

# Laminar Flame Burning Velocity of Fuels/Air Mixture at Different Pressure, Temperature and Equivalence Ratio

**S. Brusca**

*Researcher Department of Engineering University of Messina [sbrusca@unime.it](mailto:sbrusca@unime.it)*

**R. Lanzafame**

*Full Professor Department of Industrial Engineering University of Catania [rlanzafa@dii.unict.it](mailto:rlanzafa@dii.unict.it)*

**A. Marino Cugno Garrano**

*Researcher Department of Industrial Engineering University of Catania [amarin@dii.unict.it](mailto:amarin@dii.unict.it)*

**M. Messina**

*Full Professor Department of Industrial Engineering University of Catania [mmessina@dii.unict.it](mailto:mmessina@dii.unict.it)*

## Abstract

Fuel laminar flame speed is an important property in internal combustion engine modeling and combustion analysis.

The aim of this paper is to develop a mathematical model able to provide laminar flame speed for any fuel at any reagent thermodynamic condition. Therefore a mathematical investigation of laminar burning velocity in some main fuels was carried out.

Fifth order logarithmic polynomial functions were used to predict the propagating flame speed of several combusting fuels as hydrogen, methane, ethane, iso-octane, etc. at different temperature and pressure conditions.

On the basis of results obtained, the mathematical model proposed in this paper showed a higher precision in experimental data interpolation (about 2 % error) and the possibility to interpolate and use a single function for a wider operation field.

**Keywords:** Mathematical Modeling, Combustion, Laminar Burning Velocity, Fuels.

## Introduction

Laminar flame speed is among the most fundamental and intrinsic property characterizing the combustion of homogeneous fuel-air mixtures. It can be defined as the velocity, relative and normal to the flame front, with which unburned gas moves into the front and is converted into products under laminar flow conditions. A flame is correlated to the process of self-sustaining chemical reaction occurring within a space region where unburned mixture is heated and turned into products. This region, called flame front, consists of a preheat zone and a reaction zone. In preheat zone, no significant reaction or energy release occurs. A slight temperature increase of the unburned mixture is mainly due to heat transfer from the reaction zone. Exothermic chemical reactions are activated when a critical temperature is reached. In this region where the temperature increase is strong, heat

release takes place. The reaction zone is placed between the region of reaction activation and the downstream hot region where burned gas reaches equilibrium temperature.

The laminar flame speed is also an important parameter that can be used for both practical applications and theoretical model of internal combustion engines and burners. Most of combustion system mathematical models use this parameter to determine turbulent flame front velocity [1]. Both ICI and combustion turbine mathematical modeling needs to take into account laminar flame velocity in the equations. That is much more important in combustion studies of not conventional fuels [2] and synthesis gas [3, 4].

Several authors measured laminar burning speed for a wide variety of fuels as a function of equivalence ratio and highlighted its strong temperature and pressure dependence [5-10].

When air-fuel mixture temperature increases, oxidation chemical reactions are sped up bringing to a laminar burning velocity rise. A slight decrease in laminar burning velocity is observed at higher air-fuel mixture pressures, which have low influence in chemical reactions while they reduce mass and energy transfer processes in flame front.

The most common equation used to fit flame burning velocity data for hydrogen, methane, propane, iso-octane, methanol and gasoline, at different pressure and temperature of unburned mixture, is a power law of temperature and pressure where exponents are a function of equivalence ratio. The equation also depends on the laminar speed at reference conditions ( $S_{L0}$ ). Iijima et al. [5] proposed an expression for temperature and pressure exponents that depend linearly on the equivalence ratio, used by most of authors [5-10]. Metghalchi et al. [6, 7] used a second-order polynomial function of fuel ratio for laminar flame velocity at the reference conditions for methanol, isooctane, indolene and propane, while Galmiche et.al used a forth-order polynomial function for iso-octane [8]. Vereá et al. recently extended the linear power exponent of pressure to contain quadratic term of equivalence ratio. During their calculation for n-butanol,

isooctane, Liu K. et al. [9] found that it is difficult to compromise such range of equivalence ratio of interest unless the power exponent of pressure is extended to include the cubic term. Ravi et al. [10] assumed the laminar speed at reference conditions and the two exponents to be different order polynomial functions of equivalence ratio for hydrogen-oxygen mixture. To cover whole range of equivalence ratio data, Ravi et al. used different polynomial functions calculating the corresponding coefficients. In order to integrate renewable energies, such as wind energy [11-13], into generation systems, conventional power generation efficiency should be increased. Thus, studying internal combustion engine combustion is fundamental for fuel energy conversion efficiency.

Therefore, in the present work authors proposed a fifth order logarithmic polynomial for the laminar speed at the reference conditions and for both power exponents of pressure and temperature to describe the burning velocity as a function of equivalence ratio, pressure and temperature. In particular, a coefficients database of several conventional and non-conventional fuels was implemented.

The proposed method allows predicting laminar burning velocity of combusting air/fuel mixtures in several engineering applications such as Internal Combustion Engine and Gas Turbine modeling.

### Mathematical model

Laminar flame speed of fuels strongly depends on temperature and pressure. This simultaneous dependence in temperature and pressure was taken into account by authors adopting the commonly used function described by a power law expression as in equation 1.

$$S_L = S_{L0} \left( \frac{T}{T_0} \right)^\alpha \left( \frac{p}{p_0} \right)^\beta \quad (1)$$

where  $S_L$  is the laminar flame speed at arbitrary conditions of temperature  $T$  and pressure  $p$ ,  $T_0$  and  $p_0$  are the reference temperature and pressure,  $S_{L0}$  is the laminar flame speed at reference conditions,  $\alpha$  and  $\beta$  are respectively the power exponent of temperature and pressure. In this paper authors proposed fifth order logarithmic polynomial functions to define the laminar speed  $S_{L0}$  and the exponent  $\alpha$  and  $\beta$  as a function of equivalence ratio  $\phi$  (see equation 2).

$$S_L(\phi) = \left( \sum_{i=0}^5 a_i (\ln \phi)^i \right) \left( \frac{T}{T_0} \right)^{\sum_{i=0}^5 b_i (\ln \phi)^i} \left( \frac{p}{p_0} \right)^{\sum_{i=0}^5 c_i (\ln \phi)^i} \quad (2)$$

In this mathematical model used to fit experimental data of laminar flame speed, the coefficients  $a_i$ ,  $b_i$  and  $c_i$  are determined for a given fuel with the least square method. The calculation procedure of all coefficients for each fuel consists in three main steps.

The coefficients  $a_i$  are firstly obtained starting from the experimental data of the laminar flame speed at reference conditions and solving the over-determined matrix system (3).

$$Y_{10} = X A \quad (3)$$

where:

$$Y_{10} = \begin{bmatrix} S_{L0}(\phi_1) \\ S_{L0}(\phi_2) \\ \vdots \\ S_{L0}(\phi_n) \end{bmatrix} \quad (4)$$

column vector of experimental data  $S_{L0}(\phi)$  at reference temperature and pressure ( $T_0, p_0$ ) ( $j = 1, 2, \dots, n$ ) with  $n > 5$ .

$$X = \begin{bmatrix} 1 & \ln \phi_1 & (\ln \phi_1)^2 & (\ln \phi_1)^3 & (\ln \phi_1)^4 & (\ln \phi_1)^5 \\ 1 & \ln \phi_2 & (\ln \phi_2)^2 & (\ln \phi_2)^3 & (\ln \phi_2)^4 & (\ln \phi_2)^5 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \ln \phi_n & (\ln \phi_n)^2 & (\ln \phi_n)^3 & (\ln \phi_n)^4 & (\ln \phi_n)^5 \end{bmatrix} \quad (5)$$

with  $\phi_j$  data values of equivalence ratio ( $j = 1, 2, \dots, n$ )

$$A = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} \quad (6)$$

with  $a_i$  coefficients of fifth order logarithmic polynomial relative to laminar flame speed at reference conditions.

The column vector  $A$  of unknown coefficients can be easily determined by solving the matrix system 7.

$$A = (X^T X)^{-1} X^T Y_{10} \quad (7)$$

where  $X^T$  is the matrix transpose of  $X$  and  $(X^T X)^{-1}$  is the matrix inverse of  $X^T X$ .

Secondly, the temperature exponent coefficients  $b_i$  and the pressure exponent coefficients  $c_i$  are determined by the matrix system 8.

$$B = (X^T X)^{-1} X^T Y_{TP} \quad (8)$$

where:

$$B = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} \quad (9)$$

$$Y_{TP} = \begin{bmatrix} \ln \left( \frac{S_{TP}(\phi_1)}{S_{L0}(\phi_1)} \right) \\ \ln \left( \frac{S_{TP}(\phi_2)}{S_{L0}(\phi_2)} \right) \\ \vdots \\ \ln \left( \frac{S_{TP}(\phi_n)}{S_{L0}(\phi_n)} \right) \end{bmatrix} \quad (10)$$

$$X = [X_T \ X_p] \quad (11)$$

Where

$$X_T = \begin{bmatrix} \ln\left(\frac{T}{T_0}\right) & \ln\left(\frac{T}{T_0}\right) \cdot \ln\phi_1 & \ln\left(\frac{T}{T_0}\right) \cdot (\ln\phi_1)^2 & \dots & \dots & \dots & \ln\left(\frac{T}{T_0}\right) \cdot (\ln\phi_1)^5 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \quad (12)$$

$$X_p = \begin{bmatrix} \ln\left(\frac{p}{p_0}\right) & \ln\left(\frac{p}{p_0}\right) \cdot \ln\phi_1 & \ln\left(\frac{p}{p_0}\right) \cdot (\ln\phi_1)^2 & \dots & \dots & \dots & \ln\left(\frac{p}{p_0}\right) \cdot (\ln\phi_1)^5 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \quad (13)$$

with T and p arbitrary temperatures and pressures,  $S_{Tp}(\phi_k)$  experimental data of laminar speed at the arbitrary temperatures and pressures (T, p),  $\phi_k$  data values of equivalence ratio ( $k = 1, 2, \dots, m$ ),  $S_{L0}(\phi_k)$  laminar speed values at reference conditions ( $T_0, p_0$ ) calculated using equivalence ratio data  $\phi_k$  and coefficients  $a_i$  in equation 3.

### Results and discussion

In order to determine all coefficients of mathematical model proposed by authors and validate it, experimental data from literature for different fuels were used. Data fitting was performed for some fuels such as methane, ethane, iso-octane, hydrogen, dimethyl ether, tert-butanol, etc.

For the sake of simplicity, validation model results are shown only for iso-octane, since the same assessments can be extended to all other fuels.

The calculation procedure could be divided in the following main steps:

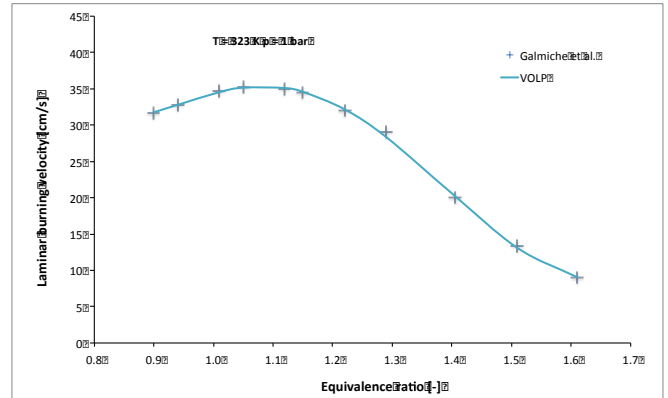
1. Determination of laminar burning velocity coefficients at reference conditions;
2. Determination of laminar burning velocity coefficients at different pressure and temperature;
3. Correlation validation at different pressure and temperature;
4. Verification of correlation extrapolation capabilities.

In the first step, the constant parameters  $a_i$  were optimized using the experimental values of laminar burning velocity at reference conditions  $T_0 = 323$  K and  $p_0 = 1$  bar [10]. The comparison between experimental data and the correlation curve is shown in Fig. 1 and highlights an average error less than 1 %.

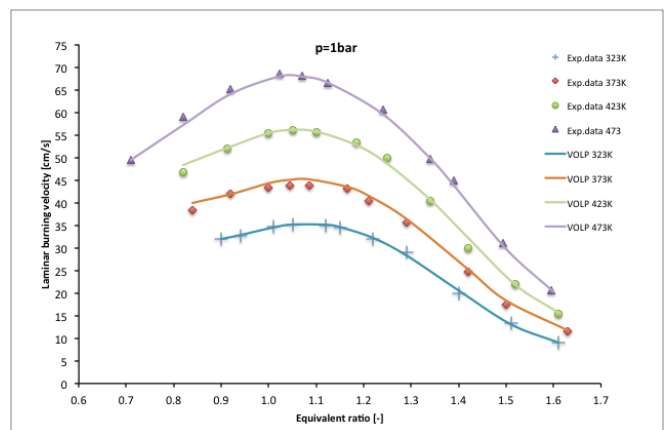
In the second step, the parameters  $b_i$  and  $c_i$  were optimized using experimental data set at reference pressure and variable temperature of 373 K, 423 K, and 473 K as well as at reference temperature and variable pressures of 2, 3, 5, and 10 bar, respectively [10]. In the graphs in Fig. 2, laminar burning velocity is reported as a function of equivalence ratio at mentioned temperatures (Fig. 2a) and pressures (Fig. 2b). In the same figures experimental data and interpolation curves are shown. It is well evident that interpolation curves match experimental data very well (average relative error of 1.63 % and 2.34 % for Fig.2a and Fig. 2b, respectively). Moreover, in Fig. 2b some extrapolation capabilities are observed for higher equivalence ratios.

In order to verify the efficacy of the proposed mathematical model several extrapolation tests at different pressures and temperatures were carried out. In Fig. 3 tests results are

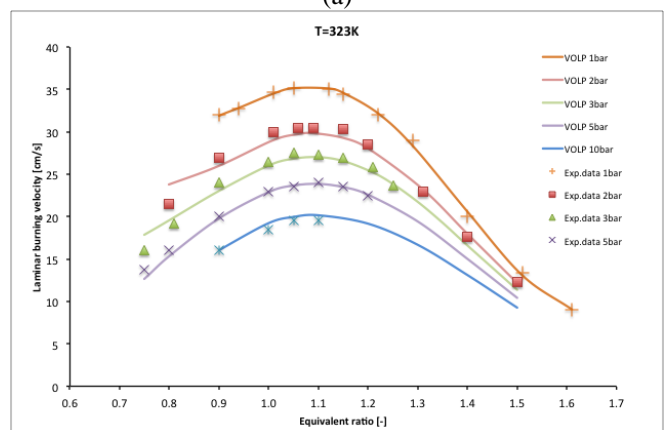
shown. In particular, Fig. 3a, b, c and d show laminar burning velocity as a function of equivalence ratio at different reactant temperatures (323 K, 373 K, 423 K and 473 K) and at different reactant pressures (2 bar, 3 bar, 5 bar and 10 bar). In the same figures experimental data and interpolation curves are reported.



**Fig.1. Experimental and calculated laminar burning velocity of iso-octane as a function of equivalence ratio at reference conditions**



(a)



(b)

**Fig.2. Experimental and calculated laminar burning velocity as a function of equivalence ratio at reference conditions**

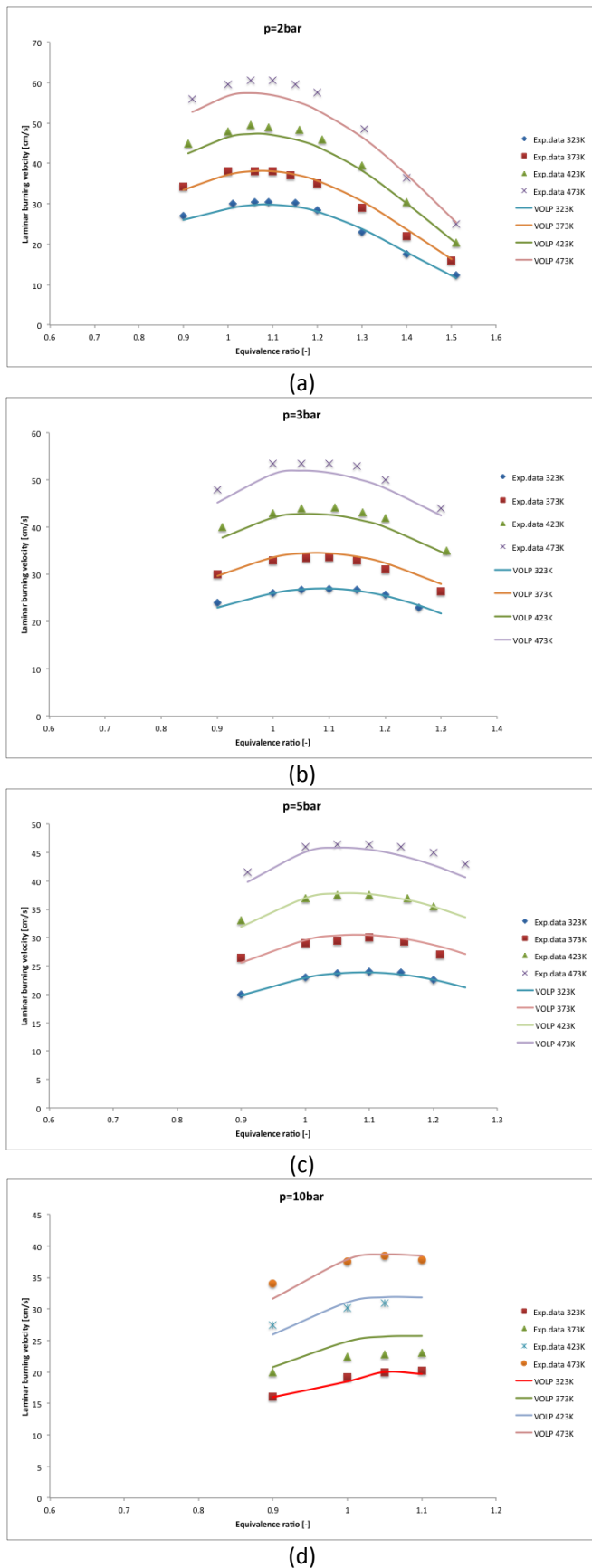


Fig.3. Experimental and calculated laminar burning velocity as a function of equivalence ratio at different pressures and temperatures

Result analysis leads to the consideration that laminar burning velocity increases with equivalence ratio up to about 1.1 and then decreases while equivalence ratio still increases. This behavior is well evident for all analyzed pressures and temperatures. Moreover, increasing reactant pressure (Fig. 2b and Fig. 3) a reduction in laminar burning velocity is observed at all equivalence ratios. The higher the pressure is the lower the laminar burning velocity. Temperature effects on laminar burning velocity are well evident in Fig. 3. A higher reactant temperature has the effect to speed up the combustion reaction increasing the laminar burning velocity. This behavior is observed for all studied reactant pressures, as well as at all equivalence ratios.

As far as the extrapolation capabilities it is concerned, it is possible to observe that extrapolating the curves for each pressure the average error increases with temperature, while increasing the pressure the extrapolation errors are almost constant for each temperature.

In conclusion, it is possible to state that the proposed mathematical model is able to predict laminar burning velocity as a function of equivalence ratio, pressure and temperature with a good agreement with experimental data. The mathematical model can be considered validated.

The new correlation model has been applied to several published experimental results for different fuels and reference, pressure and temperature coefficients have been calculated. A data summary table of laminar burning velocity was compiled (Table 1). This table contains all coefficients, reference conditions, pressure and temperature limits, equivalence ratio range, as well as allowed unit of measurement. A data summary table of laminar burning velocity was compiled. This table contains all coefficients, reference conditions, pressure and temperature limits, equivalence ratio range, as well as allowed unit of measurement. In the same table bibliographic data reference was reported.

TABLE.1. Data summary table of Laminar burning velocity

$$S_L(\phi) = \left( \sum_{i=1}^5 a_i (\ln \phi)^i \right) \left( \frac{T}{T_0} \right)^{c_1 + c_2 \ln(\phi^2)} \left( \frac{p}{p_0} \right)^{c_3 + c_4 \ln(\phi^2)}$$

acetylene						
T <sub>0</sub> [K]	p <sub>0</sub> [atm]	φ range [-]	T range [K]	p range [atm]	UOM	Ref.
298	1	0.6 – 1.8	-	1-2	cm/s	[14,15]
Coefficients	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
	136.78511185	106.60835888	-122.81180448	-99.99970747	-30.75220958	-243.79727130
	b <sub>0</sub>	b <sub>1</sub>	b <sub>2</sub>	b <sub>3</sub>	b <sub>4</sub>	b <sub>5</sub>
	-	-	-	-	-	-
	c <sub>0</sub>	c <sub>1</sub>	c <sub>2</sub>	c <sub>3</sub>	c <sub>4</sub>	c <sub>5</sub>
-0.19993383	0.29928146	-0.24935839	-3.80149819	-3.17858503	11.07670616	
benzene						
T <sub>0</sub> [K]	p <sub>0</sub> [atm]	φ range [-]	T range [K]	p range [atm]	UOM	Ref.
298	1	0.8 – 1.6	298-450	1-3	cm/s	[16,17,18]
Coefficients	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
	41.56611013	30.70705592	-141.80125318	-331.20081423	88.39415337	830.09909291
	b <sub>0</sub>	b <sub>1</sub>	b <sub>2</sub>	b <sub>3</sub>	b <sub>4</sub>	b <sub>5</sub>
	1.35872952	-2.09133865	-1.45226502	-20.34059243	-36.75455809	80.76204838
	c <sub>0</sub>	c <sub>1</sub>	c <sub>2</sub>	c <sub>3</sub>	c <sub>4</sub>	c <sub>5</sub>
-0.07369291	0.53424273	1.88410735	9.61036883	-4.47408135	-1.22107814	
carbon monoxide						
T <sub>0</sub> [K]	p <sub>0</sub> [atm]	φ range [-]	T range [K]	p range [atm]	UOM	Ref.
298	1	0.4 – 2	-	-	cm/s	[19]
Coefficients	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
	16.21398704	5.33200638	-3.42306594	6.47061936	-3.93588537	-15.01471807
	b <sub>0</sub>	b <sub>1</sub>	b <sub>2</sub>	b <sub>3</sub>	b <sub>4</sub>	b <sub>5</sub>
	-	-	-	-	-	-
	c <sub>0</sub>	c <sub>1</sub>	c <sub>2</sub>	c <sub>3</sub>	c <sub>4</sub>	c <sub>5</sub>
-	-	-	-	-	-	



tert-butanol						
T <sub>0</sub> [K]	p <sub>0</sub> [atm]	φ range [-]	T range [K]	p range [atm]	UOM	Ref.
428	1	0.8 – 1.5	428–488	1–5	cm/s	[30]
Coefficients	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
	49.60012772	12.33870721	-60.02138093	-391.50399530	-763.00223734	2371.55724619
	b <sub>0</sub>	b <sub>1</sub>	b <sub>2</sub>	b <sub>3</sub>	b <sub>4</sub>	b <sub>5</sub>
	1.31851311	0.13035354	-3.15324076	26.78102775	58.70504492	-195.12014956
c <sub>0</sub>	c <sub>1</sub>	c <sub>2</sub>	c <sub>3</sub>	c <sub>4</sub>	c <sub>5</sub>	
-0.12009181	0.34257029	-2.09267434	0.39137248	30.81232216	-54.47956552	
toluene						
T <sub>0</sub> [K]	p <sub>0</sub> [atm]	φ range [-]	T range [K]	p range [atm]	UOM	Ref.
298	1	0.8 – 1.4	298–470	1–2	cm/s	[17, 31, 32]
Coefficients	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>
	35.78407392	21.01348860	-90.99441920	-132.03193457	-199.86840684	-219.45572189
	b <sub>0</sub>	b <sub>1</sub>	b <sub>2</sub>	b <sub>3</sub>	b <sub>4</sub>	b <sub>5</sub>
	1.66576338	-0.24027649	0.47965078	-2.36407108	18.02927030	28.06813188
c <sub>0</sub>	c <sub>1</sub>	c <sub>2</sub>	c <sub>3</sub>	c <sub>4</sub>	c <sub>5</sub>	
-0.05543636	-0.00089523	0.64551729	-2.24110263	-25.73469103	68.72776722	

**Conclusions**

In this paper a study of laminar burning velocity of fuels/air mixture as a function of equivalence ratio, reactant pressure and temperature was presented.

Therefore, a mathematical methodology to interpolate and extrapolate experimental laminar burning velocity data was proposed and tested. Results analysis highlighted that simulated results, in the comparison between experimental data, presents an average relative error of about or less than 2 % at reference conditions. Thus, the proposed model is validated.

As mentioned the proposed model has some extrapolation capabilities. Thus, several tests were carried out at different pressure and temperature to test and demonstrate them. Results analysis highlighted that the proposed mathematical model is able to extrapolate data for pressure and temperature acceptable errors (maximum average error less than 5 %).

Coefficients determination for several fuels was carried out. For each studied fuel, reference, pressure and temperature coefficients were determined starting from experimental data. A data summary table of laminar burning velocity was compiled. This table contains all coefficients, reference conditions, pressure and temperature limits, equivalence ratio range, as well as allowed unit of measurement.

In conclusion, on the basis of the presented results it is possible to state that the proposed mathematical model is able to predict laminar burning velocity of fuel/air mixture for each equivalence ratio, pressure and temperature with very low errors.

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