CHEMICAL ENGINEERING TRANSACTIONS

VOL. 56, 2017

A publication of
AIDIC
The Italian Association
of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Jiří Jaromír Klemeš, Peng Yen Liew, Wai Shin Ho, Jeng Shiun Lim

ISBN 978-88-95608-47-1; **ISSN** 2283-9216

DOI: 10.3303/CET1756225

Inherent Safety Assessment Technique for Preliminary Design Stage

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Safety is defined as accidents prevention through appropriate technologies to identify and eliminate hazards before an accident occurs. Safety program that prevents hazards in the first place is preferable compared to the typical approaches of controlling the hazards upon being detected. Plants should be designed so that they are user-friendlier to the workers. This can be done by preventing the presence of the hazards in the process during its design stages. The concept of preventing hazards existence early during the design stage is called inherent safety. This paper introduces an inherent safety assessment technique for preliminary design stage (ISAPEDS) of chemical process. ISAPEDS focuses on assessing inherent safety using information available from the process flow sheet diagram (PFD). ISAPEDS is a technique that is an extension of the Numerical Descriptive Inherent Safety Technique (NuDIST) and the Graphical and Numerical Descriptive (GRAND) techniques developed by the same authors for application during research and development (R&D) design stage. There are five inherent safety parameters considered in this assessment which are operating temperature, operating pressure, flammability, explosiveness and toxicity. ISAPEDS introduces four new features as an improvement to the previous NuDIST and GRAND methods. First, instead of assessing these parameters as a standalone hazard factor, the parameters are assessed in relations to each other. For example the flammability parameter is evaluated in relations to the operating pressure while explosiveness parameter is evaluated in relations to the operating temperature. The second feature is assessing the chemicals as a mixture instead of as individual substance, which is a very rare scenarios in a typical chemical processes. Thirdly, the evaluation will be done comprehensively on each of the process equipment in the process flow diagram (PFD). The last one is the score of the safety hazards assessment in the whole process will be weighted based on the chemicals composition in the mixture. In this technique, a higher score is indicated as more hazardous compared to a lower score. A simple case study is performed on the hydrodealkylation process of toluene (HDA) focusing on three equipment which are the reactor (R101), the toluene feed drum (V101) and the low pressure phase separator (V103). The overall assessment shows that R101 is the most hazardous equipment in the process with the highest ISAPEDS score of 298.6 while V101 is the least hazardous equipment in the process with the lowest ISAPEDS score of 117.1. Among the three equipment, R101 was found to be the most hazardous in all five parameters resulting it to be the most hazardous equipment in the process section.

1. Introduction

Safety is defined as accidents prevention through appropriate technologies to identify and eliminate hazards before an accident occurs (Crowl and Louvar, 2002). Safety program that prevents hazards in the first place is preferable compared to safety program which eliminates hazards as they are detected. The concept of preventing hazards existence during design stages is referred as inherent safety. It is important to understand the hazards posed by the chemicals and process conditions in a process before any hazard preventions and mitigations can be applied. Understanding hazards can be done through hazards assessments. Various

Please cite this article as: Ahmad S.I., Hashim H., Hassim M.H., 2017, Inherent safety assessment technique for preliminary design stage, Chemical Engineering Transactions, 56, 1345-1350 DOI:10.3303/CET1756225

inherent safety assessment methods for preliminary engineering phase of process design stage had been introduced in the past few years. The most common technique is the Inherent Safety Index (ISI) (Heikkila, 1999). The ISI method includes a wide range of inherent safety parameters, divided into chemical inherent safety index and process inherent safety index. Scores for all parameters will be added into a total score to represent a process route. In ISI, a higher total score represents an inherently more unsafe process.

Risk and consequences estimation is included in a method called the Integrated Risk Estimation Tool (iRET) as proposed by Mohd Shariff et al. (2006). iRET evaluates explosion risks in a process through the integration of Microsoft Excel and HYSYS. TORCAT also applies similar technique as iRET but instead of explosion it focuses on assessing toxicity by calculating the toxic release dispersion to assess the toxic release effect (Mohd Shariff and Zaini, 2010). Mohd Shariff and Abdul Wahab (2013) proposed another similar method for elimination of fire accidents called the Inherent Fire Consequence Estimation Tool (IFCET). The Three-tier Inherent Safety Quantification (3-TISQ) (Zaini et al., 2014) focuses on evaluating the inherent safety level of a process from the perspective of toxicity parameter. This framework enables the design engineers to easily identify the critical process streams to be considered for improvement in order to avoid or minimize explosion hazards. Ahmad et al. (2014) introduces an inherent safety assessment technique called the Numerical Descriptive Inherent Safety Technique (NuDIST) which incorporates logistic functions in order to score the inherent safety level of eight parameters. The NuDIST technique was extended through the addition of root-cause analysis to determine the main contributor to the largest hazards in a process in a technique called the Graphical Descriptive Technique for Inherent Safety Assessment (GRAND) (Ahmad et al., 2016a). Both techniques focus on assessing inherent safety parameters for a process route during the research and development (R&D) phase of process design. Next, the research was further extended for application during the preliminary design stage of process design focusing on assessing inherent safety on separation equipment (Ahmad et al., 2015) as well as assessing the inherent safety level of flammability parameter in biodiesel production (Ahmad et al., 2016b).This paper introduces a new technique to inherent safety assessment called the Inherent Safety Assessment for Preliminary Engineering Design Stage (ISAPEDS). ISAPEDS involves five main safety parameters which are operating temperature, operating pressure, flammability, explosiveness and toxicity. Logistic function (Larsen and Marx, 2001) is used in this technique for score assignments due to its ability to eliminate subjective scaling in scores assignment. ISAPEDS introduces four new features. The first feature is instead of assessing these parameters as a standalone factors, the parameters are assessed in relations to each other. For example the flammability parameter is evaluated in relations to the operating pressure while explosiveness parameter is evaluated in relations to the operating temperature. The second feature is assessing the chemicals as a mixture. The third feature is the evaluation will be done according to every equipment exists in the process flow diagram (PFD). The last feature is taking mass fraction of chemical substances in unit operation to be the weightage in the final score calculation.

2. Methodology

2.1 Calculation of Flammability and Explosiveness Value According to Operating Temperature and Pressure

2.1.1 Flammability

In this technique, flash point value of a chemical is used to determine the flammability hazards of a chemical. The flash point of a liquid is defined as the lowest temperature at which it emits enough vapour to form an ignitable mixture with air (Crowl and Louvar, 2002). Liquids with lower flash points are more hazardous than liquids with higher flash points. In ISAPEDS flash point of a chemical is evaluated at the operating pressure in every equipment. The Clausius-Clapeyron equation shown in Eq(1) is used to obtain the new boiling point (TBPnew) of a chemical at designated pressure. In Eq(1), P_1 is the ambient pressure, P_2 is the designated pressure, T_2 is the new boiling point value to be obtained, T_1 is the boiling point value at ambient temperature, Δhvap is the heat of vaporisation for each chemicals and R is the gas constant.

$$\ln\frac{P_2}{P_1} = \frac{-\Delta Hvap}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \quad (1)$$

The new boiling point is then used to determine the new flash point at the designated pressure. Eq(2) (Crowl and Louvar, 2002) is used to find the new flash point value from the boiling point value obtained from Eq(1). In Eq(2), T_F is the new flash point, T_b is the new boiling point obtained from Eq(1) while a, b and c are the constants that can be obtained from Table 6.1 in Crowl and Louvar (2002).

$$T_F = a + \frac{b\left(\frac{c}{T_b}\right)^2 \left(e^{-\frac{c}{T_b}}\right)}{\left(1 - e^{-\frac{c}{T_b}}\right)^2} \tag{2}$$

2.1.2 Explosiveness

The tendency of chemicals to form an explosive mixture in air (also known as explosiveness) depends on the range between explosion limits (Heikkila, 1999). Below the Lower Explosion Limit (LEL), the mixture is too lean to burn while the mixture is too rich for combustion above the Upper Explosion Limit (UEL) (Crowl and Louvar, 2002). Thus, wider range between LEL and UEL indicates higher tendency for explosion. In ISAPEDS explosiveness of a chemical is evaluated at the operating temperature in every equipment. Eqs(3)-(4) (Crowl and Louvar, 2002) are used to calculate the new LEL and UEL value at the designated operating temperature, T. LEL_{25} and UEL_{25} are the UEL and LEL value at ambient temperature and ΔH_c is the heat of combustion for the chemical.

$$LEL_T = LEL_{25} - \frac{0.75}{\Delta Hc}(T - 25) \tag{3}$$

$$UEL_T = UEL_{25} + \frac{0.75}{\Delta Hc}(T - 25) \tag{4}$$

2.2 Treating the Chemicals as a Mixture

Eq(5) is used to calculate all the values obtained as a mixture (Crowl and Louvar, 2002) and is used as the base in producing Eqs(6)-(9). Y is the mix parameter value. For example, for flash point, explosiveness value or toxicity, m_i is the mass fraction for every chemicals involved while X_i is the individual parameter value. Eq(6) as well as Eqs(7)- (8) show the mixed value equations for flammability and explosiveness parameters.

$$Y = \frac{1}{\sum_{i=1}^{n} \frac{m_i}{X_i}} \tag{5}$$

$$T_{Fmix} = 1/\sum_{i=1}^{n} \frac{m_i}{T_{Fi}} \tag{6}$$

$$LEL_{mix} = 1/\sum_{i=1}^{n} \frac{m_i}{LEL_i} \tag{7}$$

$$UEL_{mix} = 1/\sum_{i=1}^{n} \frac{m_i}{UEL_i} \tag{8}$$

One indicator that can be used in determining the toxicity of a chemical is called threshold limit values (TLVs). In this method, threshold limit values for short-term exposure limit (TLV-STEL) are used, which is more significant for an acute toxicity type of event. A lower TLV-STEL value for a chemical indicates a higher toxicity hazard compared to a chemical with a higher TLV-STEL value. In this method, a higher score represent higher hazard imposed by the chemicals. The mixed TLV-STEL values is calculated according to Eq(9).

$$TLV - STEL_{mix} = 1/\sum_{i=1}^{n} \frac{m_i}{TLV - STEL_i} \tag{9}$$

2.3 Logistic Function for Scoring Technique

2.3.1 Logistic Function for Every Parameter

2.3.1.1 Operating Temperature

Temperature is a direct measure of the heat energy available for release (Srinivasan and Nhan, 2008). A higher operating temperature is inherently unsafe. It is assumed that the process will not contribute to hazards when operating at the ambient temperature of 25 °C. Eqs(10)-(11) represent the logistic equation for operating temperatures higher and lower than 25 °C. $S_{T>25°C}$ and $S_{T<25°C}$ are the score produced for $x_{T>25°C}$ and $x_{T<25°C}$ evaluated for operating temperatures higher and lower than 25 °C.

$$S_{T>25°C} = 100 \times \left(\frac{1}{1 + 403.43e^{-0.012x_{T>25°C}}}\right) \tag{10}$$

$$S_{T<25^\circ C} = 100 \times (1 - \left(\frac{1}{1 + 0.0025e^{-0.012x_{T<25^\circ C}}}\right)) \quad (11)$$

2.3.1.2 Operating Pressure

High pressure usage increases the amount of energy available in the plant greatly (Heikkila, 1999). Leakage of chemicals can also occur due to high operating pressure (Srinivasan and Nhan, 2008). A process with higher operating pressure is more hazardous compared to a process with low operating pressure. Eq(12) shows the logistic equation for the pressure parameter. Evaluated operating pressure, x_P will result in a score for the pressure parameter, S_P. A high pressure value is represented by a high score value, indicating a greater hazard.

$$S_P = 100 \times \left(\frac{1}{1+148.41e^{-0.2x_P}}\right) \quad (12)$$

2.3.1.3 Flammability

Liquids with lower flash points are more hazardous than liquids with higher flash points. The logistic equation for flammability is produced as Eqs(13)-(14). S_{FL} refers to the scores for the flammability parameter while x_{FL} refers to the flash point value to be evaluated.

$$S_{FL>25^\circ C} = 100 \times (1 - \left(\frac{1}{1+2.2255e^{-0.008x_{FL>25^\circ C}}}\right)) \quad (13)$$

$$S_{FL<25^\circ C} = 100 \times \left(\frac{1}{1+0.4493e^{-0.008x_{FL<25^\circ C}}}\right) \quad (14)$$

2.3.1.4 Explosiveness

Wider range between LEL and UEL indicates higher tendency for explosion which represents by logistic equation in Eq(15). In Eq(15), x_{EXP} is the explosiveness value (or the difference between UEL and LEL), while S_{EXP} is the score produced for the explosiveness value evaluated. For explosiveness parameter, higher hazard is represented with high score designation.

$$S_{EXP} = 100 \times \left(\frac{1}{1+1096.63e^{-0.14x_{EXP}}}\right) \quad (15)$$

2.3.1.5 Toxicity

A chemical with a lower TLV-STEL value is more hazardous than a chemical with a higher TLV-STEL value. Eq(16) shows the logistic equation for the toxicity parameter. The score produced is denoted as S_{TOX}, while x_{TOX} denotes the TLV-STEL value to be evaluated. Higher TLV-STEL values are represented by lower score values.

$$S_{TOX} = 100 \times (1 - \left(\frac{1}{1+403.4288e^{-0.012x_{TOX}}}\right)) \quad (16)$$

2.3.2 Total Scores

In this study, the ISAPEDS Total Score represents the final scores. This score will be used to represent the routes assessed for ranking purposes. A total score for each route is used for process ranking with lower ISAPEDS Total Score value indicates a less hazardous route compared to a route with a higher ISAPEDS Total Score value. ISAPEDS Total Score is derived using Eq(17) based on the worst-case scenario. According to Heikkila (1999), the approach of the worst case describes the most risky situation that can appear. The maximum score received by chemicals for operating temperature (S_T), operating pressure (SP), flammability (SFL), explosiveness (SEXP) and toxicity (STOX) are summed up to represent the reaction step for those particular routes.

$$\text{ISAPEDS Total Score} = S_T + S_P + S_{FL} + S_{EXP} + S_{TOX} \quad (17)$$

2.4 Root-cause Analysis to Identify the Most Hazardous Chemical

Identifying the chemicals that contributes to the largest hazard in a process route is important in determining the suitable measures that need to be taken in order to avoid any fire or explosion thus, the root-cause analysis is applied for this purpose. A chemical with the highest score in a process route might not be the most hazardous if there is only small amount of it existed in the process. Thus, the mass fraction for each chemical is used as the weighing factor to identify the most hazardous chemical. According to Eq(18), S_i is the score assigned to every chemical while y_i is the mass fraction to every chemical. After the normalized score for every chemical have been calculated, the normalized score will then be analysed and chemical with the highest normalized score is the most hazardous chemical in a process route.

$$Normalized\ Score_i = S_i \times\ y_i \tag{18}$$

3. Case Study

A simple case study is performed on the hydrodealkylation process of toluene (HDA) to produce benzene. This process is a highly exothermic reaction with operating conditions from 500 °C to 660 °C and from 20 bar to 60 bar. This assessment focused on three equipment which are the reactor (R101), the toluene feed drum (V101) and the low pressure phase separator (V103). Table 1 shows the inherent safety assessment results for the process. The results were obtained by directly inputting the parameters value into Eqs(10)-(11) for operating temperature, Eq(12) for pressure, Eqs(13)-(14) for flammability, Eq(15) for explosiveness and Eq(16) toxicity parameters. Overall ranking in Table 1 shows that reactor R101 is the most hazardous equipment among the three equipment with the highest total score of 298.6 while the toluene feed drum V101 is indicated as the safest equipment with the lowest total score of 117.1. According to Table 1, reactor R101 is the most hazardous process equipment in term of operating temperature with operating temperature value of 660 °C and the associated score of 87.21. The highest score that can be achieved is 100. Reactor R101 is also the most hazardous process equipment in term of operating pressure (24.67 atm: 48.37), flammability (39.22 °C: 61.92) and explosiveness (20.67 %: 1.62). As for toxicity parameter, all process equipment have similar score, this indicates that all process equipment above have similar level of hazards in term of chemical toxicity. As reactor R101 scores the highest in all parameters assessment, it is evaluated as the most hazardous process equipment. Thus, further analysis was done on reactor R101 to find the root-cause that contributes to the highest hazards in the process equipment.

Table 2 shows the results obtained from the root-cause analysis done on reactor R101. Mass fraction of every chemicals is used as the weightage factor in determining the most hazardous chemical for flammability, explosiveness and toxicity parameters. Chemical with the highest normalised score is the most hazardous chemical in a process route. According to Table 2, hydrogen existed in the highest amount in the process equipment with a mass fraction of 0.61 while benzene existed in the lowest amount in the process equipment with a mass fraction of 0.01. Hydrogen is the most hazardous chemical for flammability and explosiveness parameters while toluene is the most hazardous chemical in term of toxicity as shown in Table 2. Not only hydrogen existed in the highest amount in the process equipment, it is also the most flammable and explosive with the highest score for both flammability and explosiveness parameters which are 64.57 and 96.79. Since mass fraction and assessment score affect the normalized score directly, hence the normalized score value will be high when both mass fraction and assessment score values are high. However, the root-cause analysis done for toxicity parameter on reactor R101 shows different result. Toluene is analysed as the most hazardous chemical for toxicity parameter as shown in Table 2. Toluene and benzene have similar toxicity score which are 98.20 and 98.18. However, toluene existed in higher amount than benzene in reactor R101 thus toluene is indicated as the most hazardous chemical for toxicity parameter. Although hydrogen and methane existed in higher amount with mass fraction of 0.61 and 0.26 than toluene in the process equipment, hydrogen and methane have the lowest toxicity score compared to toluene and benzene resulting to hydrogen and methane as the safest chemical in term of toxicity.

Table 1: Inherent safety assessment results for the hydrodealkylation process of toluene (HDA)

	Operating Temperature (°C)		Operating Pressure (atm)		Flammability (°C)		Explosiveness (%UEL-%LEL)		Toxicity (TLV-STEL) (ppm)		Total Score	Rank
	Value	Score	Value	Score	Value	Score	Value	Score	Value	Score		
R101	660	87.21	24.67	48.37	39.22	61.92	20.67	1.62	0.17	98.200	298.6	3
V101	55	0.48	1.97	0.99	296.30	17.22	5.31	0.19	0.02	98.201	117.1	1
(V103)	38	0.39	2.96	1.20	278.01	19.40	5.70	0.20	0.08	98.201	119.4	2

Table 2: Root-cause analysis results on Reactor R101

	Chemical	Hydrogen	Methane	Benzene	Toluene
	Mass Fraction	0.61	0.26	0.01	0.12
Flammability	Score	64.57	11.55	11.15	9.11
	Normalised Score	39.43	3.04	0.07	1.09
	The Most Hazardous Chemical	Hydrogen			
Explosiveness	Score	96.79	0.41	0.21	0.20
	Normalised Score	59.10	0.11	0.00	0.02
	The Most Hazardous Chemical	Hydrogen			
Toxicity	Score	0.03	0.03	98.18	98.20
	Normalised Score	0.02	0.01	0.62	11.74
	The Most Hazardous Chemical	Toluene			

4. Conclusions

This paper presents a technique known as ISAPEDS by considering five inherent safety parameters considered in this assessment which are operating temperature, operating pressure, flammability, explosiveness and toxicity. In this technique, a high score is indicated as more hazardous compared to a low score. A simple case study is performed on the hydrodealkylation process of toluene (HDA) focusing on three equipment which are the reactor (R101), the toluene feed drum (V101) and the low pressure phase separator (V103). The overall assessment shows that R101 is the most hazardous equipment in the process with the highest ISAPEDS score of 298.6 while V101 is the least hazardous equipment in the process with the lowest ISAPEDS score of 117.1. The root-cause analysis performed on R101 shows that hydrogen is the most hazardous chemical in term of flammability and explosiveness parameters while toluene is the most hazardous chemical in term of toxicity parameter.

Acknowledgments

The authors gratefully acknowledge the Ministry of Higher Education (MOHE) and Universiti Teknologi Malaysia (UTM) for providing the research grant Vot No. Q.J130000.2446.03G52.

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