

Evaluation of lower flammability limits of fuel–air–diluent mixtures using calculated adiabatic flame temperatures

M. Vidal, W. Wong, W.J. Rogers, M.S. Mannan*

Mary Kay O'Connor Process Safety Center, Department of Chemical Engineering, Texas A&M University, Texas, USA

Available online 23 November 2005

Abstract

The lower flammability limit (LFL) of a fuel is the minimum composition in air over which a flame can propagate. Calculated adiabatic flame temperatures (CAFT) are a powerful tool to estimate the LFL of gas mixtures. Different CAFT values are used for the estimation of LFL. SuperChems™ is used by industry to perform flammability calculations under different initial conditions which depends on the selection of a threshold temperature. In this work, the CAFT at the LFL is suggested for mixtures of fuel–air and fuel–air–diluent. These CAFT can be used as the threshold values in SuperChems™ to calculate the LFL. This paper discusses an approach to evaluate the LFL in the presence of diluents such as N₂ and CO₂ by an algebraic method and by the application of SuperChems™ using CAFT as the basis of the calculations. The CAFT for different paraffinic and unsaturated hydrocarbons are presented as well as an average value per family of chemicals.

© 2005 Elsevier B.V. All rights reserved.

Keywords: Lower flammable limit (LFL); Calculated adiabatic flame temperatures (CAFT); Diluent

1. Introduction

The knowledge of material safety properties is critical for safe handling during unit operations, especially when dealing with flammable or combustible materials. There is no single parameter that defines flammability, but one that is relevant to gaseous mixtures is the flammability limit, which defines the range of fuel concentrations for flame propagation to occur. The lower flammable limit (LFL) is the minimum composition limit above which a flame can propagate. The flammability limits depend on numerous factors including, but not limited to, direction of flame propagation, mixture temperature and pressure, presence of diluents, and oxidant concentrations.

The experimental determination of flammability limits is very dependent on the apparatus and methodology used. Even though flammability limits are available in the literature for a vast group of pure chemicals [1,2], sometimes the experimental conditions are not representative of the actual conditions of the process under study. At the same time, reliable predictive methods that consider different conditions such as mixture compositions, presence of diluents, and different initial temperatures are needed. A compilation of available prediction methods can be found in the literature [3].

The purpose of this study is to: (1) investigate the applicability of a simple algebraic method in the prediction of LFL of gaseous mixtures, (2) define a specific temperature threshold for the evaluation of the LFL, and (3) compare the results obtained with experimental values and calculated with the SuperChems software [4].

2. Background: calculated adiabatic flame temperature and LFL

Calculated adiabatic flame temperature (CAFT) is the temperature that is obtained, when there are no combustion heat losses. The flammability limit is associated with a certain critical energy generation rate or with a certain level of reaction temperature. The CAFT indicates the temperature ceiling of the process [5]. The critical reaction temperature at the LFL composition can be assumed to be equivalent to the CAFT at the known LFL composition, $T_{ad,LFL}$.

In general, the CAFT of many organic substances at their LFL are similar. Some researchers agree that this temperature is around 1550 K [6] or 1200 K [7], while others believe that this temperature is in the range of 1000–1500 K [8].

Due to the similarity of critical reaction temperatures among organic substances, several researchers have selected a specific value for the prediction of the LFL or the flammability zone. For example, Mashuga and Crowl [9] found that a temperature of

* Corresponding author.

E-mail address: mannan@tamu.edu (M.S. Mannan).

1200 K is a good criterion for the prediction of the flammability zones for methane and ethylene. On the other hand, Shebeko et al. [6] selected the value of 1600 K in obtaining formulas for LFL calculations.

An assumption made when estimating LFL with CAFT is that the process occurs at constant pressure. This process occurs in the open, so the pressure is constant and the initial and final enthalpies are the same. The CAFT approach is based on the premise that the flammability limits are mostly thermal in behavior and are not highly dependent on kinetics [10]. This is true at LFL compositions but at UFL, kinetics becomes important.

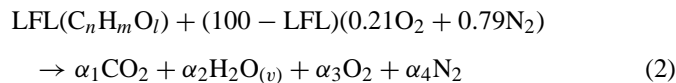
3. Prediction methodologies

3.1. Algebraic method

Mathematically, the lower flammability limit can be represented as:

$$\text{LFL} = \frac{100}{1 + \nu_{a0}} \quad (1)$$

where ν_{a0} is the number of moles of air per mole of fuel in the mixture at the LFL. In this limit, abundant oxygen is available for the combustion to be assumed complete. A general overall combustion reaction for a lean limit mixture of a typical fuel $C_nH_mO_l$ in air is:



where:

$$\begin{aligned} \alpha_1 &= \text{LFL} \times n \\ \alpha_2 &= \text{LFL} \times \frac{m}{2} \\ \alpha_3 &= 21 - \text{LFL} \left(0.21 + n + \frac{m}{4} - \frac{l}{2} \right) \\ \alpha_4 &= 79 - \text{LFL} \times 0.79 \end{aligned}$$

The flammability limit is associated with a certain critical energy generation rate or with a certain critical reaction temperature. This critical temperature can be assumed to be equivalent to the adiabatic flame temperature, $T_{ad,LFL}$ ¹ at the LFL composition and is the maximum temperature achieved due to the combustion reaction when the fuel composition is equal to the LFL. If the LFL of the fuel in air is known, the final product temperature can be evaluated from the energy balance:

$$\sum_i H_{\text{reac},i}(T_i, P) = \sum_i H_{\text{prod},i}(T_{ad}, P) \quad (3)$$

where $H_{\text{reac},i}$ and $H_{\text{prod},i}$ ² are the enthalpies of the i th component of the reactants and products, respectively, at the initial temperature T_i and final temperature $T_f = T_{ad}$.

Once a characteristic adiabatic flame temperature is known, it can be used to predict the LFL. Expanding Eq. (3) yields:

$$H_f^i + \nu_{a0}H_a^i = nH_{CO_2}^{\text{ad}} + \frac{m}{2}H_{H_2O}^{\text{ad}} - \beta H_{O_2}^{\text{ad}} + \nu_{a0}H_a^{\text{ad}} \quad (4)$$

where H_f , H_a , H_{CO_2} , H_{H_2O} ³, and H_{O_2} are the absolute mole enthalpies of fuel, air, carbon dioxide, steam, and oxygen, and β is the stoichiometric coefficient of oxygen in the reaction of complete combustion. The superscripts ‘i’ and ‘ad’ refer to the initial and adiabatic temperatures, respectively.

If Eq. (1) is substituted in Eq. (4), we can solve for the LFL:

$$\text{LFL} = \frac{100}{1 + g_f\Delta H_f + g_cn + g_Hm + g_Ol} \quad (5)$$

where the values of g_i 's are described below:

$$\begin{aligned} g_f &= \frac{1}{H_a^{\text{ad}} - H_a^i} \\ g_c &= g_f(H_c^i - H_{CO_2}^{\text{ad}} + H_{O_2}^{\text{ad}}) \\ g_H &= 0.5g_f(H_{H_2}^i - H_{H_2O}^{\text{ad}} + 0.5H_{O_2}^{\text{ad}}) \\ g_O &= -0.5g_f(H_{O_2}^{\text{ad}} - H_{O_2}^i) \end{aligned} \quad (6)$$

This methodology was previously presented by Shebeko et al. [6], where an overall adiabatic temperature of 1600 K was used for the estimation of the LFL. In this study, this methodology will be tested using the adiabatic flame temperature of each chemical and by selecting an average value for each family of chemicals.

Examining limit behavior, a flame can be extinguished by the addition of diluents, which have primarily a thermal effect. An addition of inert diluent gases to the fuel mixture changes the thermodynamic and transport properties of the fuel–air mixture. The fuel and the diluent will share the energy released by the chemical reaction. Then, for mixtures originally at the LFL concentrations, richer mixtures would be required to increase the reaction rates.

The final temperature of the reaction zone when a diluted fuel is used can be assumed to be at the same level as the final temperature of the reaction zone of the pure fuel in air at the same set of conditions [11]. Generally, knowing the $T_{ad,LFL}$ can permit the evaluation of the value of the lean limit of the fuel–diluent mixture, LFL_m , by incorporating the enthalpy of the diluent in Eq. (3).

The LFL_m for the mixture of diluted fuel in air can be estimated with:

$$\begin{aligned} \frac{1}{\text{LFL}_m} &= \frac{y_F}{\text{LFL}_F} \\ &+ \frac{(H_D^{\text{ad}} - H_D^i) - (H_a^{\text{ad}} - H_a^i) \times (1 - y_F)}{\text{LFL}_F \times (nH_{CO_2}^{\text{ad}} + \frac{m}{2}H_{H_2O}^{\text{ad}} - \beta H_{O_2}^{\text{ad}} - H_F^i - (H_a^{\text{ad}} - H_a^i))} \end{aligned} \quad (7)$$

This equation was first presented by Wierzbka et al. [12]. However, no further discussion on the determination of the reactants

¹ It should be noted that the T_{ad} presented in most combustion books is for reactions at stoichiometric conditions.

² All combustion products are assumed to be in the gas phase.

³ This enthalpy is for water vapor. Lower CAFT values are obtained when liquid water is formed.

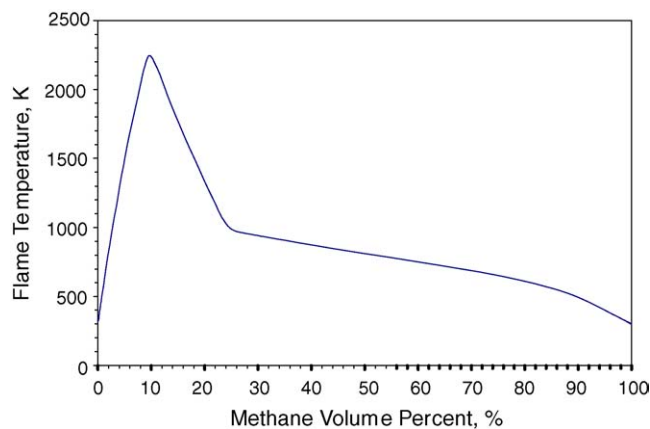


Fig. 1. Computed theoretical flame temperature for the system methane–air at 1 bar and 298 K using SuperChems Expert Version 5.62.

Table 1
LFL of methane at different threshold theoretical flame temperatures

Threshold theoretical flame temperature (K)	LFL (%)
1000	2.88
1200	3.75
1400	4.61
1482	5.04
1500	5.13
1600	5.68

The LFL values were obtained using SuperChems^{TM4} Expert version 5.62 at standard conditions.

and products enthalpies was given. In this work these enthalpies will be obtained by selecting an average constant heat capacity, which can be represented as:

$$H_i^{\text{ad}} = H_{Fi}^0(T_{\text{ref}}) + \bar{c}_p(T_{\text{ad}} - T_{\text{ref}}) \quad (8)$$

The average constant heat capacity will be obtained at an average temperature of $(T_{\text{ad}} + T_{\text{ref}})/2$, where the reference temperature, T_{ref} , is equivalent to 298.15 K.

3.2. SuperChems^{TM4} method

This methodology estimates the mixture flammability limits based on chemical equilibrium. After a mixture and a scenario are defined, a direct minimization of the Gibbs free energy is performed to obtain a graph of flame temperature versus fuel composition. An example of the flame temperature for a mixture of methane and air at 1 bar and 25 °C is presented in Fig. 1.

After this graph is obtained, a threshold theoretical flame temperature is used to determine the flammability limits. At the reported literature flammability limits (LFL of 5%), the methane–air system has a threshold theoretical flame temperature of 1500 K.

After a threshold theoretical flame temperature has been selected, a flammability envelope can be constructed. The effect of the threshold theoretical flame temperature on the LFL of methane is presented in Table 1.

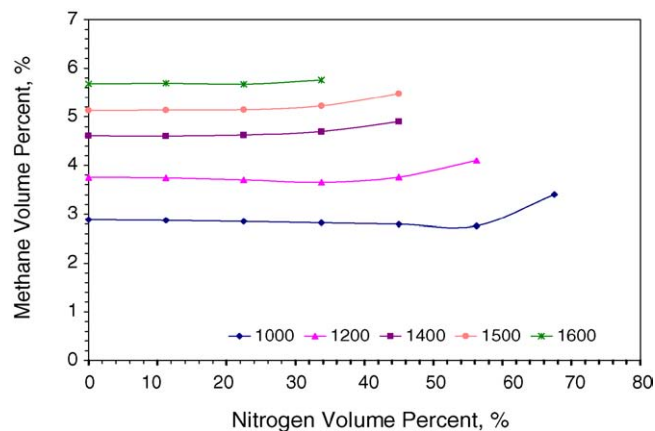


Fig. 2. Flammability envelope of methane at different threshold theoretical flame temperatures with nitrogen as diluent.

The impact of the threshold temperature on the flammability envelope is presented in Fig. 2 for a mixture of methane–air–nitrogen.

4. Results

4.1. Calculated adiabatic flame temperature

The adiabatic flame temperature at the known experimental LFL was calculated using a computer code for equilibrium products of hydrocarbon–air combustion. Eleven species were considered in the products of combustion: H, O, N, H₂, OH, CO, NO, O₂, H₂O, CO₂, and N₂. Carbon⁵ was not included as one of the products because it does not have much effect on the LFL. The experimental data on the LFL was taken from refs. [2,13]. The results for the paraffinic and unsaturated hydrocarbon families are presented in Tables 2 and 3.

These temperatures will be used to estimate the LFL by the algebraic and SuperChems^{TM4} methodologies. If an average $T_{\text{ad,LFL}}$ is taken per family group of chemicals, a value of 1590.29 K will be obtained for the paraffinic group and 1610.50 K for the unsaturated group. These average values are considered to be in agreement with the adiabatic flame temperature of 1600 K selected by Shebeko et al. [6] for organic compounds.

4.2. Algebraic

The LFL of each member of each family of chemicals was estimated by means of Eq. (5). An average heat capacity was calculated for each compound by using their corresponding calculated adiabatic flame temperature. All heat capacity values are presented in units of kJ/(kg mol K) in Tables 4–6.

The results obtained were within 0.35 and 3.35% of error⁶ for the paraffinic and unsaturated hydrocarbons, respectively.

⁵ This work is focused only on LFL and C_(s) was not included in the combustion products. For UFL calculations, kinetics becomes more important and C_(s) should be included as well as other products.

⁶ error (%) = $\frac{|\text{Experimental value} - \text{Calculated value}|}{\text{Experimental value}} \times 100$

⁴ SuperChems is a trademark of A.D. Little/ioMosaic.

Table 2
Calculated adiabatic flame temperature for the paraffinic hydrocarbons (C_nH_{2n+2}) at the LFL

Fuel	Formula	MW	LFL	$T_{ad,LFL}$ (K)
Methane	CH ₄	16.04	5.00	1482
Ethane	C ₂ H ₆	30.07	3.00	1534
Propane	C ₃ H ₈	44.09	2.10	1530
<i>n</i> -Butane	C ₄ H ₁₀	58.12	1.80	1640
<i>n</i> -Pentane	C ₅ H ₁₂	72.15	1.40	1591
<i>n</i> -Hexane	C ₆ H ₁₄	86.17	1.20	1608
<i>n</i> -Heptane	C ₇ H ₁₆	100.2	1.05	1622
<i>n</i> -Octane	C ₈ H ₁₈	114.23	0.95	1652
<i>n</i> -Undecane	C ₁₁ H ₂₄	156.3	0.68	1620
<i>n</i> -Dodecane	C ₁₂ H ₂₆	170.33	0.60	1578
<i>n</i> -Tridecane	C ₁₃ H ₂₈	184.36	0.55	1568
<i>n</i> -Tetradecane	C ₁₄ H ₃₀	198.38	0.50	1542
<i>n</i> -Pentadecane	C ₁₅ H ₃₂	212.41	0.46	1527
<i>n</i> -Hexadecane	C ₁₆ H ₃₄	226.44	0.43	1523
2-Methylpropane	C ₄ H ₁₀	58.12	1.80	1636
2-Methylbutane	C ₅ H ₁₂	72.15	1.40	1589
Neopentane	C ₅ H ₁₂	72.15	1.40	1584
2-Methylpentane	C ₆ H ₁₄	86.18	1.20	1606
2,2-Dimethylbutane	C ₆ H ₁₄	86.18	1.20	1603
2,3-Dimethylbutane	C ₆ H ₁₄	86.18	1.20	1605
2,3-Dimethylpentane	C ₇ H ₁₆	100.20	1.10	1672
2,2,4-Trimethylpentane	C ₈ H ₁₈	114.23	1.10	1816
3,3-Diethylpentane	C ₉ H ₂₀	128.26	0.70	1452
2,2,3,3-Tetramethylpentane	C ₉ H ₂₀	128.26	0.80	1587

The LFL prediction calculations were repeated by selecting an average c_p value per family of chemicals and are presented in Table 6.

The results obtained were within 0.38 and 2.26% of error for the paraffinic and unsaturated hydrocarbons, respectively.

Table 4
Predicted LFL for the paraffinic hydrocarbon family

Fuel	T_{ave} (K)	$c_{p,air}$	c_{p,CO_2}	c_{p,O_2}	$c_{p,H_2O(v)}$	LFL	Predicted LFL
Methane	889.84	32.25	52.64	32.29	39.85	5.00	5.05
Ethane	916.12	32.41	53.03	34.44	40.18	3.00	3.02
Propane	913.88	32.40	53.00	34.43	40.16	2.10	2.11
<i>n</i> -Butane	969.05	32.72	53.77	34.71	40.86	1.80	1.79
<i>n</i> -Pentane	944.81	32.58	53.44	34.59	40.55	1.40	1.40
<i>n</i> -Hexane	953.18	32.63	53.56	34.63	40.65	1.20	1.20
<i>n</i> -Heptane	960.28	32.67	53.65	34.67	40.74	1.05	1.05
<i>n</i> -Octane	974.94	32.75	53.86	34.74	40.93	0.95	0.94
<i>n</i> -Undecane	959.25	32.66	53.64	34.66	40.73	0.68	0.68
<i>n</i> -Dodecane	937.93	32.54	53.34	34.55	40.46	0.60	0.60
<i>n</i> -Tridecane	933.11	32.51	53.27	34.53	40.40	0.55	0.55
<i>n</i> -Tetradecane	920.32	32.43	53.09	34.46	40.23	0.50	0.50
<i>n</i> -Pentadecane	912.42	32.39	52.97	34.41	40.13	0.46	0.46
<i>n</i> -Hexadecane	910.49	32.38	52.95	34.41	40.11	0.43	0.43
2-Methylpropane	967.16	32.71	53.75	34.7	40.83	1.80	1.79
2-Methylbutane	943.58	32.57	53.42	34.58	40.53	1.40	1.40
Neopentane	941.03	32.56	53.39	34.57	40.5	1.40	1.40
2-Methylpentane	952.04	32.62	53.54	34.63	40.64	1.20	1.20
2,2-Dimethylbutane	950.52	32.61	53.52	34.62	40.62	1.20	1.20
2,3-Dimethylbutane	951.70	32.62	53.54	34.63	40.64	1.20	1.20
2,3-Dimethylpentane	985.22	32.81	53.99	34.79	41.07	1.10	1.09
2,2,4-Trimethylpentane	1057.22	33.19	54.89	35.12	41.98	1.10	1.08
3,3-Diethylpentane	875.02	32.16	52.4	34.2	39.66	0.70	0.71
2,2,3,3-Tetramethylpentane	942.55	32.57	53.41	34.58	40.52	0.80	0.80

Table 3
Calculated adiabatic flame temperature for the unsaturated hydrocarbons (C_nH_{2n} , C_nH_{2n-2}) at the LFL

Fuel	Formula	MW	LFL	$T_{ad,LFL}$ (K)
Ethylene	C ₂ H ₄	28.05	2.70	1369
Propylene	C ₃ H ₆	42.08	2.40	1621
Butene-1	C ₄ H ₈	56.10	1.70	1572
<i>cis</i> -Butene-2	C ₄ H ₈	56.10	1.80	1685
Isobutylene	C ₄ H ₈	56.10	1.80	1681
3-Methyl-butene-1	C ₅ H ₁₀	70.13	1.50	1632
Propadiene	C ₃ H ₄	40.06	2.60	1687
1,3-Butadiene	C ₄ H ₆	54.09	2.00	1670
1-Pentene	C ₅ H ₁₀	70.13	1.50	1635
2-Methyl-2-butene	C ₅ H ₁₀	70.13	1.40	1553

The effect of the addition of inerts in the LFL value was examined for methane and ethylene. The inerts considered were nitrogen and carbon dioxide. The calculated adiabatic temperature and Eq. (7) were used in these calculations, with results presented in Table 7.

As seen on the results, the LFL estimates obtained with an average constant c_p value are as good as the estimates obtained using the $T_{ad,LFL}$ of each compound. Therefore, the methodology can be simplified by using an average constant c_p values per group of chemicals for the determination of the enthalpies. The results are in very good agreement with the experimental results presented in ref. [12]. However, it should be noted that the LFL values are dependant on the experimental conditions. Lower flammability limits determined in closed vessels with upward propagation tend to be lower [2].

Carbon dioxide will produce smaller flammability envelopes than those for nitrogen due to its larger heat capacity. The

Table 5
Predicted LFL for the unsaturated hydrocarbon family

Fuel	T_{ave} (K)	$c_{p,air}$	c_{p,CO_2}	c_{p,O_2}	$c_{p,H_2O(v)}$	LFL	Predicted LFL
Ethylene	833.66	31.90	51.74	33.95	39.14	2.70	2.69
Propylene	959.49	32.66	53.64	34.66	40.73	2.40	2.40
Butene-1	934.90	32.52	53.30	34.54	40.42	1.70	1.75
<i>cis</i> -Butene-2	991.77	32.85	54.08	34.82	41.15	1.80	1.95
Isobutylene	989.41	32.83	54.04	34.81	41.11	1.80	1.94
3-Methyl-butene-1	890.58	32.26	52.65	34.30	39.86	1.50	1.30
Propadiene	992.56	32.85	54.09	34.83	41.16	2.60	2.60
1,3-Butadiene	983.98	32.85	54.09	34.83	41.16	2.00	2.00
1-Pentene	966.61	32.71	53.75	34.70	40.83	1.50	1.50
2-Methyl-2-butene	925.36	32.46	53.16	34.49	40.30	1.40	1.40

Table 6
Average heat capacity values per family of chemicals

Family	$c_{p,air}$	c_{p,CO_2}	c_{p,O_2}	$c_{p,H_2O(v)}$	c_{p,N_2}
Paraffinic	32.57	53.42	34.50	40.54	32.36
Unsaturated	32.59	53.45	34.59	40.59	32.38

larger the heat capacity of the diluent, the lower the adiabatic flame temperature, and the higher the amount of fuel needed for propagation.

In this methodology, the amount of inert added is associated with a dilution of the fuel. Then, the increase in the LFL is due to the amount of fuel that was substituted with an inert. For example, the LFL of pure methane is 5%. If this fuel is diluted with 20% of an inert compound, the LFL of the mixture will have to be higher to reach the minimum composition for flame propagation ($\cong \frac{5}{0.2}$).

4.3. SuperChems

A flammability diagram can be constructed after a theoretical threshold temperature has been selected. The adiabatic flame temperature of methane at its LFL composition is equal to 1482 K. If a threshold temperature of 1500 K is selected the LFL is 5.13% (see Table 1). This value can be accepted depending on the direction of the flame and the size of the vessel. A com-

Table 7
Lower flammable limit for methane–air–diluent and ethylene–air–diluent

Fuel	Diluent		LFL _m	LFL _m with average c_p	Exp. values [12]
	CH ₄	C ₂ H ₄			
80		20	6.25	6.25	6.20
50		50	10.00	10.00	9.90
20		80	24.96	24.97	24.90
80		20	6.30	6.30	6.30
50		50	10.33	10.33	10.40
20		80	28.63	28.71	–
	80	20	3.37	3.37	–
	50	50	5.40	5.40	–
	20	80	13.49	13.49	–
	80	20	3.39	3.39	3.8
	50	50	5.49	5.50	6.0
	20	80	14.47	14.52	16.5

Table 8
Lower flammable limit of methane

Vessel	LFL	Reference
10.2 cm diameter tube with 96 cm length	5.00	[1]
20 L spherical bomb	4.85	[7]

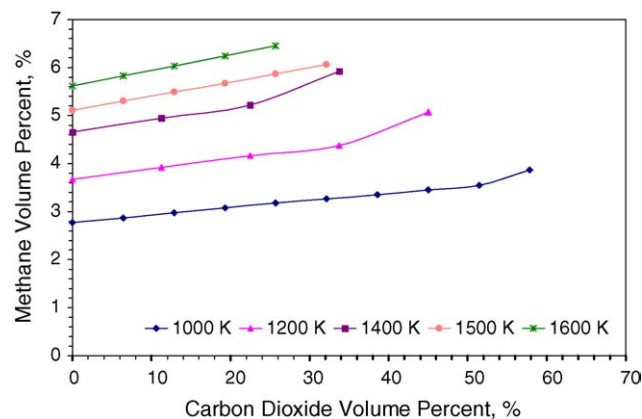


Fig. 3. Flammability envelope of methane at different threshold theoretical flame temperatures with carbon dioxide as diluent.

parison of experimental LFL values for methane is presented in Table 8.

At a temperature of 1400 K, the LFL is 4.61%, which covers a recent experimental LFL value for methane [7]. After the theoretical threshold temperature has been determined, the influence of the addition of inerts such as nitrogen and carbon dioxide can be studied through the construction of a flammability diagram as shown in Figs. 2 and 3.

Experimental LFL values for ethylene are listed in Table 9.

The ethylene–air flame temperature as a function of mixture composition is presented in Fig. 4.

The calculated adiabatic flame temperature of ethylene is 1369 K, at which the LFL of ethylene is 2.97%. According to ref.

Table 9
Lower flammability limit of ethylene

Vessel	LFL	Reference
10.2 cm diameter tube with 96 cm length	2.75	[1]
20 L spherical bomb	2.62	[7]

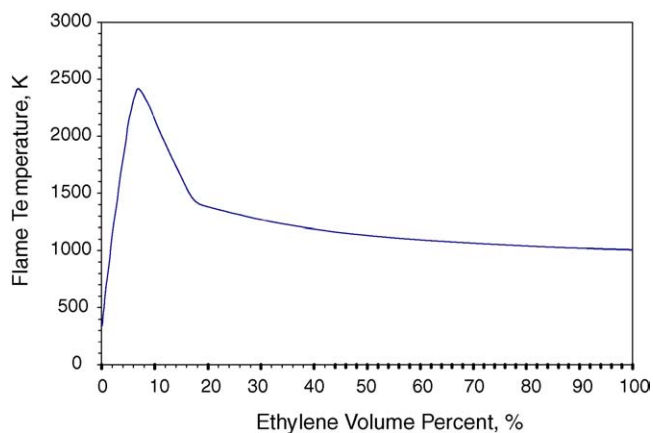


Fig. 4. Computed theoretical flame temperature for the system ethylene–air at 1 bar and 298 K using SuperChems^{TM4} Expert Version 5.62.

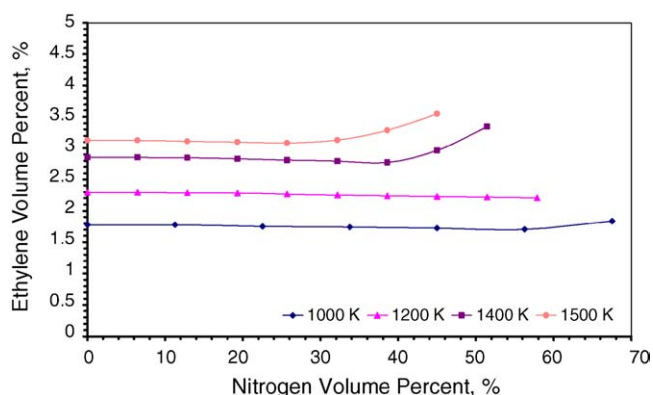


Fig. 5. Flammability envelope of ethylene at different threshold theoretical flame temperatures with nitrogen as diluent.

[1] the LFL of ethylene ranges from 2.75 to 3.4% depending on the dimensions of the experimental vessel. At 1300 K, the LFL is 2.76%.

The threshold temperature selected does not affect the estimation of the LFL of ethylene. The results obtained with each temperature overlap with each other, are shown in Figs. 5 and 6. However the amount of diluent needed to render the mixture outside the flammability range is affected by the selection

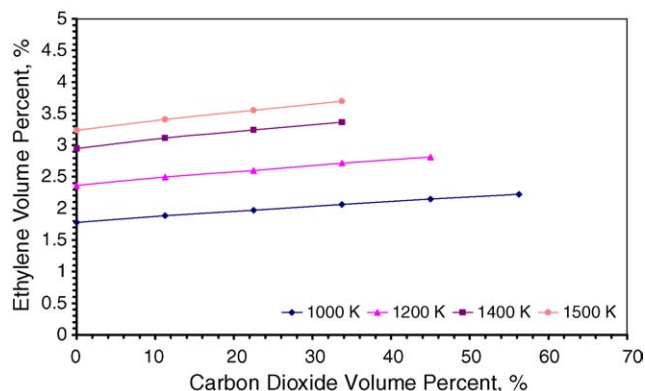


Fig. 6. Flammability envelope of ethylene at different threshold theoretical flame temperatures with carbon dioxide as diluent.

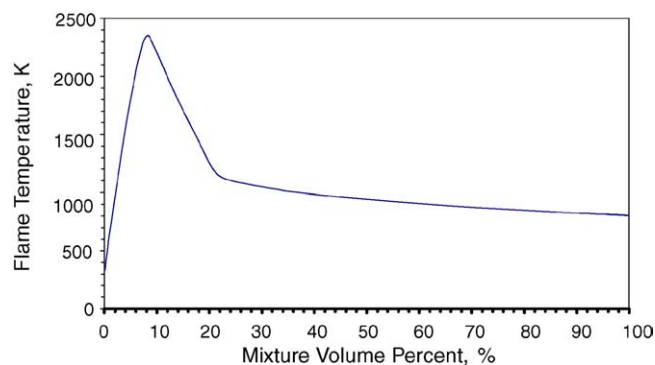


Fig. 7. Computed theoretical flame temperature for the fuel mixture 50/50 CH₄/C₂H₄–air at 1 bar and 298 K using SuperChems^{TM4} Expert Version 5.62.

of the threshold temperature. From the temperatures studied, $T = 1400$ K is the temperature that best agrees with the graphical results presented in ref. [1].

The LFL prediction of a mixture of 50/50 methane/ethylene was explored. The theoretical threshold temperature was calculated by:

$$T_{ad,mix} = \sum_i x_i T_{ad,i} = 0.5T_{ad,methane} + 0.5T_{ad,ethylene} \quad (9)$$

The adiabatic temperature for this mixture is 1426 K, at which the computed LFL composition is 3.68% as it is shown in Fig. 7. The experimental LFL for this mixture is 3.65% as reported by Mashuga [7].

5. Conclusions

The CAFT is a powerful parameter in LFL estimation methods. The algebraic methodology is used to determine the set of heat capacity values needed to obtain enthalpy and LFL values. Also, this methodology proved to be effective for the estimation of LFL of pure compounds as well as for fuel–diluent–air⁷ mixtures.

The SuperChems^{TM4} software is powerful for the study of flammability properties. In this methodology also, the CAFT can be used as the theoretical threshold temperature needed to estimate the LFL and to construct the flammability diagrams.

References

- [1] H.F. Coward, G.W. Jones, Limits of flammability of gases and vapors, Bureau Mines Bull. 627 (1952).
- [2] M.G. Zabetakis, Flammability characteristics of combustible gases and vapors, Bureau Mines Bull. 627 (1965).
- [3] M. Vidal, W.J. Rogers, J.C. Holste, M.S. Mannan, A review of estimation methods for flash points and flammability limits, Process Safety Prog. 23 (1) (March 2004) 47–55.
- [4] SuperChems^{TM4} Expert Version 2004, ioMosaic Corporation.
- [5] D.M. Himmelblau, Basic Principles and Calculations in Chemical Engineering, Prentice Hall, 2004.
- [6] Y.N. Shebeko, W. Fan, I.A. Bolodian, V.Y. Navzenya, An analytical evaluation of flammability limits of gaseous mixtures of combustible–oxidizer–diluent, Fire Safety J. 37 (2002) 549–568.

⁷ In this methodology, the diluent is associated with the fuel.

- [7] C.V. Mashuga, Determination of the combustion behavior for pure components and mixtures using a 20-l sphere, in: *Chemical Engineering*, Michigan Technological University, Michigan, 1999.
- [8] G.A. Melhem, A detailed method for estimating mixture flammability limits using chemical equilibrium, *Process Safety Prog.* 16 (1997) 203–218.
- [9] C.V. Mashuga, D.A. Crowl, Flammability zone prediction using calculated adiabatic flame temperatures, *Process Safety Prog.* 18 (1999) 127–134.
- [10] D.A. Crowl, *Understanding Explosions—Center for Chemical Process Safety*, AIChE, New York, 2003.
- [11] I. Wierzba, S.O.B. Shrestha, G.A. Karim, A thermodynamic analysis of the lean flammability limits of fuel–diluent mixtures in air, *J. Energy Res. Technol. Trans. ASME* 116 (1994) 181–185.
- [12] I. Wierzba, S.O.B. Shrestha, G.A. Karim, An approach for predicting the flammability limits of fuel/diluent mixtures in air, *J. Inst. Energy* 69 (1996) 122–130.
- [13] C.L. Yaws, *Chemical Properties Handbook*, McGraw-Hill, 1999.