# Chapter 25

# EXPLOSIVE LIMITS IN AIR, FLASH POINT AND AUTOIGNITION TEMPERATURE

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## ABSTRACT

Results for explosive (lower and upper flammable) limits in air, flash point and auto-ignition temperature are presented for organic compounds. The results are displayed in an easy-to-use table that is especially applicable for rapid engineering usage. The organic compounds encompass hydrocarbon, oxygen, nitrogen, halogen, silicon, sulfur and other chemical types.

## EXPLOSIVE LIMITS IN AIR

The results for lower (LEL) and upper (UEL) explosive limits in air are presented in Tables 25-1 and 25-2. The LEL and UEL values are the lower and upper concentrations (expressed as volume %) for flammability in air. The tabulation is based on both experimental data and estimated values.

In the data collection, a literature search was conducted to identify data source publications (1-56) for explosive limits in air. Both experimental values for the property under consideration and parameter values for estimation of the property are included in the source publications. The publications were screened and copies of appropriate data were made. These data were then keyed into the computer to provide a database for which experimental values are available. The database also served as a basis to check the accuracy of the estimation methods.

Upon completion of data collection, estimation of values for explosive limits in air was performed. The estimates are primarily based on the methods of Shebeko (17) and Jones (2). The Jones method (regression of the stoichiometric concentrations for volume % fuel in fuel plus air) is shown below:

$$C_mH_xO_y + z\,O_2 \text{ -----> } m\,CO_2 + x/2\,H_2O$$

$$\text{LEL, \%} = 0.55\,(100)/(4.76m + 1.19x + 1 - 2.38y) \quad (25\text{-}1)$$

$$\text{UEL, \%} = 3.50\,(100)/(4.76m + 1.19x + 1 - 2.38y) \quad (25\text{-}2)$$

Evaluation of these equations with normal alkanes disclosed favorable agreement of estimates and data. For lower explosive limit, very favorable agreement was obtained for small, intermediate and large size alkanes. For upper explosive limit, rough agreement was experienced for small and large size alkanes. More favorable agreement was exhibited for intermediate size alkanes.

A comparison of experimental data and estimates for lower explosion limit in air and data is shown in Figure 25-1 for normal alkanes. The graph discloses favorable agreement of data and estimates.

## EXPLOSIVE LIMITS FOR MIXTURES

The lower and upper explosive limits in air are often needed for gas mixtures. The Le Chatelier equation (2) for gas mixtures is:

$$\text{LEL}_{mixture}\text{, \%} = 1 / \sum (y_i/\text{LEL}_i) \quad (25\text{-}3)$$

$$\text{UEL}_{mixture}\text{, \%} = 1 / \sum (y_i/\text{UEL}_i) \quad (25\text{-}4)$$

where $y_i$ = mole fraction of component i on a combustible basis

## FLASH POINT AND AUTOIGNITION TEMPERATURE

The results for flash point and auto-ignition temperatures are also given in Tables 25-1 and 25-2. The flash point represents the temperature at which the liquid gives off enough vapor to flash (combust) when exposed to an external ignition source. The auto-ignition temperature is the temperature at which the substance will automatically ignite (combust) without an external ignition source. The tabulation is based on both experimental data and estimated values.

In the data collection, a literature search was conducted to identify data source publications (1-83) for flash point and auto-ignition temperature. The publications were screened and copies of appropriate data were made. These data were then keyed into the computer to provide a database for which experimental data are available. The database also served as a basis to check the accuracy of the estimation methods.

Upon completion of data collection, estimation of values for the remaining compounds was performed. The estimates are primarily based on the methods of Shebeko (22), Gmehling and Rasmussen (23) and vapor pressure methods. The vapor pressure method is based on determining the temperature at which the vapor pressure will provide an equilibrium concentration that is equal to the lower explosive limit (LEL) concentration in air. The equations are briefly given below:

$$y_i = P_i/P = LEL_i/100 \qquad (25\text{-}5)$$

where
$y_i$ = vapor concentration of component i, mole fraction
$P_i$ = vapor pressure of component i, atm
$P$ = total pressure, atm
$P_i/P$ = equilibrium concentration of component i, mole fraction
$LEL_i/100$ = lower explosive limit concentration of component i, mole fraction

Evaluation of the vapor pressure method with normal alkanes disclosed favorable agreement of estimates and data for small, intermediate and large size molecules. Evaluation with other compound types was not performed. If the lower explosive limit (LEL) used in the calculations is estimated, the estimates for flashpoint should be considered as rough values.

A comparison of experimental data and estimates for flash point and data is shown in Figure 25-2 for normal alkanes. The graph discloses favorable agreement of data and estimates.

**EXAMPLES**

The tabulated values maybe used in engineering applications involving pure components and mixtures in air. Examples are given below.

**Example 1** A process vessel contains n-pentane (C5H12) at a concentration of 2 vol % in air. Are the contents of the vessel flammable?

Inspection of the table discloses that LEL = 1.4 vol % for n-pentane. Since the vessel contents exceed the LEL for n-pentane, the contents are flammable. This is shown below:

Vessel contents of 2 vol % > LEL of 1.4 vol %

Vessel contents are flammable.

**Example 2** Estimate the lower (LEL) and upper (UEL) explosive limits in air for the gas mixture below:

| | vol % | $y_i$ (combustible basis) | $LEL_i$ | $UEL_i$ |
|---|---|---|---|---|
| Methane | 1 | 0.2 | 5.0 | 15.0 |
| Ethane | 2 | 0.4 | 3.0 | 12.5 |
| Propane | 2 | 0.4 | 2.1 | 9.5 |
| Air | 95 | --- | --- | --- |

Substitution of $y_i$, $LEL_i$ and $UEL_i$ into the equations for gas mixtures provides:

$LEL_{mixture} = 1 / \Sigma(y_i/LEL_i) = 1/(0.2/5 + 0.4/3 + 0.4/2.1) = 2.75$ vol %

$UEL_{mixture} = 1 / \Sigma(y_i/UEL_i) = 1/(0.2/15 + 0.4/12.5 + 0.4/9.5) = 11.4$ vol %

**Example 3** A process vessel at a temperature of 80 F contains liquid toluene (C7H8) in contact with air. Is the vapor in the process vessel flammable?

Inspection of the table discloses that the flash point is 40 F for toluene. Since the temperature of the process vessel contents exceeds the flash point for toluene, the vapor is flammable. This is shown below:

Vessel temperature of 80 F > Flash point of 40 F

Vapor in vessel is flammable.

**Example 4** A small quantity of residual n-tetradecane (C14H30) is in the piston bore of a piston-type compressor. If air at ambient conditions is compressed to 570 psia and 420 F, will the n-tetradecane undergo autoignition?

Inspection of the table discloses that the autoignition temperature of n-tetradecane is 392 F. Since the temperature of 420 F at the end of the compression exceeds the autoignition temperature, autoignition of the n-tetradecane will occur. This is shown below:

Compressor temp. of 420 F > Autoignition temp. of 392 F

Autoignition of n-tetradecane will occur.

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