



Theoretical estimation of the lower flammability limit of fuel-air mixtures at elevated temperatures and pressures



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ABSTRACT

We present an approach for predicting the lower flammability limits of combustible gas in air. The influence of initial pressure and temperature on lower flammability limit has been examined in this study. The lower flammability limits of methane, ethylene and propane in air are estimated numerically at the pressure from one to 100 bar and the temperature from ambient to 1200 K. It was found that the predicted LFLs of methane, ethylene and propane decrease slightly with the elevated pressure at the high temperature. The LFLs variation for methane-air mixture is 0.17, 0.18, 0.18 volume% with the initial pressure from one to 100 bar at the initial temperature of 800 K, 1000 K and 1200 K respectively, which is significantly higher than that at lower temperature. And the LFL of methane-air mixture at 1200 K and 100 bar reaches 1.03 volume% which is much lower than that at 1 bar and ambient temperature. On the other hand, the LFLs variation is 0.11–0.12 volume% for ethylene-air mixture and 0.06–0.07 volume% for propane-air mixture with the initial temperature from 800 K to 1200 K at the same range of pressure. The LFL values at high temperatures and pressures represent higher risk of explosion.

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1. Introduction

Flammability limits are significant properties that represent flammability characteristics of fuels, and also are essential for quantitative risk assessment of the explosion hazard associated with the use of these fuel-air mixtures. The fuel concentration limit, often referred to as lower flammable limit (LFL), which is the lowest concentration of a combustible gas in air that can propagate an explosion (Coronado et al., 2012; Crowl and Louvar, 2011). The flammability limits are affected by a variety of factors including temperature, pressure, oxygen concentration, ignition energy, etc. (Bond, 1991; Lian et al., 2010, 2012). Generally the flammability limits are determined experimentally, lots of data are available about the LFLs of fuel-air mixtures at atmospheric temperatures and pressures (Brandes and Möller, 2003; Cashdollar et al., 2000; Coward and Jones, 1952; Molnarne et al., 2003). These experiments are, however, greatly difficult and troublesome, especially at elevated conditions of pressure and temperature. The flammability limits are rare and unavailable for combustible mixtures at non-ambient conditions. Furthermore, some fuels will be resolved

under high temperature, the experimental determination of the LFL is unfeasible. Thus, it is necessary to find out other methods to determine the flammability limits. Some predicted models have been developed to estimate the LFL (Albahri, 2003; Shebeko et al., 2002; Shimy, 1970). It has been reported that the LFL can be predicted using adiabatic flame temperature (Mashuga and Crowl, 1999; Vidal et al., 2006). Whereas, the adiabatic flame temperature is obtained from the empirical data, and no data exist especially at high temperature and pressure.

Therefore, the purpose of this study is to estimate the adiabatic flame temperatures for combustible mixtures at various conditions by means of algebraic method, and to predict the LFLs of methane-air, ethylene-air and propane-air using adiabatic flame temperature at initial pressure up to 100 bar, along with initial temperature up to 1200 K. Then, the variation of the LFLs is investigated in this work that includes the dependence of high temperature and pressure for the fuel-air mixtures.

2. Numerical methods

2.1. LFL prediction method

The adiabatic flame temperature is the temperature that is obtained when the enthalpy remains constant. The flammability limit

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is associated with a certain critical reaction temperature, which can be assumed to be equivalent to the adiabatic flame temperature at the LFL composition and is the maximum temperature achieved due to the combustion reaction when the fuel composition is equal to the LFL. The methodology was presented by Vidal et al. (2006), mathematically formula for the LFL can be represented as:

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

where ν_{a0} is the number of moles of air per mole of fuel in the mixture at the lower flammability limit.

The approach is based on the premise that the LFL is mostly thermal in behavior (Crowl, 2003). Assuming that the reaction occurs at adiabatic condition, so the enthalpy is constant. For hydrocarbon-air combustion, the final reaction temperature can be determined from thermal balance:

$$\sum_i H_{reac,i}(T_i, P) = \sum_j H_{prod,j}(T_{ad}, P) \quad (2)$$

where $H_{reac,i}$ is the absolute enthalpy of the reactant and $H_{prod,j}$ is the absolute enthalpy of the product; T_i and T_{ad} are the initial temperature and the adiabatic flame temperature respectively.

In this paper, methane-air, ethylene-air and propane-air mixtures are considered as reactants respectively. And the products are composed of CO, CO₂, H₂O(v), N₂, O₂, H₂, NO, OH, O, H and N. There is a relation between the absolute enthalpy and the enthalpy of formation, which can be written in the form

$$H(T, P) = \Delta H_f(T_i, P) + \bar{C}_p(T - T_i) \quad (3)$$

where \bar{C}_p is the average constant heat capacity. For C_nH_m, the enthalpy of formation is given as

$$\Delta H_f(T_i, P) = \Delta H_f(T_o, P) + \left\{ \bar{C}_p[C_nH_m] - n\bar{C}_p[C] - \frac{m}{2}\bar{C}_p[H_2] \right\} \times (T_i - T_o) \quad (4)$$

where T_o is the reference temperature. Then the adiabatic flame temperature is determined by Eq. (2) using a computer code, and the equilibrium compositions of combustion products can be obtained by minimizing the free energy of the system (Cimini et al., 2005). It should be illustrated that an iterative procedure is applied to these mentioned calculation by the compiled programs. Finally, the adiabatic flame temperature at different initial condition is determined, and then the LFL is predicted by Eq. (1).

Considering various initial conditions, it is clear that the thermodynamic data of real gas is essential. However, rare data at high temperature and pressure can be obtained from database, including heat capacity, entropy, enthalpy, Gibbs free energies, etc. Therefore, thermodynamic parameters should be estimated, especially reasonable magnitude for heat capacity and enthalpy under various conditions.

2.2. Heat capacity

There are several methods to estimate the heat capacity of real gas. Lee-Kesler method (Poling et al., 2001) was used to predict the heat capacity by corresponding state principle and the graph or data sheet was applied as an assistant tool. Setzmann and Wagner (1991) developed a new equation of state to calculate the heat capacity of methane for the ranges of temperature up to 625 K and of pressure up to 1000 MPa, the results acquired by this method are satisfactory compared with experimental data. Young and Ely

(1987) studied the heat capacity of methane, ethane, propane, etc. using a mathematical form of modified Benedict–Webb–Rubin equation of state. The Peng–Robinson (PR) cubic equation of state was supposed to determine the thermodynamic properties for hydrocarbon by Poling et al. (2001), the departure function is represented as,

$$\frac{C_p}{R} = \frac{C_p^O}{R} - 1 - \frac{T}{R} \int_V^\infty \left[\left(\frac{\partial^2 P}{\partial T^2} \right)_V \right]_T dV - \frac{T}{R} \left(\frac{\partial P}{\partial T} \right)_V^2 / \left(\frac{\partial P}{\partial V} \right)_T \quad (5)$$

In this expression, C_p and C_p^O are the constant pressure heat capacity of real gas and ideal gas respectively, and R is gas constant. Smith et al. (2001) provided a general form of cubic equation of state, it is

$$p = \frac{RT}{V - b} - \frac{a(T)}{(V + \epsilon b) + (V + \delta b)} \quad (6)$$

The parameters vary with kinds of equation of state. For PR cubic equation of state, $\epsilon = 1 - \sqrt{2}$ and $\delta = 1 + \sqrt{2}$,

$$a(T) = 0.45724\alpha(T_r)R^2T_c^2/P_c \quad (7)$$

$$b = 0.07779RT_c/P_c \quad (8)$$

where P_c and T_c are the critical pressure and temperature respectively, $\alpha(T_r)$ is obtained from the following Eqs. (9) and (10),

$$\alpha(T_r) = \left[1 + m \left(1 - T_r^{1/2} \right) \right]^2 \quad (9)$$

$$m = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad (10)$$

where $T_r = T/T_c$ is the reduced temperature and ω is the acentric factor. In this section, the heat capacities of real gas at different pressures and temperatures were obtained through PR cubic equation of state using the computer program. The values of P_c , T_c and ω for different gases are taken from chemical and physics database (Lide, 2009). The results were estimated for methane, ethylene and propane by this approach, and the comparison between calculated values and experimental values (Din, 1956; Zagoruchenko and Zhuravlev, 1969) at different conditions are presented in Table 1. It has been seen that the predicted results of various gases show very close agreement at high pressure and temperature, where the range of relative deviation is 0–0.96% respect to the experimental data.

Table 1

The heat capacity at various temperatures and pressures for various gases.

Gas	P/bar	T/K	Cp/(J/mol K)		Deviation/%
			Calc. values	Exp. values	
CH ₄	1.5	300	35.89	35.95	0.17
		400	40.71	40.69	0.05
		500	46.60	46.28	0.69
		600	52.53	52.57	0.08
C ₂ H ₄	5	323	46.44	46.62	0.39
		348	48.81	48.81	0
		373	51.21	51.08	0.25
		423	55.96	55.96	0
C ₃ H ₈	2	300	75.13	75.41	0.37
		400	94.21	94.37	0.17
		500	113.1	114.2	0.96
		600	129.2	128.4	0.62

$$Deviation(\%) = \left| \frac{c_{pExp} - c_{pCalc}}{c_{pExp}} \right| \times 100.$$

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