



## Constants of explosive limits



Ali M. Nassimi<sup>a,c,\*</sup>, Mohammad Jafari<sup>b</sup>, Hossein Farrokhpour<sup>a</sup>, Mohammad H. Keshavarz<sup>b</sup>

<sup>a</sup> Department of Chemistry, Isfahan University of Technology, Isfahan 8115683111, Iran

<sup>b</sup> Department of Chemistry, Malek Ashtar University of Technology, Shahin Shahr 83145 115, Iran

<sup>c</sup> Department of Chemistry, Sharif University of Technology, 11365-9516 Tehran, Iran

### HIGHLIGHTS

- Density factor is defined as the ratio of before ignition density to after ignition density of the ignition mixture.
- This work provides an estimation method for explosive limits of various fuels.
- The assumption of a constant density factor can be used in approximating upper explosive limit.

### ARTICLE INFO

#### Article history:

Received 7 December 2016

Received in revised form 23 April 2017

Accepted 8 August 2017

Available online 9 August 2017

#### Keywords:

Explosive limit

Flammability limit

Adiabatic flame temperature

Density factor

LEL

UEL

LFL

UFL

### ABSTRACT

This work defines density factor as the ratio of before ignition density to after ignition density of the ignition mixture. This work provides an estimation method for explosive limits of various fuels under room temperature and pressure by showing that for a large universe of fuels, constant adiabatic flame temperature and density factor are appropriate approximations at the lower explosive limit while only a constant density factor might be an appropriate approximation at the upper explosive limit. Thus the assumption of a constant adiabatic flame temperature can be used in calculating lower explosive limit while the assumption of a constant density factor can be used in approximating upper explosive limit.

© 2017 Elsevier Ltd. All rights reserved.

## 1. Introduction

Flammability parameters are important safety considerations in various applications ranging from the design of combustion chambers to the design of fuel tanks. Moreover, a knowledge of the flammability parameters is used in judging fire and explosion

*Abbreviations:* LEL, lower explosive limit; UEL, upper explosive limit; EL, explosive limits; AFT, adiabatic flame temperature; TTT, theoretical threshold temperature;  $\phi$ , Equivalence ratio; CEA, chemical equilibrium with applications; HP, constant enthalpy and pressure; UV, constant internal energy and volume; LLFT, lower limit flame temperature; ULFT, upper limit flame temperature; LFT, limit flame temperature; LLDF, lower limit density factor; ULDF, upper limit density factor; LDF, limit density factor.

\* Corresponding author at: Department of Chemistry, Sharif University of Technology, 11365-9516 Tehran, Iran.

*E-mail addresses:* [ali.nassimi@utoronto.ca](mailto:ali.nassimi@utoronto.ca) (A.M. Nassimi), [jafariemamzadeh@gmail.com](mailto:jafariemamzadeh@gmail.com) (M. Jafari), [h-farrokh@cc.iut.ac.ir](mailto:h-farrokh@cc.iut.ac.ir) (H. Farrokhpour), [keshavarz7@gmail.com](mailto:keshavarz7@gmail.com) (M.H. Keshavarz).

hazards of technological processes and technological installations. Among these parameters are flash point [Keshavarz et al. \(2016\)](#), [Keshavarz and Ghanbarzadeh \(2011\)](#), [Keshavarz et al. \(2013\)](#)—the least temperature at which evaporation is enough for the vapor-air mixture above the flammable liquid to be ignitable—and explosive limits [Beyler \(2016\)](#). A mixture of a fuel and an oxidant can give rise to a self propagating flame if the oxidant/fuel ratio is within a specific range. The boundaries of this range are called explosive limits.<sup>1</sup> Lower explosive limit (LEL)—defined as the least fuel concentration capable of self-propagating a flame—and upper explosive limit (UEL)—defined as the greatest fuel concentration capable of self-propagating a flame—are properties of a fuel-oxidizer mixture. Many studies report LEL and UEL of various materials [Zabetakis \(1965\)](#), [Cashdollar et al. \(2000\)](#), [Kuchta \(1985\)](#); in practice, most ignition processes involve a mixture of fuels and/or diluents, so

<sup>1</sup> Also called flammability limits.

the explosive limits (ELs) of fuel–fuel–oxidant (air) mixtures Van den Schoor et al. (2008a,b), Miao et al. (2011), Shoshin and de Goey (2010) and fuel–oxidant–diluent mixtures Van den Schoor et al. (2009), Vidal et al. (2006) are studied. Further the effect of temperature Van den Schoor et al. (2008b), Rowley et al. (2011), Gibbon et al. (1994), Kondo et al. (2011), Mendiburu et al. (2016) and pressure Van den Schoor et al. (2008b), Gibbon et al. (1994), Van den Schoor and Verplaetsen (2007), Arnaldos et al. (2001) on ELs are studied.

Both the LEL and the UEL depend on the temperature and pressure of the fuel–oxidizer mixture, but they also depend on the size, geometry and heat conductance of the combustion vessel and on the source of ignition Coward and Jones (1952), Razus et al. (2004), Gieras et al. (2008). Measurement condition dependence causes values of ELs measured according to different standard methods to differ Smedt et al. (1999), Zlochower and Green (2009). Common standard methods for measuring explosive limits are Schroder and Molnarne (2005): (a) the US bureau of mines standard, which uses a vertical tube with an inner diameter of 5 cm and a length of 150 cm, with an electric spark or a pilot flame at the open lower end of the tube Coward and Jones (1952), (b) the ASTM 681 standard, which uses a 5 dm<sup>3</sup> spherical glass with a central 15 kV igniter ASTM E681-09 (2009), (c) the DIN 51 649 standard, which uses a cylindrical vertical glass with inner diameter of 6 cm, height of 30 cm and a 15 kV igniter located 6 cm above the tube's bottom DIN 51649-1 (1985-2004), and (d) the VDI 2263-1 standard developed for measuring dust explosion limits but also used for gaseous mixtures, which uses a 20 dm<sup>3</sup> spherical vessel with a central ignition VDI 2263 Part I (1990).

The LEL and the UEL are generally considered to be 0.5 and 3 times the stoichiometric concentration of the fuel Ma et al. (2013). Methods for calculating the LEL or the UEL make use of the standard enthalpy of combustion Suzuki (1994), Britton and Frurip (2003), normal burning velocity Macek (1976), adiabatic flame temperature (AFT) for partial combustion to CO and H<sub>2</sub>O Shebeko et al. (2002), minimum spark ignition energy Fenn (1951), ratio of stoichiometric AFT to AFT at the EL Mendiburu et al. (2016) or constancy of AFT Vidal et al. (2006), Melhem (1997), Shu et al. (2015). In calculation of flammability limits from AFT, the existence of the flammability limits is considered to be a consequence of existence of a minimum sustaining temperature for the flame—thermal theory Williams (1969). For LEL this sustaining temperature called theoretical threshold temperature (TTT) is claimed to be approximately a universal constant for every fuel Vidal et al. (2006). Thermal theory has also been extended to UEL Mashuga and Crowl (1999). TTT at the upper and lower limits of explosivity should be distinguished but since we only use the concept and will not report any values for it, the same abbreviation is used for both temperatures. If we limit our attention to specific classes of compounds, relations exist among flammability parameters, e.g., in the case of alkanes a linear relationship between molar heat of combustion and inverse of the LEL and another linear relationship between the LEL and the UEL exists Affens (1966).

To calculate explosive limits one needs an appropriate criteria for defining sustained ignition. The most obvious ignition criterion is visual criterion, i.e., the flame moves away from the ignition source EN 1839 (2012). Visual criterion is not useful for a theoretical study as the occurrence of observation of the flame propagation is difficult to quantify in a model. Surrogates of the visual criterion are pressure rise criterion based on the rise of pressure by a fixed percentage of the initial pressure EN 1839 (2012) and temperature rise criterion based on a fixed amount of rise in the temperature of the fuel–oxidizer mixture Tschirschwitz et al. (2015). The pressure rise criterion seems suitable for a study dealing with a constant internal energy and volume (UV) problem type. A UV problem type corresponds to an experimental setup where

ignition occurs in a closed vessel. The temperature rise criterion corresponds to the existence of the TTT and thus the constancy of the AFT at the ELs in a theoretical study based on thermodynamics. It can be used either for a UV or a constant enthalpy and pressure (HP) problem type.

Density factor (DF) is defined as the ratio of the density of the reactants mixture ( $\rho_r$ ) to the density of the products mixture ( $\rho_p$ ). DF is introduced to serve as an indicator of ignition. We assume equilibrium and ideal gas behavior. Mass conservation imply that DF is proportional to volume factor, i.e., ratio of after ignition to before ignition volume of the combustible mixture. Equilibrium and ideal gas assumptions imply that the volume factor is proportional to temperature factor, i.e., ratio of after ignition temperature to before ignition temperature of the combustible mixture, times mole factor.

$$DF = \frac{\rho_r}{\rho_p} = \frac{\frac{m_r}{V_r}}{\frac{m_p}{V_p}} = \frac{V_p}{V_r} = \frac{\frac{n_p RT_p}{P_p}}{\frac{n_r RT_r}{P_r}} = \frac{n_p T_p}{n_r T_r}, \quad (1)$$

where m, V, n, T and P, respectively, denote mass, volume, number of moles, temperature and pressure while indexes r and p respectively denote reactants and products.

In the following passages, we would use lower limit flame temperature (LLFT) for AFT at LEL, upper limit flame temperature (ULFT) for AFT at UEL and limit flame temperature (LFT) for AFT at either EL. Further we use lower limit density factor (LLDF) for DF at the LEL, upper limit density factor (ULDF) for DF at the UEL and limit density factor (LDF) for DF at either EL.

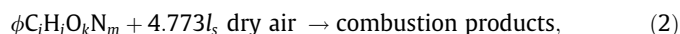
Temperature in a flame is lower than the AFT by an amount which is proportional to the amount of heat loss per unit of the limiting reactant which in turn is proportional to surface/volume ratio of the combustion vessel. LLFT and ULFT are upper bounds to the TTTs because AFT represents a situation of no heat loss from the flame. In a first approximation TTT can be approximated with LFT but this approximation is not necessary; all we need is for the difference between LFT and TTT to be constant. LFT-TTT is proportional to the heat loss which under the same measurement conditions is proportional to the TTT. Thus the constancy of this difference is implied by the constancy of the TTT. Values as high as 1800 K to as low as 1000 K are suggested for TTT. This wide variation of TTT seems to be a result of variation in the combustion test conditions Razus et al. (2004), Gieras et al. (2008).

Fuel and oxidizer contribute an amount of heat,  $\Delta H_{com}$ , together with an amount of quenching effect,  $\int_{T_0}^{T_f} C_{p,mix}(T)dT$ , where  $T_0$  and  $T_f$  are, respectively, the initial and flame temperature while  $C_{p,mix}$  is the heat capacity of product mixture Di Benedetto (2013). The AFT is derived by equating heat and quenching quantities Ma (2011).

This work considers flammables made up of the set of atoms {C, H, N, O}, among these flammables thermal theory fuel universe (TTFU) is defined as the set of flammables excluding Hydrogen (and deuterium), triple and adjacent double bond containing compounds and explosives. For TTFU the values of LLFT and ULDF are shown to concentrate around their respective mean. This mean concentration is suggested as a method for predicting explosive limits when their experimental values are not available.

## 2. Method

Assuming a fuel molecule consisting of carbon, hydrogen, oxygen and nitrogen atoms; combustion equation can be written as



where, dry air = 0.7808N<sub>2</sub> + 0.2095O<sub>2</sub> + 0.0093Ar + 0.0031CO<sub>2</sub>. (Thus molecular mass of dry air  $M_{da}$  = 29.0845.) The stoichiometric

Download English Version:

<https://daneshyari.com/en/article/6466798>

Download Persian Version:

<https://daneshyari.com/article/6466798>

[Daneshyari.com](https://daneshyari.com)