-3} T + 1.44 & p = 10 \text{ bar} \\ 1.80 \cdot 10^{-4} T^2 - 6.09 \cdot 10^{-2} T + 10.53 & p = 31.6 \text{ bar} \end{cases} \quad (14)$$

while d_2 is expressed with the formula,

$$d_2 = 0.43 \cdot \ln(p / p_0) + 1. \quad (15)$$

$$d_3 = 0 \quad (16)$$

In Figure 3, the results obtained with the corrected formulation $S_{L,C}$ are correlated with the original database values $S_{L,I}$ at 300 K. The absolute majority of the points are located close to the equality $S_{L,C}=S_{L,I}$, the correlation coefficient $r_{L,C}$ is large and a low standard deviation is achieved. The correlation obtained for this temperature agrees with the data obtained in calculations with INSFLA in the range from 200 to 800 K. The model approximates the values obtained with INSFLA with a maximum relative error of 8.3%

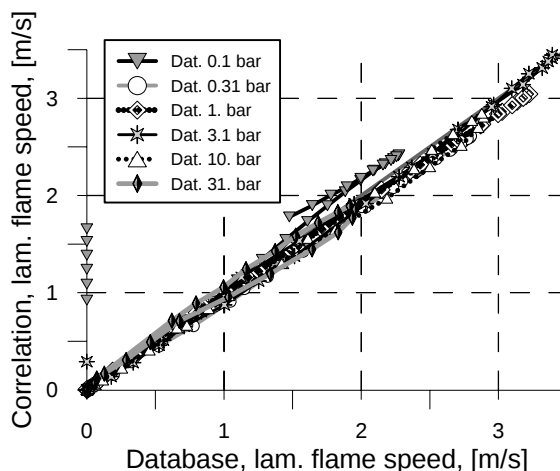


Figure 3: Correlation of approximation used for the modeling of the pressure deviations with database values at 300 K.

The dependence on the pressure obtained could be interpreted as an implicit *overall* reaction order n , if we assume $S_L \sim P^{n/2-1}$ [4]. Between 1 and 31.6 bar the d_l dependence is approximated as $d_l \approx 1.4 \cdot T/T_0 \cdot (P/P_0 - 1)$. With the previous considerations studying the dependence S_L/S_{L0} , the ratio $(P/P_0)^{n/2-1} \approx S_{L0} \cdot 0.4 \cdot \ln(P/P_0) / (1.4 \cdot T/T_0 \cdot (P/P_0 - 1))$. Finally,

$$\frac{n}{2} - 1 \approx 0.43 \cdot \ln(S_{L0}) - \frac{\ln(1.4 \cdot T/T_0 \cdot (P/P_0 - 1))}{\ln(P/P_0)} \quad (17)$$

4 Conclusions

A new correlation approximation for the evaluation of the laminar flame speed in hydrogen-air-steam mixtures was created. It is based on the data on laminar flame speeds calculated using INSFLA code with detailed chemical kinetic reaction mechanism of Warnatz and Maas [1]. The proposed approximation is generalized multi-parametric expression taking into account dependencies on equivalence ratio, temperature and pressure. The approximation is found to be valid for all the equivalence ratios inside the flammability limits, for temperatures from 200 K to 800 K and pressures between 0.1 bar and 31.6 bar. The correspondence coefficient between the proposed approximation and the values of the database in whole area of validity is 0.97.

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