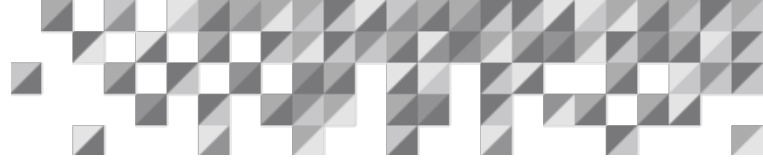


Laminar Flame Speeds Data Collection

Ensuring Reliable Data for Explosions Characterization

An ioMosaic White Paper



Introduction

Regarding vessels and tubes containing combustible gases or dust, it is important to acquire knowledge on the conditions under which a fuel and oxidizer could undergo explosive reactions. These conditions are strongly dependent on the pressure and temperature.

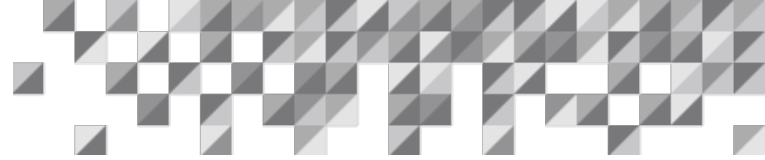
Given a premixed fuel-oxidizer system at room temperature and ambient pressure, the mixture is essentially unreactive. However, if an ignition source is applied locally and the composition of the mixture is within certain limits (the so-called flammability limits), a region of explosive reaction can propagate through the gaseous mixture due to mainly two phenomena: (1) Temperature rises substantially, (2) High concentration of radicals to form. Characterizing potential explosive reactions is one of the main objectives of hazard assessment. Safeguards to be implemented in process equipment, best process conditions, appropriate prevention and/or mitigation measures, are some of the key purposes to be clarified when handling flammable mixtures. This characterization requires knowledge of several parameters that directly influence on the explosive reaction behavior. One of these parameters is the Laminar Flame Speed, which is one of the key factors that define the kinetics of the reaction.

The present paper addresses how to characterize fuel-oxidizer explosive reactions and highlights the importance of the laminar flame speed concept. The main purpose of this study is to provide reliable data regarding laminar flame speeds with the aim to ensure accurate calculations for hazard assessment purposes.

Explosive reaction: Deflagration and Detonation Concepts

When a premixed gaseous fuel-oxidizer mixture within the flammability limits is contained in a long tube or vessel, a combustion wave will propagate down the recipient if an ignition source is present. The velocity of this wave is controlled by transport processes: (1) heat conduction and, (2) diffusion of radicals if the velocities observed are much less than the speed of sound in the unburned gaseous mixture. However, if the propagating wave undergoes a transition from subsonic to supersonic speeds, the velocity of the wave is controlled by the shock wave structure.

The propagating combustion wave is referred as a flame, and it is defined as a deflagration or detonation depending on the velocity of the wave; i.e., subsonic or supersonic, respectively.



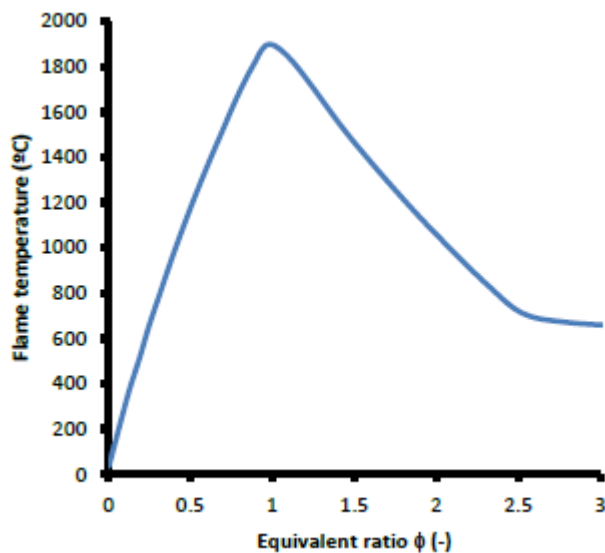
Addressing Deflagrations

The key parameters for the evaluation of combustion systems are the equilibrium product temperature and composition. If all the heat evolved in the reaction is employed solely to raise the product temperature, this temperature is called the adiabatic flame temperature. Valuable information can be extracted from a plot of *Flame Temperature* versus *fuel-oxidizer mole fraction ratio*, defining the ratio (ϕ) as follows:

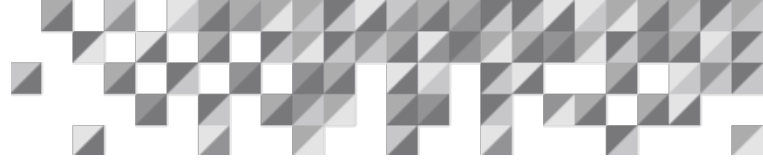
Equation 1. Fuel-oxidizer mole fraction ratio definition

$$\phi = \frac{\left[\frac{M_{fuel}}{M_{oxidizer}} \right]}{\left[\frac{M_{fuel}}{M_{oxidizer}} \right]_{stoichiometric}} = \frac{\left[\frac{N_{fuel}}{N_{oxidizer}} \right]}{\left[\frac{N_{fuel}}{N_{oxidizer}} \right]_{stoichiometric}}$$

Figure 1: Flame temperature as a function of fuel-air mole fraction ratio of a given mixture



Source: Process Safety Office® - SuperChems®



The maximum flame temperature is reached at a value of $\phi = 1$; i.e., stoichiometric ratio. In fact, the maximum flame temperature normally appears at ratios slightly higher than the stoichiometric fuel-air compositions mainly due to the preferential diffusion of oxygen into the reaction zone which shifts the composition towards stoichiometric. For example, a mixture of ethylene-air presents a maximum flame temperature at $\phi = 1.13$.

The Laminar Flame Speed Concept

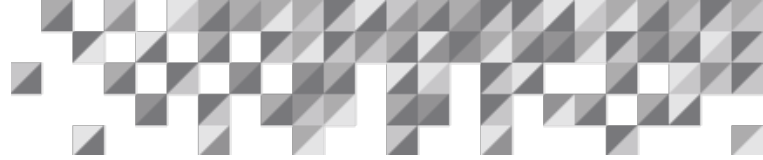
Laminar flame speed or burning velocity plays an essential role in determining several important aspects of the combustion process. This parameter is used in many areas of combustion science such as in designing burners and predicting explosions.

The burning velocity, **Su**, is defined as the velocity at which unburned gases move through the combustion wave in the direction normal to the wave surface [2]. It plays an essential role in determining several important aspects of the combustion process, among these are:

- Ignition Delay (which in turn affects the range of equivalence ratios which can be a combustion)
- Thickness of the wall quench layers (which are a primary source of unburned hydrocarbons),
- Minimum Ignition Energy; i.e., smallest amount of energy needed to propagate aflame for a given system

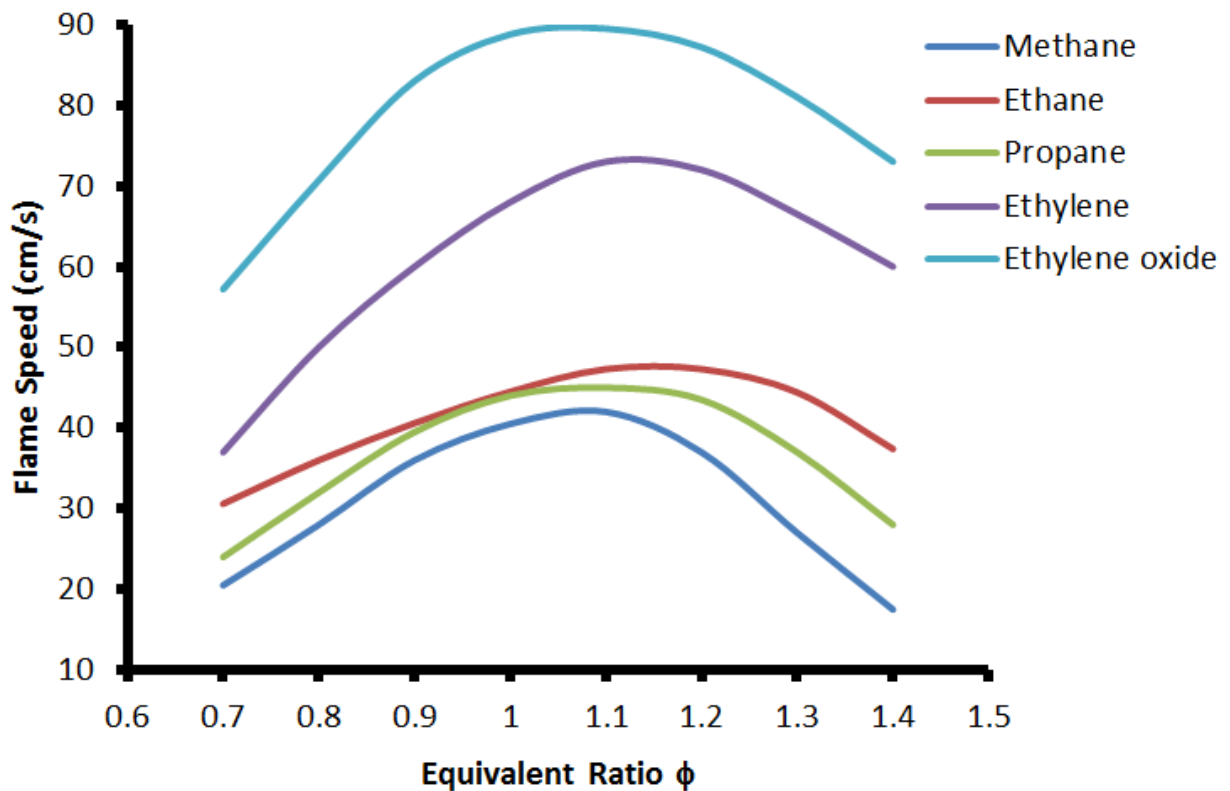
Additionally, it is found that a detailed knowledge of laminar premixed flames will provide insights into such properties as heat release rates, flammability limits, propagation rates, quenching, and emissions characteristics [3]. The methods used to measure burning rates and flame speeds can be characterized as either constant pressure or constant volume

- Constant pressure methods are limited to a relatively narrow range of temperatures and are most useful for obtaining data at atmospheric pressure.
- Constant volume methods cover a wider range of temperatures and pressures and provide a range of data along an isentropic in a single experimental run. In addition, corrections for flame geometry or heat loss are generally quite small. These methods have been used for several investigators [4], [5], [6], [7]. These methods use a spherical vessel with central ignition and rely on measurements taken after the early stages of flame propagation, during which there is a significant pressure rise. The advantage of measuring the burning velocity using the closed vessel over other methods is that, from a single test, burning velocities can be calculated over a wide range of temperatures and pressures.



Laminar flame speeds, equivalence ratios, diluent concentrations, pressures and temperatures have been collected for a wide variety of fuels-oxidizer mixtures [2], [11]. Taking into account reported experimental data, it is evident how sensitive is the laminar flame speed of fuel-oxidizer mixtures respect to the following parameters: (1) chemical composition, (2) Pressure, and (3) Temperature. Figure 2 and Figure 3 illustrate how laminar flame speeds depend on the equivalent ratio and pressure, respectively.

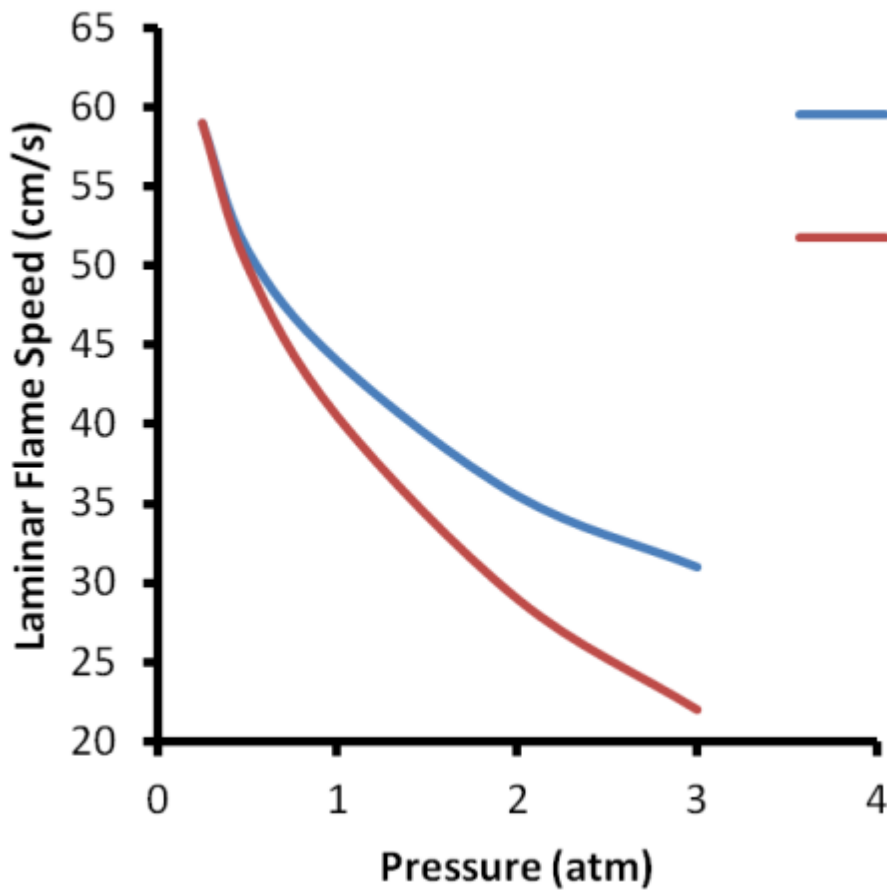
Figure 2: S_L ($\text{cm}\cdot\text{s}^{-1}$) vs. ϕ



Source: Process Safety Office® - SuperChems®

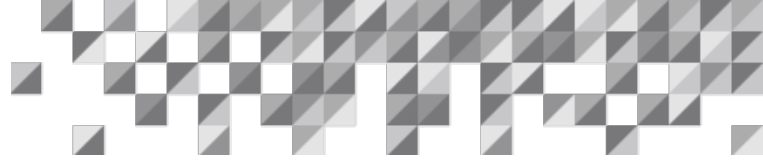


Figure 3: S_L ($\text{cm}\cdot\text{s}^{-1}$) vs. P (atm)



Source: Process Safety Office® - SuperChems®

This sensitivity is commonly described by a power law expression. Metghalchi and Keck [5], [6] calculated burning velocities from several fuels at different unburned densities and temperatures at constant volume. Results fitted to the following relation:



Equation 2. Metghalchi and Keck power law for modeling laminar flame speeds

$$S_L^0 = S_{L,ref}^0 \left[\frac{T_u}{T_{u,ref}} \right]^\alpha \left[\frac{P}{P_{ref}} \right]^\beta (1 - 2.1Y_{dil}) \quad P \geq P_{ref}$$

$$S_{L,ref}^0 = B_m + B_\phi (\phi - \phi_m)^2$$

$$\alpha = 2.18 - 0.8(\phi - 1)$$

$$\beta = -0.17 + 0.22(\phi - 1)$$

S_L^0 : laminar flame speed [$\text{cm}\cdot\text{s}^{-1}$]

$S_{L,ref}^0$: reference laminar flame speed [$\text{cm}\cdot\text{s}^{-1}$] (please refer to appendix)

P : pressure [e.g., atm, bar]

P_{ref} : reference pressure [e.g., atm, bar]

$T_{u,ref}$: reference temperature [e.g., °C, K]

T_u : unburned gas temperature [e.g., °C, K]

ϕ : equivalent ratio [-]

B_m : maximum flame speed attained at equivalence ratio ϕ_m [$\text{cm}\cdot\text{s}^{-1}$]

B_ϕ : quantifies the dependence of flame speed on equivalence ratio [-]

Y_{dil} : mass fraction of diluents [-]

α : temperature exponent [-]

β : pressure exponent [-]

Addressing potential hazardous scenarios due to explosions, it is common to establish a conservative criterion via considering stoichiometric ratios of fuel-oxidizer mixtures involved ($\phi = 1$). Following equation 2, it is easy to define both the temperature and pressure exponents; i.e., $\alpha = 2.18$, and $\beta = -0.17$. However, if it is considered more convenient to work with the equivalent ratio that satisfies maximum flame speed (B_m), it is necessary to calculate α and β per each specific mixture under study.

Advanced Modeling Deflagrations

SuperChems® presents an algorithm for direct minimization of the Gibbs free energy which can be used to perform a wide variety of simultaneous multiphase physical and chemical equilibrium estimates. Calculations are performed at each time step to determine the combustion reaction products, flame temperature, reactant temperature, and pressure. The algorithm uses a modified cubic equation of state for both the liquid and vapor phases. This equation of state provides analytic derivatives and the ability to perform direct minimization of the Gibbs free energy at high



pressure and for highly non-ideal systems and systems with strong solution effects. Detailed description of the method can be found in [1]. This algorithm can be used to perform a wide variety of simultaneous multiphase physical and chemical equilibrium estimates. Some applications are the following:

- Estimation of flammability limits for vapor and multiphase systems. The effects of pressure, temperature, inerts, and composition are well predicted for a variety of systems. This method has been proven as a very useful tool for fire and explosion hazard assessment studies and for providing guidance to flammability testing [1].
- Hugoniot combustion curves and identification of upper and lower Chapman-Jouguet points for detonation characterization (out of the scope of this paper).
- Deflagration dynamics

Focusing on modeling deflagrations, a detailed one-dimensional model for the prediction of overpressures in cubic, rectangular, and spherical geometries has been developed and implemented into SuperChems®. The non-ideal behavior of burnt and unburnt gaseous components is accounted for during high pressure venting and multi-reaction chemical equilibrium. In the derivation of the model, the following assumptions are made [12]:

- The gas mixture is uniform in composition
- The thickness of the flame in the reaction zone is negligible
- The burning rate accelerates when the flame front becomes wrinkled at a critical expansion ratio corresponding to a critical Reynolds number.
- Burnt and unburnt gases are treated assuming non-ideal gas behavior using a modified cubic equation of state.
- When venting occurs, unburnt gases are vented until the flame area reaches the vent at which time burnt gases are vented.

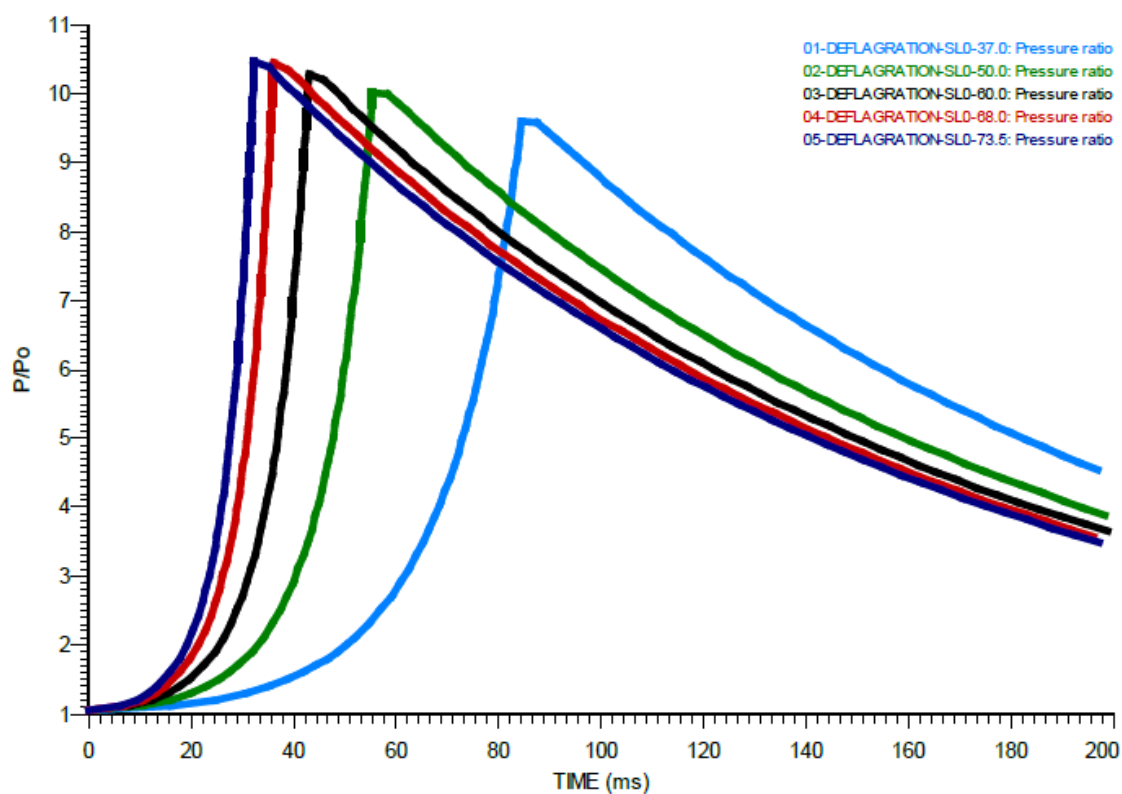
The deflagration dynamics model accounts for the variation of the laminar flame speed according to the previous cited work developed by Metghalchi and Keck [5], [6].

The following example illustrates an explosion in a given vented vessel with a fuel-oxidizer mixture. Five (5) different values of laminar flame speeds have been taken into account in the calculations with the aim to highlight how the simulation depends on this parameter; i.e., how explosion potential varies with temperature, pressure and equivalent ratio. The laminar flame speeds used for the simulation are 73.5, 68.0, 60.0, 50.0, and 37.0 cm·s⁻¹. Results are given as pressure profile (see Figure 4) and deflagration severity profile (see Figure 5); i.e., taking into account the deflagration index in (bar·m·s⁻¹), parameter defined as the product of the maximum pressure rise



and the cube root of the volume, and which is considered valuable for the actual comparison purposes.

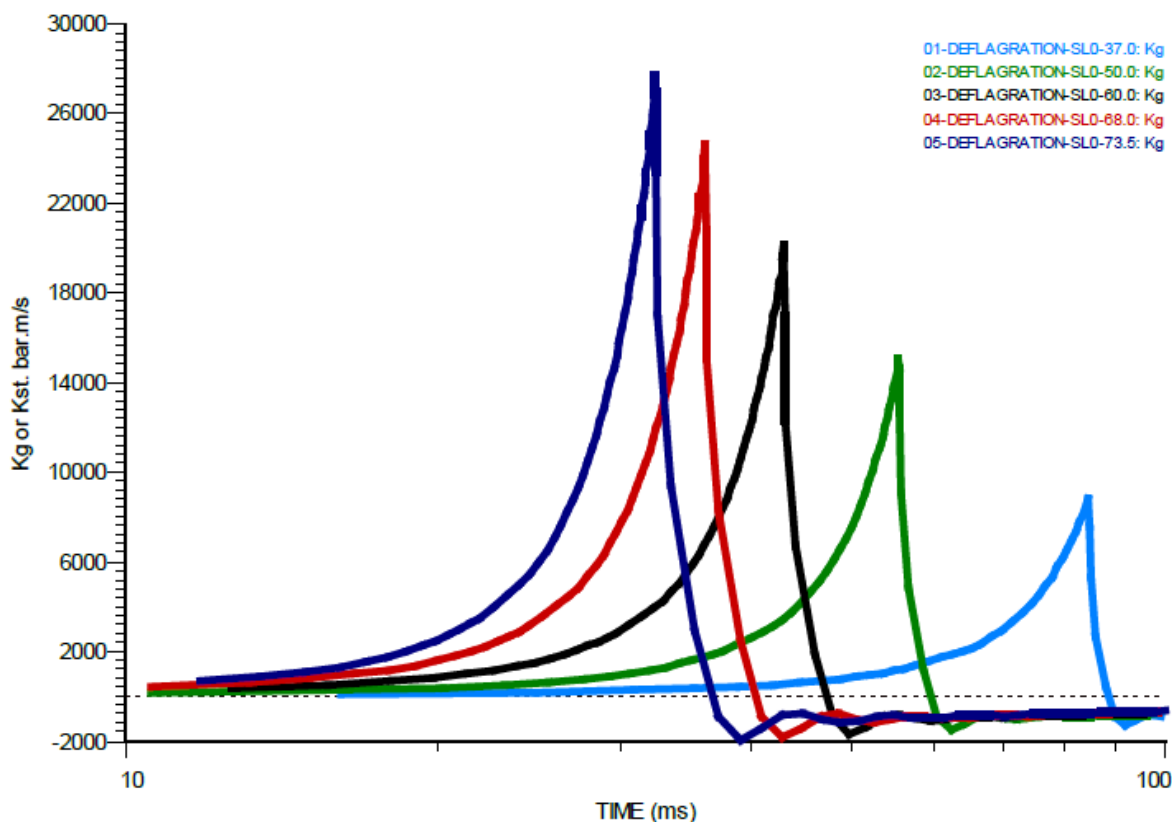
Figure 4: Deflagration Pressure Profile



Source: Process Safety Office® - SuperChems®



Figure 5: Deflagration Severity Profile

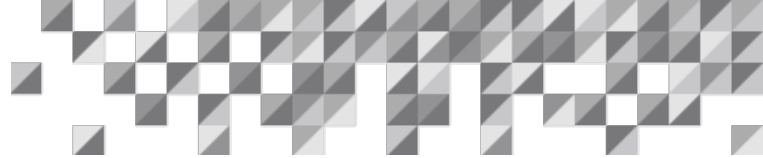


Source: Process Safety Office® - SuperChems®

Conclusions

The laminar flame speed is a key variable for explosion characterization purposes. Modeling these phenomena allows acquiring valuable information for hazard assessment; e.g., venting sizing for partial deflagrations in vessels containing gases or dusts, minimum length of a pipe to avoid detonation, hazard characterization and classification of fuel-oxidizer mixtures, minimum ignition energies estimation, quenching distances.

Laminar flame speed depends on the fuel-oxidizer mixture composition, temperature and pressure. Relatively small variations of these parameters entail substantial variations on flame speeds. Illustrated Figure 4 and Figure 5 evidence this sensitivity. It is for this reason that is necessary to ensure reliable data for performing simulations that require the use of flame speeds.



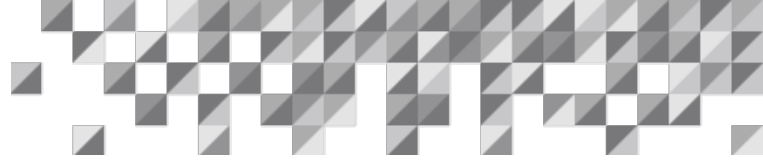
After briefly introducing explosive reaction characterization, the appendix of the present paper presents a valuable data collection concerning flame speeds for different equivalent ratios. Additionally, both the temperature and pressure exponents; i.e., α and β have been calculated taking into account the maximum flame speed (sometimes slightly superior to the stoichiometric ratio $\phi = 1$). This data is convenient when addressing hazard assessment purposes; thus, working with worst credible scenarios.

The compilation of laminar flame speed data given has been extracted from [2]. These data collection is due to Gibbs and Calcote [8]. The data are for premixed fuel–air mixtures at 25°C and 100°C and 1 atm pressure. Examples of more recent data have also been included from Law [9], and Vagelopoulos et al. [10].



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Additional Resources

1. Jordi Dunjó, Ph.D., 2014
2. Daniel Nguyen, P.E., 2014
3. Michelle Murphy, Partner, ioKinetic, LLC, 2014



Appendix

Table A1. Burning Velocities of Various Fuels at 25°C Air-Fuel Temperature and 1 atm (0.31 mol.% H₂O in Air). Burning Velocity S_L in cm/s as a Function of Equivalence Ratio ϕ . Exponent α and exponent β have been calculated for ϕ_{max} according to [5] and [6].

Fuel	Equivalent Ratio ϕ								S_L (cm/s)		T exponent	P exponent	Source
	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	$S_{\max}$	ϕ at $S_{\max}$	α	β	
Saturated Hydrocarbons													
Ethane	30.6	36.0	40.6	44.5	47.3	47.3	44.4	37.4	47.6	1.14	2.07	-0.14	[8]
	22.0	29.0	36.5	42.5	43.0	42.5	40.0	27.5	—	—	—	—	[9]
Propane	—	—	42.3	45.6	46.2	42.4	34.3	—	46.4	1.06	2.13	-0.16	[8]
	24.0	32.0	39.5	44.0	45.0	43.5	37.0	28.0	—	—	—	—	[9]
	23.0	30.0	37.0	39.0	41.0	40.5	33.5	25.0	—	—	—	—	[10]
n-Butane	—	38.0	42.6	44.8	44.2	41.2	34.4	25.0	44.9	1.03	2.16	-0.16	[8]
Methane	—	30.0	38.3	43.4	44.7	39.8	31.2	—	44.8	1.08	2.12	-0.15	[8]
	20.5	28.0	36.0	40.5	42.0	37.0	27.0	17.5	—	—	—	—	[9]
	17.0	25.0	33.0	38.0	38.5	34.0	24.0	13.5	—	—	—	—	[10]
n-Pentane	—	35.0	40.5	42.7	42.7	39.3	33.9	—	43.0	1.05	2.14	-0.16	[8]
n-Heptane	—	37.0	39.8	42.2	42.0	35.5	29.4	—	42.8	1.05	2.14	-0.16	[8]
2,2,4-Trimethylpentane	—	37.5	40.2	41.0	37.2	31.0	23.5	—	41.0	0.98	2.20	-0.17	[8]
2,2,3-Trimethylpentane	—	37.8	39.5	40.1	39.5	36.2	—	—	40.1	1.00	2.18	-0.17	[8]
2,2-Dimethylbutane	—	33.5	38.3	39.9	37.0	33.5	—	—	40.0	0.98	2.20	-0.17	[8]
Isopentane	—	33.0	37.6	39.8	38.4	33.4	24.8	—	39.9	1.01	2.17	-0.17	[8]
2,2-Dimethylpropane	—	—	31.0	34.8	36.0	35.2	33.5	31.2	36.0	1.10	2.10	-0.15	[8]
Unsaturated Hydrocarbons													
Acetylene	—	107.0	130.0	144.0	151.0	154.0	154.0	152.0	155.0	1.25	1.98	-0.12	[8]
	—	107.0	—	136.0	—	151.0	—	155.0	—	—	—	—	[9]
Ethylene	37.0	50.0	60.0	68.0	73.0	72.0	66.5	60.0	73.5	1.13	2.08	-0.14	[8]
	37.0	48.0	60.0	66.0	70.0	72.0	71.0	65.0	—	—	—	—	[9]
Propylene	—	62.0	66.6	70.2	72.2	71.2	61.0	—	72.5	1.14	2.07	-0.14	[8]



Fuel	Equivalent Ratio ϕ								S_L (cm/s)		T exponent	P exponent	Source
	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	S_{max}	ϕ at S_{max}	α	β	
1,3-Butadiene	–	–	42.6	49.6	55.0	57.0	56.9	55.4	57.2	1.23	2.00	-0.12	[8]
n-1-Heptene	–	46.8	50.7	52.3	50.9	47.4	41.6	–	52.3	1.00	2.18	-0.17	[8]
Propylene	–	–	48.4	51.2	49.9	46.4	40.8	–	51.2	1.00	2.18	-0.17	[8]
n-2-Pentene	–	35.1	42.6	47.8	46.9	42.6	34.9	–	48.0	1.03	2.16	-0.16	[8]
2,2,4-Trimethyl-3-pentene	–	34.6	41.3	42.2	37.4	33.0	–	–	42.5	0.98	2.20	-0.17	[8]
Substituted Alkyls													
Methanol	–	34.5	42.0	48.0	50.2	47.5	44.4	42.2	50.4	1.08	2.12	-0.15	[8]
Isopropyl alcohol	–	34.4	39.2	41.3	40.6	38.2	36.0	34.2	41.4	1.04	2.15	-0.16	[8]
Triethylamine	–	32.5	36.7	38.5	38.7	36.2	28.6	–	38.8	1.06	2.13	-0.16	[8]
n- Butyl chloride	24.0	30.7	33.8	34.5	32.5	26.9	20.0	–	34.5	1.00	2.18	-0.17	[8]
Allyl chloride	30.6	33.0	33.7	32.4	29.6	–	–	–	33.8	0.89	2.27	-0.19	[8]
Isopropyl mercaptan	–	30.0	33.5	33.0	26.6	–	–	–	33.8	0.94	2.23	-0.18	[8]
Ethylamine	–	28.7	31.4	32.4	31.8	29.4	25.3	–	32.4	1.00	2.18	-0.17	[8]
Isopropylamine	–	27.0	29.5	30.6	29.8	27.7	–	–	30.6	1.01	2.17	-0.17	[8]
n- Propyl chloride	–	24.7	28.3	27.5	24.1	–	–	–	28.5	0.93	2.24	-0.19	[8]
Isopropyl chloride	–	24.8	27.0	27.4	25.3	–	–	–	27.6	0.97	2.20	-0.18	[8]
Silanes													
Tetramethylsilane	39.5	49.5	57.3	58.2	57.7	54.5	47.5	–	58.2	1.01	2.17	-0.17	[8]
Trimethylethoxysilane	34.7	41.0	47.4	50.3	46.5	41.0	35.0	–	50.3	1.00	2.18	-0.17	[8]
Aldehydes													
Acrolein	47.0	58.0	66.6	65.9	56.5	–	–	–	67.2	0.95	2.22	-0.18	[8]
Propionaldehyde	–	37.5	44.3	49.0	49.5	46.0	41.6	37.2	50.0	1.06	2.13	-0.16	[8]
Acetaldehyde	–	26.6	35.0	41.4	41.4	36.0	30.0	–	42.2	1.05	2.14	-0.16	[8]
Ketones													
Acetone	–	40.4	44.2	42.6	38.2	–	–	–	44.4	0.93	2.24	-0.19	[8]
Methyl ethyl ketone	–	36.0	42.0	43.3	41.5	37.7	33.2	–	43.4	0.99	2.19	-0.17	[8]



Fuel	Equivalent Ratio ϕ								S_L (cm/s)		T exponent	P exponent	Source
	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	S_{max}	ϕ at S_{max}	α	β	
Esters													
Vinyl acetate	29.0	36.6	39.8	41.4	42.1	41.6	35.2	–	42.2	1.13	2.08	-0.14	[8]
Ethyl acetate	–	30.7	35.2	37.0	35.6	30.0	–	–	37.0	1.00	2.18	-0.17	[8]
Ethers													
Dimethyl ether	–	44.8	47.6	48.4	47.5	45.4	42.6	–	48.6	0.99	2.19	-0.17	[8]
Diethyl ether	30.6	37.0	43.4	48.0	47.6	40.4	32.0	–	48.2	1.05	2.14	-0.16	[8]
Dimethoxymethane	32.5	38.2	43.2	46.6	48.0	46.6	43.3	–	48.0	1.10	2.10	-0.15	[8]
Diisopropyl ether	–	30.7	35.5	38.3	38.6	36.0	31.2	–	38.9	1.06	2.13	-0.16	[8]
Thio ethers													
Dimethyl sulfide	–	29.9	31.9	33.0	30.1	24.8	–	–	33.0	1.00	2.18	-0.17	[8]
Peroxides													
Di-tert -butyl peroxide	–	41.0	46.8	50.0	49.6	46.5	42.0	35.5	50.4	1.04	2.15	-0.16	[8]
Aromatic Compounds													
Furan	48.0	55.0	60.0	62.5	62.4	60.0	–	–	62.9	1.05	2.14	-0.16	[8]
Benzene	–	39.4	45.6	47.6	44.8	40.2	35.6	–	47.6	1.00	2.18	-0.17	[8]
Thiophene	33.8	37.4	40.6	43.0	42.2	37.2	24.6	–	43.2	1.03	2.16	-0.16	[8]
Cyclic Compounds													
Ethylene oxide	57.2	70.7	83.0	88.8	89.5	87.2	81.0	73.0	89.5	1.07	2.12	-0.15	[8]
Butadiene monoxide	–	6.6	47.4	57.8	64.0	66.9	66.8	64.5	67.1	1.24	1.99	-0.12	[8]
Propylene oxide	41.6	53.3	62.6	66.5	66.4	62.5	53.8	–	67.0	1.05	2.14	-0.16	[8]
Dihydropyran	39.0	45.7	51.0	54.5	55.6	52.6	44.3	32.0	55.7	1.08	2.12	-0.15	[8]
Cyclopropane	–	40.6	49.0	54.2	55.6	53.5	44.0	–	55.6	1.10	2.10	-0.15	[8]
Tetrahydropyran	44.8	51.0	53.6	51.5	42.3	–	–	–	53.7	0.93	2.24	-0.19	[8]
Tetrahydrofuran	–	–	43.2	48.0	50.8	51.6	49.2	44.0	51.6	1.19	2.03	-0.13	[8]
Cyclopentadiene	36.0	41.8	45.7	47.2	45.5	40.6	32.0	–	47.2	1.00	2.18	-0.17	[8]
Ethylenimine	–	37.6	43.4	46.0	45.8	43.4	38.9	–	46.4	1.04	2.15	-0.16	[8]



Fuel	Equivalent Ratio ϕ								S_L (cm/s)		T exponent	P exponent	Source
	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	S_{max}	ϕ at S_{max}	α	β	
Cyclopentane	31.0	38.4	43.2	45.3	44.6	41.0	34.0	–	45.4	1.03	2.16	-0.16	[8]
Cyclohexane	–	–	41.3	43.5	43.9	38.0	–	–	44.0	1.08	2.12	-0.15	[8]
Inorganic Compounds													
Hydrogen	102.0	120.0	145.0	170.0	204.0	245.0	213.0	290.0	325.0	1.80	1.54	0.01	[8]
	124.0	150.0	187.0	210.0	230.0	245.0	–	–	–	–	–	–	[9]
Carbon disulfide	50.6	58.0	59.4	58.8	57.0	55.0	52.8	51.6	59.4	0.91	2.25	-0.19	[8]
Carbon monoxide	–	–	–	–	28.5	32.0	34.8	38.0	52.0	2.05	1.34	0.06	[8]
Hydrogen sulfide	34.8	39.2	40.9	39.1	32.3	–	–	–	40.9	0.90	2.26	-0.19	[8]



Table A2. Burning Velocities of Various Fuels at 100°C Air-Fuel Temperature and 1 atm (0.31 mol.% H₂O in Air). Burning Velocity **S** as a Function of Equivalence Ratio **φ** in cm/s. Exponent **α** and exponent **β** have been calculated for **φ_{max}** according to [5] and [6].

Fuel	Equivalent Ratio ϕ								S_L (cm/s)		T exponent	P exponent	Source
	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	S_{max}	ϕ at S_{max}	α	β	
Propargyl alcohol	–	76.8	100.0	110.0	110.5	108.8	105.0	85.0	110.5	1.08	2.12	-0.15	[8]
Propylene oxide	74.0	86.2	93.0	96.6	97.8	94.0	84.0	71.5	97.9	1.09	2.11	-0.15	[8]
Hydrazine *	87.3	90.5	93.2	94.3	93.0	90.7	87.4	83.7	94.4	0.98	2.20	-0.17	[8]
Furfural	62.0	73.0	83.3	87.0	87.0	84.0	77.0	65.5	87.3	1.05	2.14	-0.16	[8]
Ethyl nitrate	70.2	77.3	84.0	86.4	83.0	72.3	–	–	86.4	1.00	2.18	-0.17	[8]
Butadiene monoxide	51.4	57.0	64.5	73.0	79.3	81.0	80.4	76.7	81.1	1.23	2.00	-0.12	[8]
Carbon disulfide	64.0	72.5	76.8	78.4	75.5	71.0	66.0	62.2	78.4	1.00	2.18	-0.17	[8]
n -Butyl ether	–	67.0	72.6	70.3	65.0	–	–	–	72.7	0.91	2.25	-0.19	[8]
Methanol	50.0	58.5	66.9	71.2	72.0	66.4	58.0	48.8	72.2	1.08	2.12	-0.15	[8]
Diethyl cellosolve	49.5	56.0	63.0	69.0	69.7	65.2	–	–	70.4	1.05	2.14	-0.16	[8]
Cyclohexan monoxide	54.5	59.0	63.5	67.7	70.0	64.0	–	–	70.0	1.10	2.10	-0.15	[8]
Epichlorohydrin	53.0	59.5	65.0	68.6	70.0	66.0	58.2	–	70.0	1.10	2.10	-0.15	[8]
n-Pentane	–	50.0	55.0	61.0	62.0	57.0	49.3	42.4	62.9	1.05	2.14	-0.16	[8]
n -Propyl alcohol	49.0	56.6	62.0	64.6	63.0	50.0	37.4	–	64.8	1.03	2.16	-0.16	[8]
n-Heptane	41.5	50.0	58.5	63.8	59.5	53.8	46.2	38.8	63.8	1.00	2.18	-0.17	[8]
Ethyl nitrite	54.0	58.8	62.6	63.5	59.0	49.5	42.0	36.7	63.5	1.00	2.18	-0.17	[8]
Pinene	48.5	58.3	62.5	62.1	56.6	50.0	–	–	63.0	0.95	2.22	-0.18	[8]
Nitroethane	51.5	57.8	61.4	57.2	46.0	28.0	–	–	61.4	0.92	2.24	-0.19	[8]
Iso-octane	–	50.2	56.8	57.8	53.3	50.5	–	–	58.2	0.98	2.20	-0.17	[8]
Pyrrole	–	52.0	55.6	56.6	56.1	52.8	48.0	43.1	56.7	1.00	2.18	-0.17	[8]
Aniline	–	41.5	45.4	46.6	42.9	37.7	32.0	–	46.8	0.98	2.20	-0.17	[8]
Dimethyl formamide	–	40.0	43.6	45.8	45.5	40.7	36.7	–	46.1	1.04	2.15	-0.16	[8]