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Case Study

Theoretical Estimation of Flash Point for Industrial Scale Applications

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ABSTRACT

Flash point plays a Important Role in Industrial Chemical process. it is Necessary that Consuming a Batch Process in large scale. Theoretical Approach plays a Crucial role that to Estimate the behaviour of Minimum Flash point. That to determine the fire and explosion hazards of a liquid. Accurate estimation of flash point is essential for assessing fires and explosion hazards, particularly in large-scale batch operations. The identification of this behaviour is critical, because a hazardous situation results from taking the lowest component flash point value as the mixture flash point. an estimate of the mixture flash point is needed. A procedure to estimate the flash point of binary mixtures is discussed. This work presents a procedure for estimating the flash point of two or more components in a binary liquid mixture by applying Le Chatelier's mixing rule.

INTRODUCTION

Theoretical estimation of flash points has long been a subject of interest in chemical engineering and safety science, as it provides a predictive framework for assessing flammability without reliance on direct measurement [2]. Early theoretical approaches were based on empirical correlations linking flash points to fundamental properties such as boiling point, molecular weight, and vapor pressure. These models, while limited in scope, established the foundation for predictive estimation in hydrocarbon systems [1]. The flash point is the temperature at which the vapor pressure of a liquid (or mixture) produces enough vapor to reach the Lower Flammable Limit (LFL) in air [9]. The vapor pressure depends directly on the concentration of each component in the liquid phase. Estimation of Minimum Flash Point Behaviour. Some mixtures exhibit a flash point lower than either pure component. This occurs because the vapor composition at certain concentrations produces a more flammable mixture than expected. Identifying this behaviour is critical for safety [7]. In This Discussion some Mixtures are having with Examples Methanol–

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Water Mixture Pure methanol has a flash point of nearly 11 °C. Adding water increases the flash point because water dilutes methanol vapor concentration. Same as with Octane–Ethanol Mixture Pure octane has a higher flash point (~-4 °C). Adding ethanol lowers the flash point at certain concentrations due to synergistic vapor composition effects [5]. The determination of flash points in liquid mixtures is a critical aspect of chemical safety, process design, and environmental protection [11]. While ideal solutions can often be described using simplified thermodynamic models, most real world mixtures exhibit non ideal behaviour due to molecular interactions, differences in polarity, and deviations from Raoult's law. These complexities make the prediction of flash points in non ideal systems both challenging and essential. To approach this activity, we use the Van Laar equation By Approaching this theoretical Methods we can easily predictable in Large scale industrial Areas with out any Instrumentation or Experimental Procedures [2]. This paper is more useful for industrial scale without any cost proposals / cost consumption in Chemical manufacturing Fields. The introduction of activity coefficient models—such as Van Laar, Wilson, NRTL, and UNIQUAC—marked a significant advance, enabling predictions that accounted for non ideal solution behaviour and molecular interactions. In recent decades, computational methods and machine learning have further expanded predictive capabilities, allowing estimation for complex mixtures, biofuels, and hazardous solvents without exhaustive experimentation [6].

II. Theoretical Background:

The estimation of flash points through theoretical methods relies on fundamental thermodynamic principles and mixture rules that describe vapor–liquid equilibrium and flammability limits [4]. Unlike experimental determination, these approaches provide predictive capability for complex mixtures, particularly those exhibiting non-ideal behaviour [1].

2.1 Raoult's Law (Ideal Solutions)

For an ideal liquid mixture, the partial vapor pressure of each component is proportional to its mole fraction in the liquid phase and its pure component vapor pressure:

$P_i = x_i \cdot P_i^{sat}(T)$

where:

P_i = partial vapor pressure of component i

x_i = mole fraction of component i in the liquid phase

$P_i^{sat}(T)$ = saturation vapor pressure of pure component i at temperature T

2.2 Activity Coefficient Models (Non-Ideal Solutions)

Real mixtures often deviate from Raoult's law due to molecular interactions. Activity coefficients (γ_i) are introduced to account for non-ideality:

$$\mathbf{P_i = x_i \cdot \gamma_i \cdot P_i^{sat}(T)}$$

2.3 Le Chatelier's Mixing Rule (Flammability Limit)

The flash point corresponds to the temperature at which the vapor composition reaches the lower flammable limit (LFL). For mixtures, the effective LFL can be estimated using Le Chatelier.

III. Methodology

The estimation of flash point for binary mixtures requires combining thermodynamic principles with flammability rules. In this study, the methodology integrates

Step by Step approaches are Consider as

3.1 Overview:

•**Mole fraction Determination**: To quantify mixture composition
•**Le Chatelier's mixing Rule**: To estimate effective flammability limits.

•**Antoine equation**: To calculate vapor pressures

•**Raoult's law:** To determine total vapor pressure of the mixture

3.2 Calculation:

Applying Le-Chatelier's Rule:

Example -1: Acetone + Methanol:

Data consideration For This Calculation for Acetone =1850 Litres, Methanol= 930 Litres.
Molecular Weight of Acetone = 58.08 g/mol
Molecular Weight of Methanol = 32.04 g/mol
Le Chatelier Law: 1/Total Flash Point (mix) =∑ (xi/Total flash Point)
•Convert Acetone in to Kg's = 1850 L × 0.785 Kg/m^3
Convert Acetone in to Kg's = 1452.25 Kg
• Convert Methanol in to Kg's = 930 L × 0.791 Kg/m^3
Convert Methanol in to Kg's = 735.63 Kg

•Step-1 Finding No, of Moles in Acetone:

$$n(A) = \frac{Weight}{Mol.Wweight}$$

$$n(A) = \frac{1452250\ g}{58.08\ g/mol}$$

n(A) = 25004.30 mole

• Finding No, of Moles in Methanol:

$$n(B) = \frac{Weight}{Mol.Wweight}$$

$$n(B) = \frac{735630\ g}{32.04\ g/mol}$$

n(B) = 22959.73 mole

•Step-2 Finding Mole Fraction:

Mole Fraction of Acetone:

$$x(A) = \frac{nA}{nA+nB}$$

$$x(A) = \frac{25004.30\ mole}{25004.30\ mole+22959.73}$$

x(A) = 0.521%

Mole Fraction of Methanol:

$$x(B) = \frac{nB}{nA+nB}$$

$$x(B) = \frac{22959.73\ mole}{25004.30\ mole+22959.73}$$

x(B) = 0.478%

Now Applying Le-Chatelier Rule:

$$\frac{1}{Total\ Flash\ point} = \frac{Mole\ fraction\ of\ Acetone}{Flash\ point\ of\ Acetone} + \frac{Mole\ fraction\ of\ Methanol}{Flash\ point\ of\ Methanol}$$

$$\frac{1}{Total\ Flash\ point} = \frac{0.521}{(273+(-20°C)} + \frac{0.478}{(278+13°C)}$$

$$\frac{1}{Total\ Flash\ point} = \frac{0.521}{253\ K} + \frac{0.478}{284\ K}$$

$$\frac{1}{Total\ Flash\ point} = 0.0020592 + 0.0016830$$

$$= 0.0037422\ K^{-1}$$

$$= \frac{1}{0.0037422}$$

$$= 267.222\text{-}273$$

Total Flash Point = -5.77 °C

After Successfully Reaching the Estimation of Flash point we Have another Important Calculation for Estimation of Vapour Pressure of the Mixture By using Antonie Equation and Applying the Raoult's Law to reach this Approach

The Antoine equation Calculation for Acetone:

A= 7.0244; B= 1161; C= 224

The Antoine equation Calculation for methanol:

A= 8.08097; B= 1582.271; C= 239.726
Vapour Pressure of Acetone:

$\text{Log P} = A - \frac{B}{T+C}$

$\text{Log}_{10} P = 7.0244 - \frac{1161}{-5.77°c+224}$

$\text{Log}_{10} P = 7.0244 - \frac{1161}{218.3}$

$\text{Log}_{10} P = 7.0244 - 5.318$

$\text{Log}_{10} P = 1.706$

Vapour pressure = 10^1.706

Vapour pressure = 50.81 mmHg × 0.1333

Vapour pressure = 6.77 Kpa

Vapour Pressure of Methanol:

$\text{Log P} = A - \frac{B}{T+C}$

$\text{Log}_{10} P = 8.08097 - \frac{1582.271}{-5.77°c+239.726}$

$\text{Log}_{10} P = 8.0897 - \frac{1582.271}{233.956}$

$\text{Log}_{10} P = 8.08097 - 6.7631$

Vapour Pressure = 10^1.326

$\text{Log}_{10} P = 21.212$ mmHg × 0.1333

Vapour Pressure = 2.8276 Kpa

Now Applying the Raoults Law:

$P_{Total} = X_{Methanol} . P^0_{Methanol} + X_{Acetone} . P^0_{Acetone}$

$P_{Total} = 0.478 .2.8276 + 0.521 .6.77$

$P_{Total} = 4.872$ Kpa

$P_{Total} = \frac{4.872}{0.1333}$

$P_{Total} = 36.542$ mmHg × 0.00135

$P_{Total} = 0.0493$ Kg/cm^2 of Vapour Pressure at -5.77°C in mixture flash point.

Example-2: Acetone + Water:

Data consideration For This Calculation for Acetone =1250 Litres, Water= 520 Litres.
Molecular Weight of Acetone = 58.08 g/mol
Molecular Weight of Water = 18 g/mol

Le Chatelier Law: 1/Total Flash Point (mix) =∑ (xi/Total flash Point)

•Convert Acetone in to Kg's = 1250 L × 0.785 Kg/m^3

Convert Acetone in to Kg's = 981.25 Kg

• Convert Water in to Kg's = 520 L × 1.0 Kg/m^3

Convert Water in to Kg's = 520 Kg

•Step-1 Finding No, of Moles in Acetone:

$n(A) = \frac{Weight}{Mol.Wweight}$

$n(A) = \frac{1250000\ g}{58.08\ g/mol}$

n(A) = 21522.038 **mole**

• Finding No, of Moles in Water:

$n(B) = \frac{Weight}{Mol.Wweight}$

$n(B) = \frac{520000\ g}{\frac{18}{g/mol}}$

n(B) = 28888.88 mole

•Step-2 Finding Mole Fraction:

Mole Fraction of Acetone:

$\mathbf{x(A) = \frac{nA}{nA+nB}}$

$\mathbf{x(A) = \frac{21522.038\ mole}{21522.038\ mole+28888.88}}$

x(A) = 0.42%

Mole Fraction of Water:

$x(B) = \frac{nB}{nA+nB}$

$x(B) = \frac{28888.88\ mole}{21522.038\ mole+28888.88}$

x(B) = 0.57%

Now Applying Le-Chatelier Rule:

$$\frac{1}{Total\ Flash\ point} = \frac{Mole\ fraction\ of\ Acetone}{Flash\ point\ of\ Acetone} + \frac{Mole\ fraction\ of\ WAter}{Flash\ point\ of\ WAter}$$

$$\frac{1}{Total\ Flash\ point} = \frac{0.42}{(273+(-20°C)} + \frac{0.57}{(273+0°C)}$$

$$\frac{1}{Total\ Flash\ point} = \frac{0.42}{253\ K} + \frac{0.57}{273\ K}$$

$$\frac{1}{Total\ Flash\ point} = 0.001660 + 0.00208$$

$$= 0.00374\ K^{-1}$$

$$= \frac{1}{0.0037422}$$

$$= 267.379\text{-}273$$

Total Flash Point = -5.62 °C

Now Applying the Raoult's Law to reach this approach

The Antoine equation Calculation for Acetone:

A= 7.0244; B= 1161; C= 224

The Antoine equation Calculation for Water:

A= 8.07131; B= 1730.63; C= 233.426

Vapour Pressure of Acetone:

$\text{Log P} = A - \frac{B}{T+C}$

$\text{Log}_{10} P = 7.0244 - \frac{1161}{-5.62°c+224}$

$\text{Log}_{10} P = 7.0244 - \frac{1161}{218.3}$

$\text{Log}_{10} P = 7.0244 - 5.316$

$\text{Log}_{10} P = 1.707$

Vapour pressure = 10^1.706

Vapour pressure = 51.04 mmHg × 0.1333

Vapour pressure = 6.80 Kpa

Vapour Pressure of Water:

$\text{Log P} = A - \frac{B}{T+C}$

$\text{Log}_{10} P = 8.0713 - \frac{1730.63}{-5.77°c+233.42}$

$\text{Log}_{10} P = 8.0713 - \frac{1730.63}{233.956}$

$\text{Log}_{10} P = 8.0713 - 6.7631$

Vapour Pressure = 10^1.3082

Vapour Pressure = 20.332 mmHg × 0.1333

Vapour Pressure = 2.7103 Kpa

Now Applying the Raoults Law:

$P_{Total} = X_{Acetone} . P^0_{Acetone} + X_{Water} . P^0_{Water}$

$P_{Total} = 0.42 .6.80 + 0.57 .2.7103$

$P_{Total} = 4.400$ Kpa

$P_{Total} = \frac{4.400}{0.1333}$

$P_{Total} = 33.014$ mmHg × 0.00135

$P_{Total} = 0.0488$ Kg/cm^2 of Vapour Pressure at -5.77°C in mixture flash point.

Example-3: Isopropyl Alcohol + Water:

Data consideration For This Calculation for IPA=1000 Litres, Water= 890 Litres.

Molecular Weight of IPA = 60.10 g/mol

Molecular Weight of Water = 18 g/mol

Le Chatelier Law:

1/Total Flash Point (mix) =∑ (xi/Total flash Point)

•Convert IPA in to Kg's = 1000 L × 0.785 Kg/m^3

Convert IPA in to Kg's = 785 Kg

• Convert Water in to Kg's = 890 L × 1.0 Kg/m^3

Convert Water in to Kg's = 890 Kg

•Step-1 Finding No, of Moles in IPA:

$n(A) = \frac{Weight}{Mol.Wweight}$

$n(A) = \frac{1000000\ g}{60.10\ g/mol}$

n(A) = 16638.93 mole

• Finding No, of Moles in Water:

$n(B) = \frac{Weight}{Mol.Wweight}$

$n(B) = \frac{890000\ g}{18\ g/mol}$

n(B) = 49444.44 mole

•Step-2 Finding Mole Fraction:

Mole Fraction of IPA:

$x(A) = \frac{nA}{nA+nB}$

$x(A) = \frac{16638.93\ mole}{16638.93\ mole+49444.44}$

x(A) = 0.25%

Mole Fraction of Water:

$x(B) = \frac{nB}{nA+nB}$

$x(B) = \frac{49444.44\ mole}{16638.93\ mole+49444.44}$

x(B) = 0.74%

Now Applying Le-Chatelier Rule:

$$\frac{1}{\frac{Mole\ fraction\ of\ Water}{Flash\ point\ of\ Water}} = \frac{Mole\ fraction\ of\ IPA}{Flash\ point\ of\ IPA} +$$

$$\frac{1}{Total\ Flash\ point} = \frac{0.25}{(273+(12°C)} + \frac{0.74}{(273+0°C)}$$

$$\frac{1}{Total\ Flash\ point} = \frac{0.25}{285\ K} + \frac{0.74}{273\ K}$$

$$\frac{1}{Total\ Flash\ point} = 0.000877 + 0.00271$$

$$= 0.00358\ K^{-1}$$

$$= \frac{1}{0.003587}$$

$$= 278.78\text{-}273$$

Total Flash Point = 5.78 °C

Now Applying the Raoult's Law to reach this approach

The Antoine equation Calculation for IPA:

A= 6.86618; B= 1360.13; C= 197.592

The Antoine equation Calculation for Water:

A= 8.07131; B= 1730.63; C= 233.426

Vapour Pressure of IPA:

$\text{Log } P = A - \frac{B}{T+C}$

$\text{Log}_{10} P = 6.86618 - \frac{1360.13}{5.78°c+197.592}$

$\text{Log}_{10} P = 6.86618 - \frac{1360.13}{203.372}$

$\text{Log}_{10} P = 6.86618 - 6.6878$

$\text{Log}_{10} P = 0.1783$

Vapour pressure = 10^0.1783

Vapour pressure = 1.5076 mmHg × 0.1333

Vapour pressure = 0.2009 Kpa

Vapour Pressure of Water:

$\text{Log } P = A - \frac{B}{T+C}$

$\text{Log}_{10} P = 8.0713 - \frac{1730.63}{5.78c+233.42}$

$\text{Log}_{10} P = 8.0713 - \frac{1730.63}{239.2}$

$\text{Log}_{10} P = 8.0713 - 7.2350$

Vapour Pressure = 10^0.8363

Vapour Pressure = 6.8596 mmHg × 0.1333

Vapour Pressure = 0.9145 Kpa

Now Applying the Raoults Law:

$P_{Total} = X_{IPA} \cdot P^0_{IPA} + X_{Water} \cdot P^0_{Water}$

$P_{Total} = 0.25 .0.2009 + 0.74 .0.9145$

$P_{Total} = 0.7269$ Kpa

$P_{Total} = \frac{0.7269}{0.1333}$

$P_{Total} = 5.4518$ mmHg × 0.00135

$P_{Total} = 0.00736$ Kg/cm^2 of Vapour Pressure at 5.78°C in mixture flash point.

IV. RESULTS & DISCUSSION

The theoretical estimation of flash points for binary mixtures was carried out using Le Chatelier's mixing rule, Raoult's law, and the Antoine equation. The calculated flash points, vapor pressures, and mole fractions are summarized

Table 1. calculated Flash Point vs Total Vapour Pressure vs Mole fraction

Mixture	Calculated Flash Point	Total Vapour Pressure	Mole Fraction
Acetone + Methanol	-5.77°C	0.0493 Kg/cm2	0.52, 0.47%
Acetone + Water	-5.62°C	0.0488 Kg/cm2	0.42%, 0.57%
IPA + Water	5.78°C	0.0073 Kg/cm2	0.25%, 0.74%

Table.2: Effect of Water in Component Flash Vs Mixture Flash

Solvent	Component Flash Point	Mixture Flash Point (°C)	Effect of water
Acetone	-20°C	-5.62°C	Raise in Flash Point
IPA	12°C	5.78°C	Raise in Flash Point
Methanol	11°C	-	-

Table.3: Theoretical Observation in Components in Mixture:

Mixture	Observed trend	Theoretical Observation
Acetone + Methanol	Lowest flash point (-5.77 °C)	More flammable than either pure component alone.
Acetone + Water	Flash point raised	Water dilutes acetone vapor concentration
IPA + Water	Flash point raised significantly	Strong hydrogen bonding suppresses vaporization

4.1 Flash Point Behaviour

The acetone–methanol mixture exhibited the lowest flash point (-5.77 °C), indicating a synergistic effect between the two solvents. This result highlights that mixtures can sometimes be more flammable than either pure component, a critical consideration for industrial safety [1]. In contrast, the IPA–water mixture showed a significantly higher flash point (5.78 °C), consistent with the diluting effect of water on flammable vapor concentration [10]. The rise in flash point for the acetone–water mixture reflects the role of water in diminishing vapor-phase flammability through dilution and molecular interactions [6]

4.2 Vapor Pressure effect

The total vapor pressures calculated for acetone–methanol and acetone–water mixtures were similar (~0.049 kg/cm²), whereas the IPA–water mixture exhibited a much lower vapor pressure (0.0073 kg/cm²). This reduction reflects the strong hydrogen bonding interactions between water and IPA, which suppress vaporization and increase the flash point. These findings confirm that molecular interactions significantly influence nonideal behaviour, deviating from predictions based solely on Raoult's law.

4.3 Theoretical Validation

The application of Le Chatelier's mixing rule successfully predicted effective flammability limits for all mixtures studied. The Antoine equation provided reliable vapor pressure estimates, which, when combined with Raoult's law, yielded consistent results. The observed deviations in flash point behaviour underscore the importance of incorporating activity coefficient models for nonideal systems, particularly in mixtures involving polar solvents such as alcohols and water.

4.4 Industrial Impact

Process safety perspective, the results emphasize that relying on the lowest component flash point is insufficient for hazard assessment. Mixtures such

as acetone–methanol can exhibit unexpectedly low flash points, increasing fire and explosion risks in large-scale batch operations. Conversely, water-containing mixtures demonstrate elevated flash points, offering potential safety advantages in industrial formulations. Theoretical estimation methods thus provide a cost-effective and rapid approach to predicting flash points, reducing reliance on experimental determination while ensuring compliance with safety standards.

4.5 FUTURE SCOPE

The present study demonstrates the utility of theoretical models for binary mixtures, further refinement using advanced activity coefficient models (e.g., NRTL, UNIQUAC) and computational methods is recommended. Extending this methodology to ternary and multicomponent mixtures will enhance predictive accuracy for complex industrial systems, including biofuels and pharmaceutical solvents.

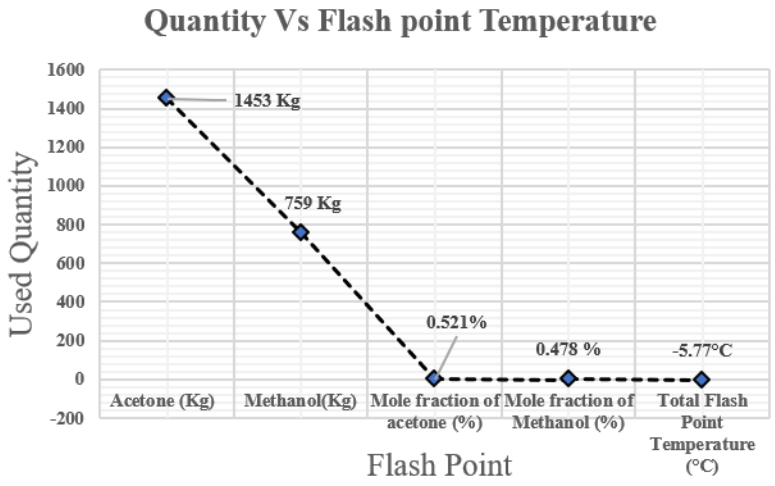

Fig.1 Explained that the Comparison Between Acetone+ Methanol used quantity, Mole Fraction of both Solvents and Final Flash Point Temperature.

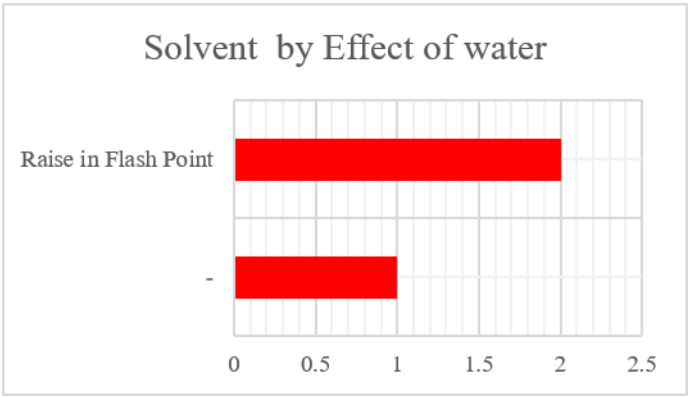

Fig.2 Explained that the Effect of Water in Solvent

Water has a very high flash point (close to 100 °C) and low volatility compared to organic solvents. When mixed with solvents like acetone, methanol, or isopropyl alcohol, water reduces the partial vapor pressure of the flammable component [8]. This dilution effect means fewer flammable

molecules enter the vapor phase, raising the overall flash point of the mixture. Water forms strong hydrogen bonds with polar solvents (e.g., alcohols). These interactions reduce the tendency of solvent molecules to escape into the vapor phase. as a result, mixtures such as IPA–water show significantly higher flash points than pure IPA. Water addition generally makes mixtures safer by raising flash points and lowering vapor pressures. In industrial practice, water is sometimes deliberately added to reduce fire hazards in solvent systems [7]. However, the effect depends on concentration: small amounts of water may not significantly change flammability, while higher proportions can strongly suppress ignition risk.

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