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Inherent Safety Assessment Technique for Separation Equipment in Preliminary Engineering Stage

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This paper highlights the development of new numerical approach for inherent safety assessment for separation process during the preliminary engineering stage of a typical petrochemical process lifecycle. Currently, existing inherent safety assessment technique for preliminary engineering phase did not specify the type of equipment they are applicable to as most of the methods can be used for any types of equipment generally. Aside from that, their assessment parameters are not exclusive to a certain type of unit operations. This new technique offers an inherent safety assessment focusing on chemicals safety during separation process. Parameters related to chemicals involved in separation process such as volatility, toxicity, flammability as well as explosiveness will be discussed. This technique will be constructed using logistic function which offers not only hazard assessment numerically but also graphically visualizes the effect of inherent safety parameters in designing an inherently safer process. The proposed technique can be used to effectively identify the level of hazards involved in process equipment besides highlighting the potential source of hazards in the process through numerical and graphical approach.

1. Introductions

Understanding the hazards posed by a process during process design stage is important in developing an inherently safer and user-friendlier chemical plant to prevent accidents. Hazards identification can be done through the implementation of inherent safety assessment technique which can be done throughout the process design stage. The Prototype Index for Inherent Safety (PIIS) (Lawrence, 1996), the simple graphical method (Gupta and Edwards, 2003) and the IRET method (Mohd Shariff et al., 2006) are a few examples of the inherent safety assessment technique available.

The PIIS method evaluates seven inherent safety parameters which are temperature, pressure, inventory, yield, toxicity, explosiveness and flammability for selection of process routes during research and development (R&D) phase of process design stage. Using the same case study as in the PIIS method, Gupta and Edwards (2003) introduced a simple graphical approach for inherent safety assessment. In this technique, parameters are plotted individually for each step in a process route. The parameters in this method can be expanded to be considered for factors such as economic, health, regulatory or pollution control. The iRET technique is more applicable for inherent safety assessment during preliminary engineering phase of process design stage which is comprised of mass and energy flow rate (Mohd Shariff et al., 2006). The iRET method focuses on assessing risks caused by explosion. Another similar technique proposed by Mohd Shariff and Abdul Wahab (2013) focuses on minimizing the consequence of fire accidents called the Inherent Fire Consequence Estimation Tool (IFCET).

A risk register was constructed by Balfe et al., (2014) for application in an electricity generation organisation. A risk register is a monitoring tool for organisations that can be used to reduce risks during initial safety assessments and also during operations.

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Currently, existing inherent safety assessment technique for preliminary engineering phase did not put any indication on the type of equipment they can assess as most of the method can be used for any types of equipment generally. Aside from that, their assessment parameters are not exclusive to a certain type of unit operations. To overcome these shortcomings, this new technique offers an inherent safety assessment for preliminary engineering phase for chemicals safety evaluation during separation process. Parameters related to chemicals involved in separation process such as volatility, toxicity, flammability as well as explosiveness will be discussed.

2. Parameter Involved

This paper will discussed the inherent safety parameters involved in evaluating chemicals involved in separation process.

a) Volatility Parameter
   Boiling point is chosen for determining the scores for volatility parameter as it is the temperature at which the liquid will turn to vapour which often used in distillation. The lower the boiling point, the easier for the liquids to turn to vapour. This is preferable as it will avoid the separation process at higher temperature. The farther the operating temperature from the ambient temperature (25°C), the more hazardous will the process be (Srinivasan and Nhan, 2008).
b) Toxicity Parameter
   If any flame or explosion occurs, there is high possibility for chemicals substance with high toxicity to leak causing harm to nearby populations (Gupta and Edwards, 2003). Thus, toxicity are often included in most inherent safety assessment methods. In this method, threshold limit values for short-term exposure limit will be used (TLV-STEL) which is more significant for acute toxicity type of event. Lower TLV-STEL value for a chemical indicates larger toxicity hazard compared to chemical with higher TLV-STEL value.
c) Flammability Parameter
   In this method, flammability is measured according to flash point of a liquid. Flash point of a liquid is defined as the lowest temperature at which it emits enough vapour to form ignitable mixture with air (Crowl and Louvar, 2002). Thus, liquids with lower flash point exposes more hazard compared to liquids with higher flash point.
d) Explosiveness Parameter
   The tendency of chemicals to form an explosive mixture in air or also known as explosiveness depends on the range between explosion limits (Crowl and Louvar, 2002). Under 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

3. Brief Introduction to Logistic Function

The scores that will be used in this technique will be constructed through the application of logistic equation. The general equation for logistic equation is as shown in Eq(1) (Larsen and Marx, 2001). There are three main constant parameters in logistic equation which are C, B and A.

$$y = C \times \left(\frac{1}{1 + Ae^{-Bx}}\right) \quad (1)$$

C indicates the upper limit of the curve. The upper limit will give a restriction on the output value of y, this means that y value will only be equal or less than C value. This characteristic is suitable for score establishment. As an example, if C value is set as 100, the maximum value for output y can only be 100 at most. Another two constant parameters aside from C is A and B. B affects the slope of the logistic curve represented by Eq(2) through m value which represent the slope inclination for the curve to be made while A affects the mid-point of the logistic curve represented by Eq(3) through k value which is the x-axis value at y=C/2. Both k and m value obtained is applied into Eq(2) and (3) to obtain the value for B and A.

$$m = \frac{BC}{4} \quad (2)$$

$$A = e^{Bk} \quad (3)$$

, k is the x-point at y =C/2.

4. Methodology

As mentioned in section 3, there are three main constant needed in developing a logistic function which are constant A, B and C. Constant A is affected by k value while constant B is affected by m value as shown in Eq(2) and (3). As for constant C, we will set it to be 100 so that the scores produced will be 100 at most. In this technique, the scores produced will be noted as y in the logistic function while the parameters values to be evaluated is noted as x as shown in Eq(1). One logistic function need to be developed for every inherent safety parameters to be evaluated. This section will propose steps that need to be taken to develop a logistic function.

1) Data needed for every parameter is collected.
2) The data is analyzed for two purposes which are;
    a. Mean Value of the Data
    b. Upper and Lower Boundary of the Data
3) The mean value identified will be used as the k value while the upper and lower boundary of the data will be used in identifying the suitable m value. The m value is considered suitable when the scores produces (y value) is unique for every parameter values (x value).
4) Both k and m values identified will be applied in Eq(1), (2) and (3) to produce the desired logistic function for the inherent safety parameter.
5) Using parameter values ranging from the lower boundary data to the upper boundary data as the x value into the logistic function produced in Step 4, a set of scores which can be represented into a logistic curve will be produced.
6) Step 1 until 5 will be repeated for every inherent safety parameters identified.

5. Results and Discussion

5.1 Volatility Parameter

Boiling points for 952 chemicals (Green and Perry, 2008) were analyzed for mean values as well as the highest and the lowest boiling points value available in the data. This was done with the assumptions that chemicals with boiling temperature similar to the temperature (25 °C) is less hazardous compared to process in higher ambient temperature (Srinivasan and Nhan, 2008). Eq(4) shows the logistic functions produced for volatility parameter. Figure 1(a) shows the logistic curve for scoring of volatility parameter produced for separation equipment. In Figure 1, higher scores indicate higher hazards.

$$S_V = 100 \times (\left(\frac{1}{1 + 58.14e^{-0.022x}}\right)) \quad (4)$$

Toxicity Parameter

Threshold Limit Value (TLV) is not intended to define the “safe” and “unsafe” level. Thus, the logistic function is simply made so that the scores starts with 0 ppm TLV-STEL with the highest score of 100. In this method, higher score represent higher hazard imposed by the chemicals. Eq(5) shows the logistic equation for toxicity parameter. Figure 1(b) shows the scores plotted with higher TLV-STEL values is represented by lower score values.

$$S_{TOX} = 100 \times (1 - \left(\frac{1}{1 + 403.4288e^{-0.012x}}\right)) \quad (5)$$

5.2 Flammability Parameter

The logistic equation for flammability parameter produced is as Eq(6). Lower flash point contributes to higher hazard. The scores will begins at 100 score point for low flash point value that is more hazardous and ends at 0 score point for higher flash point value which is safer. Then, a curve as in Figure 1(c) is plotted. Figure 1(c) indicates that lower flash point temperature results in higher score.

$$S_{FL} = 100 \times (1 - \left(\frac{1}{1 + 3.03e^{-0.02x}}\right)) \quad (6)$$

5.3 Explosiveness Parameter

There is one assumption in constructing scores for explosiveness parameter. Since both UEL and LEL is expressed in percent by volume (vol %), thus the 50 % range between UEL and LEL is taken as the mid-score for explosiveness scores which indicates both not very safe and not very hazardous either. Scores for explosiveness parameter is represented by the logistic equation as shown in Eq(7). Lastly, a curve as in Figure 1(d) is plotted with higher range between UEL and LEL indicates higher hazard with high score designation.

$$S_{EXP} = 100 \times \left(\frac{1}{1 + 1096.63e^{-0.14x}}\right) \quad (7)$$

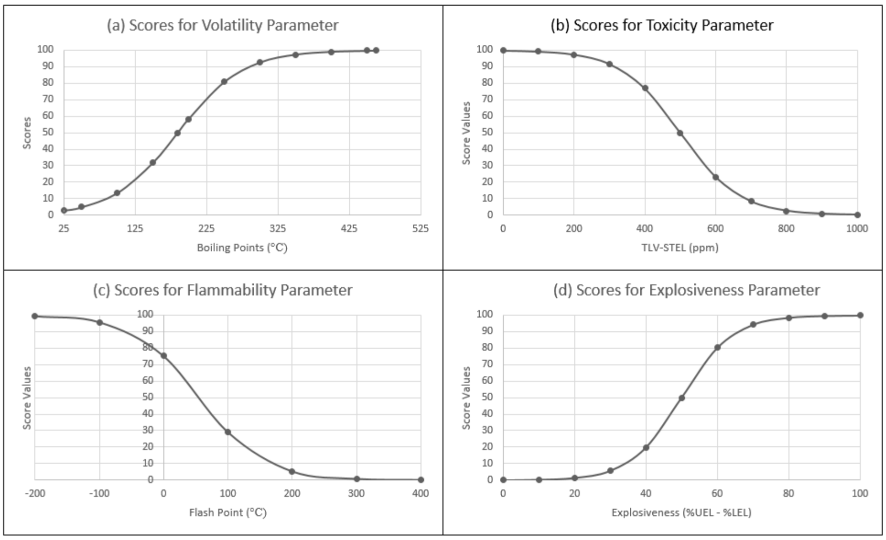

Figure 1: Scores for Chemical Inherent Safety Evaluation for Separation Equipment

5.4 Calculation of the Chemical Inherent Safety Evaluation Total Scores for Separation Equipment

The total score will be calculated for each chemical evaluated in the process. This suggests that each chemical that is evaluated using this technique will have their individual score consists of the four parameters which are volatility, toxicity, flammability, and explosiveness. Lower total score value indicates a less hazardous chemicals compared to chemicals with a higher total score value. The total score for is calculated according to Eq(8). The calculation of the total score is made based on the worst case scenario as used in the PIIS (Edwards and Lawrence, 1993), the ISI (Heikkila, 1999), the i-Safe (Palaniappan et al., 2002a, b) and the Inherent Chemical Process Properties Data (Hassim and Ali, 2009) methods. According to Heikkila (1999), the approach of the worst case describes the most risky situation that can appear. The score for volatility (S_V), explosiveness (S_{EXP}), toxicity (S_{TOX}) and flammability (S_{FL}) are summed up and the maximum score received by a chemical is taken to represent the reaction step for those particular routes.

$$\text{Total Score} = S_V + S_{EXP} + S_{TOX} + S_{FL} \quad (8)$$

6. Case Study: Reactor Effluent for a Toluene Hydrodealkylation Process

A case study was done to illustrate the usage of this technique by applying this technique to the reactor effluent for a toluene hydrodealkylation process (Seider, et al., 2010). The chemicals involved for separation are hydrogen, methane, benzene, toluene and biphenyl. These chemicals were evaluated according to the volatility, toxicity, flammability and explosiveness parameters and the scores for every parameters were totaled up using Eq(8). Table 1 shows the total scores evaluated for every chemicals as well as their inherent safety ranking with Rank 1 indicates the safest chemical while Rank 5 indicates the most hazardous chemicals. Figure 2 shows the graphical representation of the assessment results.

Table 1: Assessment Results for Toluene Hydrodealkylation Process

Chemical	Effluent (kgmol/h)	Mol fraction	Initial Total Score	Final Total Score	Rank
Hydrogen	586	0.45	102	46.1	4
Methane	529	0.41	197	80.3	5
Benzene	127	0.10	273	26.8	3
Toluene	53	0.04	271	11.1	2
Biphenyl	1	0.00	296	0.3	1
Total	1,297				

*Rank 1 is the safest while rank 5 is the most hazardous

According to Table 1, hydrogen is assessed as the safest chemical with the initial total score of 102 while biphenyl is assessed as the most hazardous chemical with the initial total score of 296. Initially, Biphenyl scores the highest in three parameters which are volatility, toxicity and explosiveness. In this technique, higher score indicates higher hazards. In volatility parameter evaluation biphenyl scores the highest with the boiling point value of 255 °C and a score of 82 as shown in Figure 2(a), As for toxicity parameters, biphenyl also scores the highest with the TLV-STEL value of 0.6 ppm and a score of 99.8. Biphenyl ranks as the most hazardous chemical in term of toxicity parameter as well as the other chemicals which are toluene and benzene with the score of 99.8 and 99.7 as shown in Figure 2(b). Aside from volatility and toxicity parameters, biphenyl also scores the highest in explosiveness parameter evaluation with explosiveness limits (UEL %-LEL %) of 5.2 % and a score of 99.81 as shown in Figure 2(d). However, Figure 2(d) also shows that two other chemicals which are benzene and toluene also have similar level of hazards with the score of 99.80 and 99.79. As for flammability parameter, methane is evaluated as the most hazardous with flash point value of -119.6 °C and a score of 97.1 as shown in Figure 2(c). According to the chemicals composition in the effluent stream as shown in Table 1, biphenyl in the stream is only 1 kmol/h compared to other chemicals with composition higher than 50 kmol/h. Thus, in real practice biphenyl might possess lower level of hazards compared to other chemicals. Due to biphenyl amount which is small compared to others, weighing factor which is the mol fraction is taken into considerations for this assessment. The final total score indicates biphenyl is the safest chemical with final total score of only 0.3 while methane is indicated as the most hazardous chemical with final total score of 80.3.

7. Conclusions

The technique proposed in this paper is suitable to be used in assessing the inherent safety of chemicals undergoing separation process during the process design stage. The four parameters evaluated in this technique is the volatility, toxicity, flammability as well as the explosiveness parameters. This technique provides inherent safety assessment using easily obtained chemical data with simple execution through the usage of logistic function. Graphical representation provided in this technique enable users to easily identify the most hazardous chemical substance even for those who are not familiar with the concept of inherent safety. A case study was done to illustrate the usage of this technique. Inherent safety assessment on the chemicals involved in separation from the reactor effluent for a toluene hydrodealkylation process was done with methane evaluated as the most hazardous chemical and biphenyl as the safest chemical. Several improvements need to be done to this technique in order to ensure a more efficient inherent safety assessment for separation process during process design stage for example the consideration of the type of separation equipment, involvement of solvent usage as well as the operating conditions of the separation process.

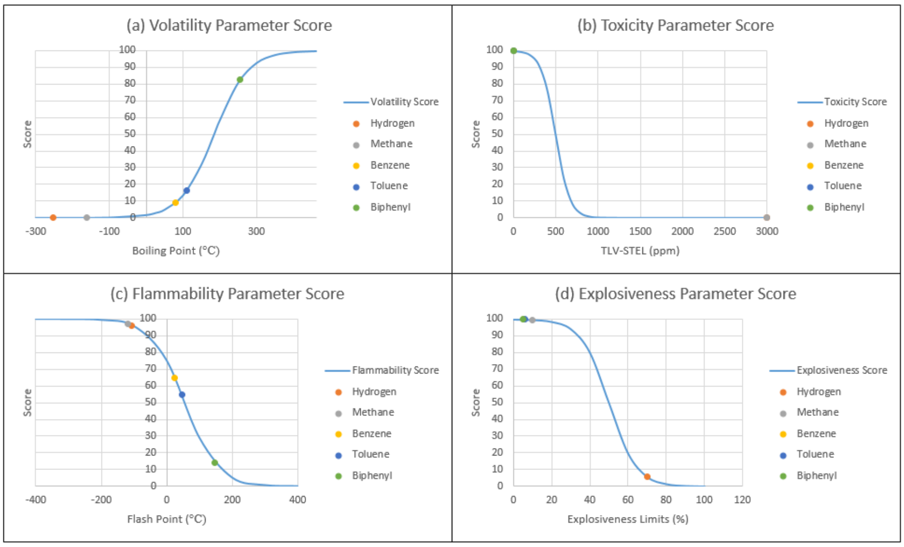

Figure 2: Graphical Representation of Assessment Results according to Parameters

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