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Calculating limiting oxygen concentration of gas mixtures

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Abstract: The limit values for the fuel concentration in the air-flammable fuel mixture are LEL (lower explosive limit) and UEL (upper explosive limit). The addition of an inert component to the fuel / air mixture determines the increase and decrease of the LEL, until no explosion occurs. The maximum oxygen quantity of the non-combustible - air - inert fuel mixture is LOC (limited oxygen concentration), an important safety property. Investigation of a comprehensive set of data on the flammability at high temperature and ambient pressure obtained from documented sources was carried out for systems containing nitrogen, carbon dioxide and water (steam) such as inert ingredients. Determining the LOC for gas mixtures with different ratios requires step-by-step testing. To solve that problem, the author used Lechateler calculation method to calculate LOC for the ratio of gas mixture and compared the results of experimental equipment.

Keywords: Loc, lower exlosion limit, upper exlosion limit.

1. Introduction

The effect of increasing the concentration of inert gas can be understood by viewing the inert as thermal ballast that quenches the flame temperature to a level below which the flame cannot exist. Carbon dioxide is therefore more effective than nitrogen due to its higher molar heat capacity.The concept has important practical use in fire safety engineering[1-9]. For instance, to safely fill a new container or a pressure vessel with flammable gases, the atmosphere of normal air (containing 20.9 volume percent of oxygen) in the vessel would first be flushed (purged) with nitrogen or another non-flammable inert gas, thereby reducing the oxygen concentration inside the container.

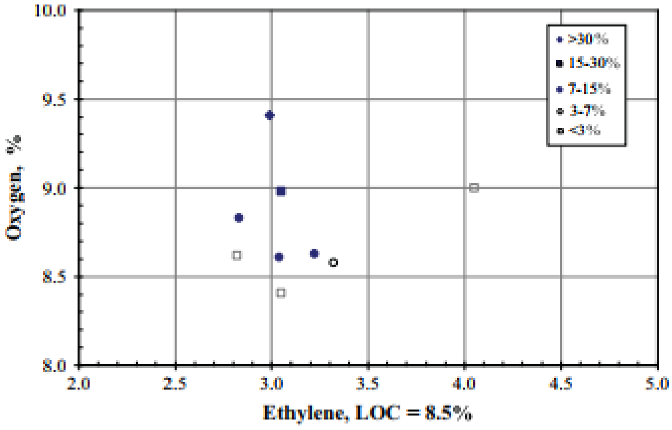

Fig.1. *The LOC of Ethylene in air with added* N_2.

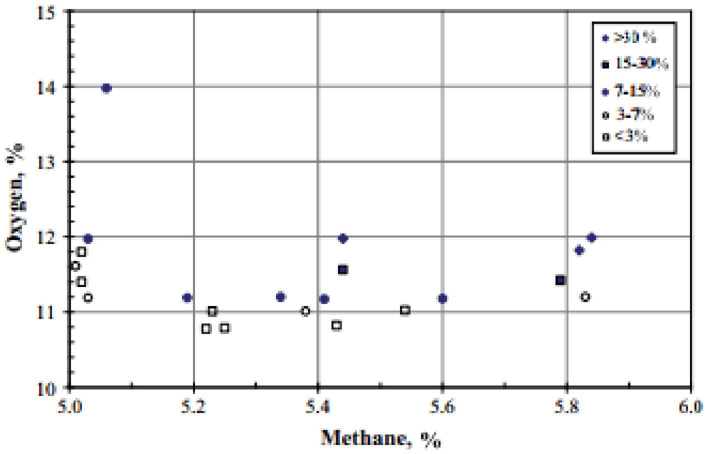

Fig.2. *The LOC CH_4 in air with added N_2.*

When the oxygen concentration is below the LOC, flammable gas can then be safely admitted to the vessel, because the possibility of internal explosion has been eliminated. The limiting oxygen concentration is a necessary parameter when designing hypoxic air fire prevention systems[10-16].

Table 1. Flammability /LOC

Gas/ Vapor	*Formula*	*Component*	*N_2 - Air Mixture*	*CO_2 - Air Mixture*
Alkanes	CH_4		11.1	13.1
	C_2H_6		9.5	11.9
	C_3H_8		10.7	12.8
	C_4H_{10}		10.6	13.0
Alkenes	C_2H_4		8.5	10.2
	C_3H_6		10.0	12.6
	C_4H_8		10.1	12.5
Aromatics	C_6H_6		11.4	12.4
	C_7H_8		9.5	
	C_8H_{10}		9.0	
Alcohols	CH_3OH		8.5	10.5
	C_2H_5OH		9.0	11.5
	C_3H_7OH		8.7	

2. Object and subject of research

Explosion chambers are used for measurement of explosion characteristics of flammable dusts, gases, vapors and hybrid mixtures, such as maximum explosion pressure, maximum rate of pressure rise, lower and upper explosibility limits and limiting oxygen concentration. There are standard size of the explosion chambers for testing dust explosions – 20 liters (CA20L).

Fully automated and remote-controlled machinery:

• Robust design with 30 barg of operating and 40 barg of testing pressures

• The CA 20L may be equipped with heating for measurements under elevated temperatures up to 200 °C

• CA 20L could be delivered with instrumentation for measurement of explosion parameters of gases and vapors according to EN 15967 (maximum pressure and rate of pressure rise), according to EN 14756 (LOC) and EN 1839 (explosion limits).

3. Target of research

Flammable limits are used not only in safety analysis but also in combustion science. In both cases, it's important that limits measured in the laboratory agree closely with the limits observed in large volumes of gas. Although wider flammable limits might be claimed to be "more conservative" it's not the job of a test laboratory to include safety factors in the test method. Such safety factors should be included during application of data, not during measurement. With respect to closed vessel tests, having lost sight of the flame it's important not to lose sight of the objective, namely to select test criteria that correctly predict the flammable limits pertaining to large volumes of gas mixture. Since these sentiments were published in 2002, European test methods have continued to generate flammable limit data outside the envelope of compositions within which flames can propagate through large volumes of test mixture. Meanwhile, although the 7% pressure rise "ignition criterion" used in ASTM E2079 has been shown to be valid during 120-L "reference quality" tests, the scope of these tests was limited to only five gases under normal atmospheric conditions. Also, it's been found that the 7% pressure rise criterion must often be increased when using smaller test vessels, especially at elevated temperatures and pressures. The need for a larger pressure rise criterion under certain conditions is recognized by ASTM E2079. Not only is there a provision for a "baseline" pressure rise to which the standard 7% value is added, but the pressure rise criterion can be substantially increased based on "exploratory tests in the vicinity of limit mixtures." However, since the procedure for selecting nonstandard pressure rise criteria is vague, test laboratories may prefer to err on the side of a conservative result.

4. Literature analysis

Flammability limits of five selected combustible gases were investigated. Actually, the investigation was made for methane, . The observed data were analyzed using the extended Le Chatelier's formula. As a result, the mixing effect on the flammability limits of individual gases was found to be adequately interpreted using the extended Le Chatelier's formula. However, contrary to the cases of nitrogen and carbon dioxide dilutions, it was not possible to appropriately interpret the mixing effects on all gases simultaneously using a common set of parameter values.

5. Research methods

As noted previously, the lower flammability limit (LFL) for mixtures of fuels is adequately given by the Le Chatelier rule:

$$L_{mixt} = \frac{1}{\sum \frac{x_i}{L_i}} \qquad (1)$$

Where: L_{mixt} is the LFL of the fuel mixture,
L_i is the LFL of fuel component i,
x_i is the mole fraction of the fuel component.

The LOC of fuel mixtures can be derived from (1) by defining:

$$L_i^* = \frac{(LOC)_i}{R_i} \quad (2) \qquad L_{mixt}^* = \frac{(LOC)_{mixt}}{R^*} \qquad (3)$$

Where (LOC)i is the experimental value for LOC of component i,
$(LOC)_{mixt}$ is the calculated LOC for the fuel mixture,

R_i is the stoichiometric molar ratio of oxygen to fuel i.
R* is the stoichiometric ratio of oxygen to the fuel mixture.
Substituting formula the LOC into the modified Le Chatelier and rearranging terms gives: For a 2-component mixture (a,b):

$$(LOC)_{mixt} = \frac{(x_a R_a + x_b R_b)}{\frac{x_a R_a}{(LOC)_a} + \frac{x_b R_b}{(LOC)_b}} \quad (4)$$

6. Research results

For experimentation and calculation, we used samples including alcohol, hydrocarbons and other groups to perform the determination of LOC by various methods.

Table 2. LOC: fuel mixtures containing methane

Fuel: $\%CH_4$	$CH_4 - H_2$		$CH_4 - CO$	
	LOC_{exp}	LOC_{cal}	LOC_{exp}	LOC_{cal}
0	4.6	5.1	5.1	5.1
10	6.5	5.6	6.1	6.1
35	8.3	7.6	7.4	7.3
50	9.1	10	10.9	10.2
70	10.1	9.8	10.8	10.6
100	11.1	11.1	11.1	11.1

The results are shown in **Table 2**.
The average absolute error included in tables is defined as:

$$A.A.E = \sum_{i=1}^{N} \frac{\left| T_i^{\exp} - T_i^{cal} \right|}{N} \quad (4)$$

Where:
N is the number of exprerimental data,
the T_i^{exp} is the exprerimental by Explosion chambers,
T_i^{cal} is the calculated flash point.

7. Prospects for further research development

The aim of this study was, to develop a model for predicting flammability limits for hydrocarbons and mixtures, with nitrogen as inert gas. A model was made using a simple combustor with mass flow controllers. They control the mole fractions of fuel, air, and nitrogen as well as the pulse of hydrogen radicals used to ignite the mixture. This way it was possible to simulate the ignition of hydrocarbons and mixtures, as well as to simulate the dilution effect of adding nitrogen to the mixture. Results obtained from the model were compared to experimental data. The model was able to predict flammability limits somewhat precisely for methane and propane, while ethane had some difficulties predicting the upper flammability limit and limiting oxygen concentration.

8. Conclusion

The study also generally confirms the results of the flammability tube messurements on the LFLs. The results of the comparison between CA 20L with a calculation with a permissible error are given. That shows that the efficiency in using the calculation method by the Le Chatelier rule plays an important role in fire safety.

References:

1) ASTM International, 2008b. ASTM International Standard test methods for limiting oxygen (oxidant) concentration in gases and vapors.

2) Brandes and Ural, 2008. Ural. Towards a global standard for flammability determination.

3) Kondo et al., 2006. Extended Le Chatelier's formula and nitrogen dilution effect on the flammability limits.

4) Kondo et al., 2008. S. Kondo, K. Takizawa, A. Takahashi, K. Tokuhashi, A. Sekiya. A study on flammability limits of fuel mixtures.

5) Schroder and Molnarne, 2005. Flammability of gas mixtures. Part I: fire potential.

6) E. Brandes, W. Moller, Sicherheitstechnische Kenngr ¨ oßen, Band 1 ″ (Brennbare Flussigkeiten und Gase), Wirtschaftsverlag NW, Bremer- ¨ haven, 2003.

7) M. Molnarne, Th. Schendler, V. Schroder, Sicherheitstechnis- ¨ che Kenngroßen Band 2 (Explosionsbereiche von Gasgemischen), ″ Wirtschaftsverlag NW, Bremerhaven, 2003.

8) [3] prEN 14756, Determination of the limiting oxygen concentration (LOC) for gases and vapours, CEN/TC 305 (2003).

9) EN 1839, Determination of Explosion Limits of Gases and Vapours, Beuth Verlag GmbH, 2003.

10) O. Fuß, M. Molnarne, V. Schroder, A. Sch ¨ onbucher, Determination of ¨ new group contributions to calculate limiting oxygen concentrations, Chem. Eng. Technol. 26 (2003) 428–433.

11) O. Fuß, M. Molnarne, A. Schonbucher, V. Schr ¨ oder, Limiting oxygen ¨ concentrations of combustible gases and vapours, Chem. Ing. Technik 75 (2003) 101–104.

12) O. Fuß, M. Molnarne, A. Schonbucher, V. Schr ¨ oder, Determination of ¨ new increments for the calculation of limiting oxygen concentrations, Chem. Ing. Technik 74 (6) (2002) 827–832.

13) D. Markus, H. Schildberg, W. Wildner, G. Krzdalic, U. Maas, Flammability limits of premixed methane/methanol/air flames, Comb. Sci. Technol. 175 (2003) 2095–2105.

14) D. Markus, U. Maas, Calculation of explosion limits with detailed reaction kinetics, Chem. Ing. Technik 76 (2004) 289–292.

15) G. Melhem, A detailed method for estimating mixture flammability limits using chemical equilibrium, Proc. Safety Progr. 16 (1997) 203.

16) D. Razus, M. Molnarne, O. Fuß, Limiting oxygen concentration evaluation in flammable gaseous mixtures by means of calculated adiabatic flame temperatures, Chem. Eng. Process. 43 (2004) 775– 784