Safety Assessment Curve (SAC) for Inherent Safety Assessment in Petrochemical Industry

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Numerical Descriptive Inherent Safety Technique (NuDIST) for inherent safety assessment in petrochemical industry

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ABSTRACT

This paper discusses the development of a new approach of inherent safety assessments called the Numerical Descriptive Inherent Safety Technique (NuDIST). Most current methods for assessing inherent safety use an index-based method. Among the disadvantages of such methods are the use of scaling in which hazards are divided into physical or chemical properties with subjective ranges and discontinuity at the sub-range boundaries. This new technique uses numerical assessment methods, can overcome the limitations inherent in the index-based methods and provides insights into the effect of safety parameters, i.e. temperature, pressure, heat of reaction, process inventory, flammability, explosiveness, toxicity and reactivity for the petrochemical industry. The results of the assessment can be used to easily identify the safest route among several alternatives for chemical synthesis or process retrofitting in addition to, highlighting potential sources of hazards. The proposed technique was tested using the methyl methacrylate manufacturing process. This test highlights the superiority of the Numerical Descriptive Inherent Safety Technique (NuDIST) over index-based methods. The results show that among the six routes of the MMA manufacturing process, the tertiary butyl alcohol (TBA) based route has the lowest total score and is considered the safest route, whereas the ethylene via propionaldehyde (C2/PA) based route has the highest score.

Keywords: Safety assessment; Numerical method; Inherent safety; Petrochemical industry; Process screening; Subjective Scaling

1. Introduction

Errors by operators and equipment failures are recognised as major causes of accidents in all industries. Many strategies have been introduced to reduce or minimise their consequences. However, it is difficult for operators to continuously maintain an error-free performance, throughout their work-lifetime. Thus, plants should be built so that they are user-friendly and able to endure deviations from ideal performance by operators and equipment failures without serious impacts on safety, output or efficiency (Kletz and Amyotte, 2010). Plants should be ideally designed so that none or only small amounts of hazardous materials leaks out. Another approach is to use the hazardous materials at lower operating conditions to prevent hazard conflagrations. This results in inherently safer plants. Although hazard reduction plays a major role in designing a user-friendly plant, it is important to understand the potential process hazards. Identification and understanding of process hazards are critical tasks, and they should be addressed before investigating hazards avoidance and risk reduction (Kletz and Amyotte, 2010). Understanding hazards can be done through hazards assessment, which includes cause and effect studies.

Therefore, the main focus of this study is to develop a new inherent safety assessment techniques that will contribute to understanding the hazards of chemical processes. In the next chapter, a brief introduction to the current inherent safety assessment methods is given. This is

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followed by detailed descriptions of the development and validation of the new method. Lastly, a case study of methyl methacrylate (MMA) manufacturing routes is used to test the new method.

2. Existing methods for inherent safety assessment

As mentioned previously, plants should be built so that they are user-friendly and able to prevent accidents from happens. Process safety evaluation during the very early design stage will assist in selecting the safer process route among several alternatives. The route with less hazardous chemicals and operating conditions obviously will result in inherently safer and user-friendly plant. Most current safety assessment methods for evaluation of process design stage are mostly index-based method such as the PIIS (Edwards and Lawrence, 1993), ISI (Heikkila, 1999), SHE Method (Koller et al., 2000), i-Safe (Palaniappan et al., 2002a, b) and also Inherent Chemical Process Properties Data (Hassim and Ali, 2009). The first inherent safety index, developed by Edwards and Lawrence is the Prototype Index for Inherent Safety (PIIS) (Edwards and Lawrence, 1993; Lawrence, 1996) considers seven parameters of a process: temperature, pressure, inventory, yield, toxicity, explosiveness and flammability. Each parameter is divided into ten sub-ranges. These ten sub-ranges are then scored on a numerical scale. In the PIIS, the route with highest numerical score is considered the least safe route.

Other than the PIIS, another method that also evaluates inherent safety is the Inherent Safety Index (ISI) by Heikkila (1999). The ISI consists of two indices, a chemical inherent safety index and a process inherent safety index. The chemical inherent safety index is further divided into two groups which are sub-index for reaction hazards and sub-index for hazardous substances. The process inherent safety index also consists of two sub-indices, one for process conditions and the other for the process system. The scores for some of the parameters involved in this method are assigned numerical values based on existing indices such as the Mond Index (Tyler, 1985) for toxic exposure and the Dow Fire and Explosion Index (Dow F&EI) (Dow Chemical Company, 1987) for the pressure parameter. The calculations of the ISI are made on the basis of a worst case situation and like the PIIS, a low index value represents an inherently safer process.

Other than the methods that only focus on safety, the SHE method (Koller et al., 2000) compares the various safety, health and environmental performances of each process route. The safety parameters include mobility, fire and explosion, acute toxicity, reaction and decomposition (focusing on the probability for undesired reaction or decomposition) and reaction and decomposition (evaluating the probable energy potential). Irritation and chronic toxicity are evaluated under the health aspect. Five parameters are included for the environmental aspect: water-mediated effects, degradation, air-mediated effects, solid waste and accumulation. The assessment is completed with the calculation of each index value for each parameter with the relevant fate index, resulting in the Effective Dangerous Property ($EDP_{i,j}$). In estimating the magnitude of SHE effects, the $EDP_{i,j}$ is converted to an exponential scale and multiplied with the relevant mass, m_{ij}, to obtain the Potential of Danger ($PoD_{i,j}$). The $PoD_{i,j}$ can be totalled for all chemicals present in the process, resulting in a total potential of danger of the process for each of the SHE parameters.

In a method proposed by Palaniappan et al. (2002a, b), the i-Safe method (Palaniappan et al., 2002a, b), alternative process routes are compared based on their inherent safety level through the Overall Safety Index (OSI) value. The OSI is the sum of the Overall Chemical Index (OCI) and the Overall Reaction Index (ORI). The OCI consists of four parameters: flammability, toxicity, explosiveness and the National Fire Protection Association (NFPA) reactivity rating. The ORI also consists of four parameters: temperature, pressure, yield and heat of reaction. As for processes with only one main reaction, the Total Chemical Index (TCI) is calculated as the sum of the parameters in the Individual Chemical Index (ICI).

Other than the SHE methods, Hassim and Ali (2009) also introduced a method for evaluating safety, health and environmental aspects called the Inherent Chemical Process Properties Data. This method evaluates safety, health and environmental problems through the use of the Inherent Safety Index (ISI) for the safety assessment, the Inherent Occupational Health Index (IOHI) for health hazards and the Environmental Hazard Index (EHI) for the environmental aspect. Multi-criteria decision making is performed by using the Simple Additive Weighting (SAW) method. A lower total score indicates better safety, health and environmental properties for a process. The application of this method is flexible as this method enables users to choose a more benign route either by individual criteria assessments (e.g., safety only) or an integration of all three aspects (safety, health and environmental). Users can also create a custom assessment of their plant, for example, by prioritising safety over the other two factors through assigning greater weight to the safety assessment (Hassim and Ali, 2009).

An index-based method is simple to use because it limits the set of effects of a process by using subjective scaling and subjective weighing in scoring sub-indices (Nhan, 2006). However, index-based methods experiences many shortcomings as highlighted by Srinivasan and Nhan (2008). One shortcoming is scaling in which the physical or chemical properties are divided into subjective ranges with each range assigned subjective scores potentially biased by human judgement. For example, in the method used by Lawrence (1996), the properties are divided into ten equal sub-ranges implying that all chemical or physical values in each particular sub-range possess the same hazard level, which may not be true. Another shortcoming from subjective scaling is the discontinuity at the sub-range boundaries (Gupta and Edwards, 2003). Usually the difference between the lower boundary of a sub-range and the upper boundary of another sub-range is only one value away. Because a score is assigned to each sub-range, a process in which one value is higher than another process may be interpreted as possessing a higher hazard rating when both processes may have similar hazard levels.

Inherent Benign-ness Index (IBI) (Srinivasan and Nhan, 2008) and the Hierarchical Fuzzy Model for the evaluation of inherent safety (Gentile, 2004) are two examples of inherent safety assessment methods that eliminates the shortcomings of index-based method including the subjective scaling in their methods. The Inherent Benign-ness Index (IBI) (Srinivasan and Nhan, 2008) compares the various safety, health and environmental performances of each process route. Fifteen safety, health and environmental parameters are considered in this method: for safety, reactivity, explosiveness, flammability, heat of reaction, pressure, process yield and temperature; for health the Human Toxicity Potential by Ingestion (HTPI), the Terrestrial Toxicity Potential (TTP) and the Human Toxicity Potential by Inhalation or the Dermal Exposure (HTPE); and for environmental, the Aquatic

Toxicity Potential (ATP), the Acidification Potential (AP), the Global Warming Potential (GWP), the Ozone Depletion Potential (ODP) and the Photochemical Oxidation Potential (PCOP). All fifteen parameters are normalised from 0 to 1 so that the scores can be totalled to determine the Cumulative Index for each route. A less benign route is represented by a larger index.

Besides the IBI method, another method that eliminates the shortcoming of subjective scaling in its inherent safety evaluation is produced by Gentile (2004). Gentile (2004) produced a hierarchical fuzzy model for inherent safety evaluation. In this method, each parameter is represented by a linguistic variable. The linguistic variable range is divided into fuzzy sets. Fuzzy modelling is able to interpret numerical and linguistic information in a mathematical approach. Besides, fuzzy logic can deal with high uncertainty associated with process safety. According to Gentile (2004), fuzzy logic is easy to understand and it is expected that non safety-specialised design engineers are able to identify potential hazards in the design stage. Hazards evaluation is based on a scale of [0 1]. Absolute absence of hazard is indicated by 0 while 1 indicates extreme hazard. This method covers three main aspects which are fire and explosions, human and environmental toxicity, and design hazards.

Table 1 – Summary of the pros and cons of different available inherent safety assessment methods reviewed.

Year	Method	Author(s)	Advantage	Disadvantage
1993	Prototype Index for Inherent Safety (PIIS)	Edwards and Lawrence	Easy to execute assessment.	Subjective scaling scoring method.
1999	Inherent Safety Index (ISI)	Heikkila	Easy to execute assessment.	Subjective scaling scoring method.
2000	SHE method	Koller et al.	Easy to execute assessment.	Subjective scaling scoring method.
2002	i-Safe method	Palaniappan et al.	Easy to execute assessment.	Subjective scaling scoring method.
2003	Simple Graphical Method	Gupta and Edwards	Eliminates subjective scaling. Use graphical representation instead of scoring scales.	Only focus on flammability, explosiveness as well as toxicity parameters.
2004	Hierarchical Fuzzy Model for the evaluation of inherent safety	Gentile	Eliminates subjective scaling. Enables interpretation of numerical and linguistic information in a mathematical approach.	Complex development method.
2006	Integrated Risk Estimation Tool (iRET)	Mohd Shariff et al.	Eliminates subjective scaling. Incorporation of process design simulator is helpful in designing inherently safer design process.	However, it is not suitable to be used in assessing inherent safety during research and design stage due to limited amount of data available.
2008	Inherent Benign-ness Index (IBI)	Srinivasan and Nhan	Eliminates subjective scaling. Incorporation of Principal Component Analysis (PCA) for a hollistic inherent safety assessment.	Complex development method.
2009	Inherent Chemical Process Properties Data	Hassim and Ali	Easy to execute assessment.	Subjective scaling scoring method.
2009	Process Route Index (PRI)	Leong and Mohd Shariff	Eliminates subjective scaling. Consider the influence of process temperature and pressure on explosiveness. Incorporation of process design simulator is helpful in designing inherently safer design process.	Less suitable in assessing inherent safety during research and design stage due to limited amount of data available.
2010	Toxic Release Consequence Analysis Tool (TORCAT)	Mohd Shariff and Zaini	Eliminates subjective scaling. Incorporation of process design simulator is helpful in designing inherently safer design process.	Focus only on toxicity parameter. Less suitable in assessing inherent safety during research and design stage due to limited amount of data available.
2012	Process Stream Index (PSI)	Mohd Shariff et al.	Eliminates subjective scaling. Focus on safety assessment on the process stream.	Less suitable in assessing inherent safety during research and design stage due to limited amount of data available.
2013	Inherent Fire Consequence Estimation Tool (IFCET)	Mohd Shariff and Abdul Wahab	Eliminates subjective scaling. Incorporation of process design simulator is helpful in designing inherently safer design process.	Focus only on fire hazard. Less suitable in assessing inherent safety during research and design stage due to limited amount of data available.

In order to eliminate the shortcomings of index-based method, the IBI (Srinivasan and Nhan, 2008) incorporates a multivariate statistical approach known as Principal Component Analysis (PCA) while the Hierarchical Fuzzy Model (Gentile, 2004) incorporates fuzzy logic approach. Although both methods eliminates the shortcoming of index-based method successfully, they have complex construction steps which might be difficult to understand to those who are not familiar with the concept of PCA and fuzzy logic.

In contrast to index based method, Gupta and Edwards (2003) introduced the graphical approach for inherent safety assessment. Graphical approach provides simple evaluation of inherent safety as well as easy to interpret. Parameters evaluated in this method are plotted individually for each step in a process route without any mathematical operation. Gupta and Edwards (2003) only considers five parameters in their method which are temperature, pressure, flammability, explosiveness and toxicity. In such a case that if there are chemicals released in a fire or explosion, it would be chemicals with the highest toxicity hazard that will affect the exposed population the most. Thus, the flammability (F), explosiveness (E) and toxicity (T) value to be plotted is the sum of the highest values for FET in that route. The advantage of this method is one can expand the parameters to be considered for example economic, regulatory, pollution control or health aspects (Gupta and Edwards, 2003). This method proves to be successful in eliminating the shortcoming of subjective scaling. This method was constructed in order to produce a simpler way for inherent safety assessment. Although this method is successful in achieving its aim, the graphical representation of this method is hard to interpret for decision making.

Execution of inherent safety assessment can also be done using process design simulator for example HYSYS software as incorporated by Mohd Shariff et al. (2006) in Integrated Risk Estimation Tool (iRET). Other methods that follows the same execution approach as iRET is Process Route Index (PRI) (Leong and Mohd Shariff, 2009), Toxic Release Consequence Analysis Tool (TORCAT) (Mohd Shariff and Zaini, 2010), Process Stream Index (PSI) (Mohd Shariff et al., 2012) and also Inherent Fire Consequence Estimation Tool (IFCET) (Mohd Shariff and Abdul Wahab, 2013). Incorporation of process design simulator is helpful in designing inherently safer design process. However, it is not suitable to be used in assessing inherent safety during research and design stage due to limited amount of data available. Instead of using a complex execution method, this research proposed an inherent safety assessment method called the Numerical Descriptive Inherent Safety Technique (NuDIST) which incorporates logistic function in its execution which is simpler and suitable to be used during research and development stage. This is the first attempt of using logistic function in hazard score assignments for inherent safety assessment. Previously, logistic function has always been used in other fields of study for example economics and medicine. Incorporation of logistic function in scores assignment also enables the elimination of subjective scaling problem that exists in the index-based method. The NuDIST, a new numerical method for inherent safety assessment in the petrochemical industry, was developed to provide a non-discrete, continuous scoring rubric. This paper will focus on the proposed inherent safety assessment technique from two perspectives: process safety and chemical safety. Table 1 shows the summary of the pros and cons of available inherent safety assessment methods discussed previously.

3. Methodology

3.1. *Development of Numerical Descriptive Inherent Safety Technique (NuDIST) through logistic equations*

The Numerical Descriptive Inherent Safety Technique (NuDIST) is developed through the application of logistic equations. The general equation is shown in Eq. (1) (Larsen and Marx, 2001). In this case, the y variable represents the scores for each parameter value, while the parameter value is represented by the x variable. There are three main constants in the equation, which are C, B and A. C indicates the maximum limit of the scores wherein the y value is always less than or equal to C. This characteristic is suitable for score establishment. For example, if the C value is set to 100, the maximum value for output y is 100. Parameter B is determined by Eq. (2) through the m value. Parameter A is calculated by Eq. (3) through the k value. In developing NuDIST, both the m and k values are obtained from the data gathered from sources mentioned in Table 2.

$$y = \frac{C}{1 + Ae^{-Bx}} \tag{1}$$

$$B = \frac{4m}{C} \tag{2}$$

$$A = e^{Bk} \tag{3}$$

There were two values that is extracted from the data collected. The first value is the mean value while the second

Table 2 – Parameters and the data sources.

Safety assessment	Parameters	Data sources
Chemical safety	Flammability	Lawrence (1996), Weiss (1986), Pohanish (2004), Crowl and Louvar (2002) and Yaws et al. (1997)
	Explosiveness	Lawrence (1996), Weiss (1986), Pohanish (2004), Crowl and Louvar (2002) and Yaws et al. (1997)
	Toxicity	Lawrence (1996), Weiss (1986), Pohanish (2004) and Rosenfeld and Feng (2011)
	Reactivity	Material Safety Data Sheet (MSDS) and National Fire Protection Association (2013)
Process safety	Temperature $T > 25\,^{\circ}C$ $T < 25\,^{\circ}C$	Chauvel and Lefebvre (1989) Hassim and Hurme (2010) Lawrence (1996)
	Pressure	Chauvel and Lefebvre (1989), Hassim and Hurme (2010) and Lawrence (1996)
	Heat of reaction $H_R > 0$ kJ/mol $H_R < 0$ kJ/mol	Chauvel and Lefebvre (1989) Nhan (2006) Green and Perry (2008)
	Process inventory	Chauvel and Lefebvre (1989), Hassim and Hurme (2010) and Lawrence (1996)

Table 3 – Extracted mean and cumulative slope values.

Group	Parameters	Mean value	Cumulative curve slope value
Chemical safety	Flammability	−218.96	55.3
	Explosiveness	8.31	0.0545
	Toxicity	85.73	2.3273
	Reactivity	0	103.2
Process condition safety	Temperature		
	$T > 25\,^{\circ}C$	210.6953	25.309
	$T < 25\,^{\circ}C$	−210.6953	−25.309
	Pressure	24.64	0.0604
	Heat of reaction		
	$H_R > 0$ kJ/mol	200.35	0.2
	$H_R < 0$ kJ/mol	−432.656	4.7091
	Process inventory	85	7.4

value is the slope value obtained from the cumulative curves. These two values will then be applied to the logistic function as k-value and m-value respectively. The steps in constructing cumulative curve are as follows:

(1) Data for every parameter is sorted according to their range. The range size is ten for parameters such as process inventory and explosiveness as their values only varied from 0 to 100 while the range size for the other parameters is 100 as their values have no limits.
(2) After all data have been sorted into their designated range, the number of processes of chemicals in each range is calculated resulting to a single number of frequency for each range.
(3) Cumulative curves for every parameter is developed by plotting the data ranges against the frequency calculated.
(4) The slope values for every cumulative curves is extracted to be used in the development of logistic functions.

Table 3 shows the extracted mean and cumulative curve slope values for every parameter.

Both m and k values gathered from the previous step is applied to the general equation of logistic function. As mentioned previously, the cumulative curve slope value will be used as the m-value while mean value will be used as the k-value in the logistic equation. Application of m and k values to Eqs. (2) and (3) respectively will result to the values of constants B and A which will be then applied to Eq. (1). Logistic equation for every parameter is produced after both B and A values were found. Constant C is taken to be 100 so that the highest score of GRAND evaluation for every parameter is 100. However, when both m and k values in Table 3 were applied to Eqs. (2) and (3) there were no results produced. This might be due to the large value of m which make it difficult for the exponential function in the logistic equation to calculate. Thus, the m value is lowered for every parameter for the curves to be constructed. The m values were lowered with restrictions of minimum and maximum values obtained from the data for every parameter. Table 4 shows the minimum and maximum values obtained from the data for every parameter.

This step was done through trial and error. The main purpose for the construction of NuDIST is to eliminate the shortcoming of subjective scaling. The m value was lowered with assumptions that the logistic equations will produce different scores for different parameter values at least within the minimum and maximum boundaries of parameter values as stated in Table 4. This assumption was made as majority of petrochemical processes reactions and chemical properties will fall within the minimum and maximum boundaries from the data gathered. The final m and k values is tabulated in Table 5. Besides subjective scaling elimination, another advantage of using logistic function is its flexibility. Application of logistic function in this technique enables each equations to be tailored to own preferences for example company's own historical chemical and process data. This can be done by manipulating both m and k values in the equations.

Table 4 – Maximum and minimum values from the data sources in Table 2.

Group	Parameters	Minimum value	Maximum value
Chemical safety	Flammability	−187.8	385
	Explosiveness	0.7	98
	Toxicity	0.006	1250
	Reactivity	0	4
Process condition safety	Temperature		
	$T > 25\,^{\circ}C$	25	850
	$T < 25\,^{\circ}C$		
	Pressure	1	641.5
	Heat of reaction		
	$H_R > 0$ kJ/mol	12	750
	$H_R < 0$ kJ/mol	−2320	−15
	Process inventory	50	100

Table 5 – Final *k* and *m* value used in logistic functions.

Group	Parameters	*k* value	*m* value
Chemical safety	Flammability	55.386	0.005
	Explosiveness	50	0.0345
	Toxicity	500	0.003
	Reactivity	2	0.7
Process condition safety	Temperature		
	$T > 25\,^{\circ}C$	500	0.003
	$T < 25\,^{\circ}C$	−500	0.003
	Pressure	25	0.05
	Heat of reaction		
	$H_R > 0$ kJ/mol	400	0.004
	$H_R < 0$ kJ/mol	−1000	−0.0015
	Process Inventory	60	0.03

3.2. *Process and chemical safety assessment*

NuDIST consists of two parts: process safety and chemical safety. There are four parameters considered for chemical safety assessment: flammability, explosiveness, toxicity and reactivity; and four parameters for process safety: temperature, pressure, heat of reaction and process inventory. The assessment scores for all parameters were produced through the application of logistic equations as shown in Eq. (1) by adjusting the *k* and *m* values in Eqs. (2) and (3).

3.2.1. *Chemical safety parameter*

3.2.1.1. *Flammability parameter.* Flammability can be defined as how easily a material burns in air (Heikkila, 1999; King and Hirst, 1998). In this method, flammability is measured according to the flash point of a liquid. The flash point of a liquid is defined as the lowest temperature at which the liquid emits enough vapour to form an ignitable mixture with air (Crowl and Louvar, 2002). The flammability of liquids depends on the lower flammability limit of the material and its vapour pressure for most temperatures (Heikkila, 1999). Thus, liquids with lower flash points present greater hazard risks compared with liquids with higher flash points.

After applying both values of *m* and *k* from Table 5 into Eqs. (1)–(3), the logistic equation for flammability parameter is produced as Eq. (4). However, a small alteration must be made to the equation to indicate that a lower flash point contributes to higher hazard. The equation is subtracted from 1 before being multiplied by coefficient C, as shown in Eq. (5). With this alteration, a lower flash point value will result in higher score, which indicates a higher hazard.

$$S_{FL} = 100 \times \left(\frac{1}{1 + 3.77e^{-0.024x}}\right) \tag{4}$$

$$S_{FL} = 100 \times \left(1 - \left(\frac{1}{1 + 3.77e^{-0.024x}}\right)\right) \tag{5}$$

3.2.1.2. *Explosiveness parameter.* Explosiveness or the tendency for chemicals to form an explosive mixture in air depends on the range between explosion limits (Heikkila, 1999; Crowl and Louvar, 2002). Under the Lower Explosion Limit (LEL), the mixture is too lean to burn; above the Upper Explosion Limit (UEL), the mixture is too rich for combustion (Crowl and Louvar, 2002). Thus, a wider range between the LEL and UEL indicates a greater tendency for explosion.

Because both the UEL and LEL is expressed in percent by volume (vol%), the 50% range between UEL and LEL is a mid-score indicating neither a safe nor a hazardous condition. Thus, the *k* value for the explosiveness parameter is 50, as shown in Table 5. By applying values from Table 5 to Eqs. (1)–(3), the logistic equation in Eq. (6) is produced.

$$S_{EXP} = 100 \times \left(\frac{1}{1 + 1096.63e^{-0.14x}}\right) \tag{6}$$

3.2.1.3. *Toxicity parameter.* According to Crowl and Louvar (2002), toxicity is a property of the agent describing its effect on biological organisms. One indicator that can be used in determining the toxicity of a chemical is the threshold limit values (TLVs), established by the American Conference of Governmental Industrial Hygienists (ACGIH). In this method, the threshold limit values for short-term exposure limit (TLV-STEL) is used, which is more applicable for acute toxicity type events. The TLV-STEL is the maximum concentration to which workers can be exposed for a continuous period up to 15 min without suffering intolerable irritation, chronic or irreversible tissue change, narcosis of sufficient degree to increase accident proneness, impaired self-rescue or materially reduce worker efficiency, provided that no more than four excursions per day are permitted, with at least 60 min between exposure periods, and provided that the daily TLV-TWA is not exceeded (Crowl and Louvar, 2002). A lower TLV-STEL value for a chemical indicates a larger toxicity hazard compared to chemical with higher TLV-STEL values.

The Threshold Limit Value (TLV) is not intended to designate "safe" and "unsafe" levels. Thus, this method is simply made so that a 0 ppm concentration will result in the highest score of 100. By this method, higher scores represent greater hazards posed by the chemicals. If chemicals with lower TLV-STEL values are more hazardous than chemicals with higher TLV-STEL values, the equation is subtracted from 1 before multiplication by 100, yielding Eq. (7).

$$S_{TOX} = 100 \times \left(1 - \left(\frac{1}{1 + 403.4288e^{-0.012x}}\right)\right) \tag{7}$$

3.2.1.4. *Reactivity parameter.* In this method, the NFPA reactivity rating is used to measure reactivity. The NFPA rating is readily available from the chemical Material Safety Data Sheet (MSDS). The hazard rating index for reactivity is summarised in Table 6.

To establish the logistic function for the reactivity parameter, an NFPA rating of 2 is assumed as the mid-score, or the

Table 6 – Hazard rating index: reactivity ("NFPA Hazard Rating System, 2013").

Rating	Indication	Explanation
0	Stable	Not reactive when mixed with water.
1	Caution	May react if heated or mixed with water but not violently.
2	Warning	Unstable or may react violently if mixed with water.
3	Danger	May be explosive if shocked and, heated under confinement or mixed with water.
4	Danger	Material that is capable of detonation or explosive decomposition or explosive reaction at normal temperature and pressures. This degree should include materials which are sensitive to mechanical or localised thermal shock at normal temperatures and pressures.

k value, due to its indication as a medium level hazard. The *m* value for the reactivity parameter is taken as 0.7 so that the score values ranges from 0 to 100 for an NFPA rating of 0–4. The logistic equation for the reactivity parameter is as shown in Eq. (8).

$$S_{R} = 100 \times \left(\frac{1}{1 + 270.43e^{-2.8x}}\right) \quad (8)$$

3.2.2. *Process safety parameter*

3.2.2.1. *Temperature parameter.* Temperature is a direct measure of the heat energy available for release (Srinivasan and Nhan, 2008). A higher operating temperature is inherently unsafe. The use of high temperatures implies that the plant is under thermal stress (Heikkila, 1999). Thus, a process with a higher operating temperature is more hazardous compared with a process with a lower operating temperature.

The logistic equation for the temperature parameter is constructed from 233 petrochemical process data (Chauvel and Lefebvre, 1989). Two equations were developed for operating temperatures greater than 25 °C and lower than 25 °C. The *m* value for both operating temperatures is obtained by constructing a cumulative curve, as shown in Table 5. After both values of *m* and *k* have been determined, the values are applied to Eqs. (1)–(3) which results in Eqs. (9) and (10) for operating temperatures higher and lower than 25 °C, respectively.

$$S_{T>25\,^{\circ}C} = 100 \times \left(\frac{1}{1 + 403.43e^{-0.012x}}\right) \quad (9)$$

$$S_{T<25\,^{\circ}C} = 100 \times \left(1 - \left(\frac{1}{1 + 0.0025e^{-0.012x}}\right)\right) \quad (10)$$

3.2.2.2. *Pressure parameter.* High pressure usage greatly increases the amount of energy available in the plant (Heikkila, 1999). The combination of high pressures and high temperatures or aggressive materials poses serious issues in the construction materials. Chemical leakages can also occur due to high operating pressures (Srinivasan and Nhan, 2008). Thus, a process with a higher operating pressure is more hazardous compared with a process with a lower operating pressure. Eq. (11) shows the logistic equation for the pressure parameter.

$$S_{P} = 100 \times \left(\frac{1}{1 + 148.41e^{-0.2x}}\right) \quad (11)$$

3.2.2.3. *Heat of reaction parameter.* High reaction enthalpy is a chemical property that increases the explosion potential (Heikkila, 1999). A positive heat of reaction value indicates an endothermic reaction, while a negative heat of reaction value indicates an exothermic reaction. Thus, there are two logistic equations for the heat of reaction parameter: below 0 kJ/mol representing exothermic reactions and over 0 kJ/mol representing endothermic reactions. The heat of reaction is calculated by taking the difference between the heat of formations of the reactants and products (Heikkila, 1999; Felder and Rousseau, 2000). Srinivasan and Nhan (2008) state that when a large quantity of heat is released or absorbed in a reaction, the reaction is potentially hazardous. Thus, in this method the score is higher when the heat of reaction value moves from zero.

The *k* values in the logistic equation for the heat of reaction parameter for both conditions are represented by values in Table 5. Eqs. (12) and (13) show the logistic equations produced for both cases of the heat of reaction parameters.

$$S_{HR>0\,kJ/mol} = 100 \times \left(\frac{1}{1 + 601.85e^{-0.016x}}\right) \quad (12)$$

$$S_{HR<0\,kJ/mol} = 100 \times \left(\frac{1}{1 + 403.43e^{0.006x}}\right) \quad (13)$$

3.2.2.4. *Process inventory parameter.* A low inventory reduces potential accident severity (Heikkila, 1999). However, during design stages it is difficult to determine the exact inventory amount required for each chemical used in the process. Thus, to obtain an estimation of the chemical inventory required for plant operation, the reaction yield is used to predict the inventory parameter (Srinivasan and Nhan, 2008). According to Felder and Rousseau (2000), the yield can be defined as the amount of desired product formed if there were no side reactions involved and the limiting reactant had completely reacted. Yield is usually measured according to the percentage yield (% yield). A high percentage yield indicates a higher amount of desired product formed indicating less amount of raw material inventory is needed.

For the process inventory parameter, after applying both values of *m* and *k* from Table 5 to Eqs. (1)–(3), and subtracting the equation from 1 before multiplication by coefficient C, the logistic equation for the process inventory parameter is produced as Eq. (14). A lower percentage yield indicates a greater hazard risk.

$$S_{PI} = 100 \times \left(1 - \left(\frac{1}{1 + 1339.43e^{-0.12x}}\right)\right) \quad (14)$$

3.2.3. *NuDIST Total Score*

The NuDIST Total Score is calculated for each route evaluated in the process. This suggests that each route that is evaluated using this method has an individual total score that includes both the total scores of the chemical safety parameters and the process safety parameters. The individual total score for each route is important for process ranking purposes so that users may determine which route is safest. This approach is also applied in other methods, for example, the PIIS method (Edwards and Lawrence, 1993), the ISI method (Heikkila, 1999), the IBI method (Srinivasan and Nhan, 2008), the SHE method (Koller et al., 2000) and the Inherent Chemical Process Properties Data (Hassim and Ali, 2009). A lower NuDIST Total Score value indicates a less hazardous route compared with a route with a higher NuDIST Total Score value. The total scores for

Table 7 – Chemical safety assessment results for MMA manufacturing process routes.

Symbol	Route	FL Score	EXP Score	TOX Score	REAC Score	Chemical Safety Total Score (CSTS)	Ranking
R1	ACH	99	10	100	50	258	3
R2	C2/PA	98	94	100	50	342	6
R3	C2/MP	97	84	99	50	330	4
R4	C3	98	84	100	50	332	5
R5	i-C4	84	6	99	50	240	1
R6	TBA	84	6	99	50	240	1

FL, flammability; EXP, explosiveness; TOX, toxicity; REAC, reactivity.

both chemical safety and process safety will need to be determined before calculating the NuDIST Total Score.

The total score for Chemical Safety is calculated according to Eq. (15). The calculation of the Chemical Safety Total Score (CSTS) is based on the worst case scenario (Edwards and Lawrence, 1993; Heikkila, 1999; Palaniappan et al., 2002a, b; Hassim and Ali, 2009). According to Heikkila (1999), the worst case describes the riskiest possible situation. The score for flammability (S_{FL}), explosiveness (S_{EXP}), toxicity (S_{TOX}) and reactivity (S_R) are summed up and the maximum score received by a chemical is used to represent the reaction step for that particular routes.

$$CSTS = (S_{FL})_{max} + (S_{EXP})_{max} + (S_{TOX})_{max} + (S_R)_{max} \quad (15)$$

In calculating the Process Safety Total Score (PSTS), the scores for temperature (S_T), pressure (S_P), heat of reaction (S_{HR}) and process inventory (S_{PI}) parameters are totalled up as shown in Eq. (16). If there are several reaction steps, the modular scores from all reaction steps in a route are taken into account.

$$PSTS = (S_T)_{max} + (S_P)_{max} + (S_{HR})_{max} + (S_{PI})_{max} \quad (16)$$

After both the Chemical Safety Total Score and the Process Safety Total Score have been determined, the NuDIST Total Score can be calculated by summing up the scores as shown in Eq. (17).

$$\text{NuDIST Total Score} = CSTS + PSTS \quad (17)$$

4. MMA manufacturing process case study

As a case study, the proposed method was applied to six processing routes for methyl methacrylate (MMA) production. The six routes are:

(1) acetone cyanohydrin (ACH) based route
(2) ethylene via propionaldehyde (C2/PA) based route
(3) ethylene via methyl propionate (C2/MP) based route
(4) propylene (C3) based route
(5) tertiary butyl alcohol (TBA) based route
(6) isobutylene (i-C4) based route

4.1. *Chemical safety assessment*

Chemical safety assessments were conducted for all chemicals involved in each of the six routes of the MMA manufacturing process. Table 7 shows NuDIST assessment results for the chemical safety assessments in the MMA manufacturing routes for all four chemical safety parameters: flammability (FL), explosiveness (EXP), toxicity (TOX) and reactivity (REAC).

Table 7 shows that both R5 and R6 have the lowest chemical safety total score (CSTS), 240. A lower score is desired in this technique as lower scores represent lower hazards. Both R5 and R6 have the lowest score compared with the other routes for flammability, explosiveness and toxicity. Chemicals that contributed to both the scores of R5 and R6 are methacrolein, methanol and methacrylic acid for the flammability, explosiveness and toxicity parameters, respectively. In this assessment, because both R5 and R6 were represented by the same chemicals, they have the same CSTS score. The highest score of 342 was obtained by R2 and therefore ranked as the most hazardous route compared with the others. Although R2 had a lower flammability score compared with that of R1, R2 had a higher explosiveness score compared with R1 (94 and 10, respectively). This indicated that R2 is the most hazardous route compared with the other five routes. A high explosiveness score for R2 was due to the presence of hydrogen with an explosiveness value of 70.1% compared with hydrogen cyanide (R1) with an explosiveness value of 34.4%. All routes had the same reactivity score of 50. This shows that all routes consist of chemicals with an NFPA reactivity rating of no greater than 2.

4.2. *Process safety assessment*

A process safety assessment involving the temperature (T), pressure (P), heat of reaction (HR) and process inventory (PI) parameters was performed for all six routes of the MMA manufacturing process. Table 8 shows the process safety assessment results for the MMA manufacturing process.

Table 8 shows R6 as the safest route in the process safety assessment, followed by R5, R3, R4, R2 and R1 with scores of 92, 131, 163, 199, 232 and 241, respectively. R6 has the lowest score in all four parameters assessment compared with the other five routes; thus, it was regarded as the safest route. Though R1 has a low score for the pressure and process inventory parameters assessment, it had the highest scores in the temperature and heat of reaction parameters compared with the other routes. The highest operating temperature of R1 is 1200 °C, while the operating temperature in R6 is 350 °C at most. This indicates that R1 is the most hazardous route among the six routes. R3 and R4 have the highest score in the pressure parameter assessment with operating pressures of 100 atm compared with the other routes. However, both R3 and R4 have low scores for the other three parameter assessments and are ranked third and fourth, respectively.

Table 8 – Process safety assessment results for MMA manufacturing process routes.

Symbol	Route	T Score	P Score	HR Score	PI Score	Process Safety Total Score (PSTS)	Ranking
R1	ACH	100	3	100	38	241	6
R2	C2/PA	11	99	66	57	232	5
R3	C2/MP	34	100	20	9	163	3
R4	C3	11	100	66	22	199	4
R5	i-C4	17	3	21	90	131	2
R6	TBA	11	3	21	57	92	1

T, temperature; P, pressure; HR, heat of reaction; PI, process inventory.

4.3. *NuDIST Total Score*

For the NuDIST Total Score, both the Chemical Safety Total Score and the Process Safety Total Score were added together and the results are shown in Table 9. Among the six routes, R6 was the safest route with the lowest NuDIST Total Score of 332, while R2 was the most hazardous route with the highest NuDIST Total Score of 574. This was supported by both the CSTS and PSTS scores which are also presented in Table 9. R6 has the lowest scores for both CSTS and PSTS, while R2 has the highest scores for both CSTS and PSTS.

4.4. *Results comparison with other methods*

The assessment results for the MMA manufacturing process of NuDIST were compared with the assessment results of the PIIS method (Edwards and Lawrence, 1993; Lawrence, 1996) and Inherent Benign-ness Index (IBI) (Srinivasan and Nhan, 2008). These methods were chosen due to the similarity in the assessed parameters and the common assumption of the worst case scenario. The worst case scenario is the riskiest situation that can occur (Heikkila, 1999) and is usually applied in inherent safety assessment methods by taking the maximum score received by a chemical substance or a step reaction to represent the overall process route. Table 10 shows the assessment results of MMA manufacturing process routes by NuDIST, the PIIS, the Inherent Chemical Process Properties Data and the IBI methods. In Table 10, the safest route is indicated with the number 1 while the most hazardous route is indicated with the number 6.

As shown in Table 10, both the NuDIST and the PIIS methods agree that the TBA-based route is the safest route among the six routes followed by i-C4-based route. The PIIS method assessment identified the ACH-based route as the most hazardous route while the NuDIST evaluation indicated the C2/PA-based route as the most hazardous. This difference is because of the assumptions used in the summation of all scores to produce each total route. In the PIIS method, all scores are added together for each reaction step. Then, scores for every reaction steps in the process route are totalled for the final score. Instead of considering the hazards according to the evaluated parameter, the PIIS method only considers the evaluation according to the number of reaction steps. Thus, a less hazardous route with many reaction steps might result in a higher total score compared to a more hazardous route with fewer reaction steps. In NuDIST, the maximum score for each parameter are totalled up to produce the total index score representing that particular route of assessment. By taking the maximum score for each parameter, the CSTS and PSTS consider at most four hazardous chemicals and four operating conditions in each route as indicated in Eqs. (15) and (16). As an example for chemical safety assessment in a route, step reaction 1 might have chemical with maximum score in explosiveness parameter while step reaction 2 might have chemical with maximum score in toxicity parameter. These chemicals from different step reaction may represent the route for CSTS calculation due to their highest score compared to other chemicals. This is also the same with process safety evaluation. In a route, step reaction 1 might have the highest score for temperature parameter while the next step reaction might have the highest score in another parameter. Instead of considering the total process hazard based on the number of reaction steps in a route, the NuDIST considers the total hazard based on the number of hazardous chemicals and operating conditions in a route regardless of the number of the reaction steps. This ensures that no hazardous chemicals or operating conditions from routes with lesser number of reaction steps are ignored. As an example, C2/PA based route has lesser number of step reaction which is four compared to ACH based route with six step reactions. However, C2/PA based route contains more hazardous chemicals and operating conditions in terms of explosiveness, pressure and process inventory parameters than ACH based route as shown by scores tabulated in Tables 7 and 8. This also indicates that the NuDIST assessment results is unaffected by the number of reaction steps in a route thereby making the assessment more accurate.

Inherent safety evaluation of the MMA manufacturing process routes by the NuDIST and the Inherent Benign-ness Index (IBI) resulted to the same hazard level for TBA and i-C4 based routes as shown in Table 10. Both of these methods agree that the TBA based route is the safest route among the six

Table 9 – Numerical Descriptive Inherent Safety Technique (NuDIST) total score for MMA manufacturing process routes.

Symbol	Route	Chemical Safety Total Score (CSTS)	Process Safety Total Score (PSTS)	NuDIST Total Score
R1	ACH	258	241	499
R2	C2/PA	342	232	574
R3	C2/MP	330	163	493
R4	C3	332	199	531
R5	i-C4	240	131	371
R6	TBA	240	92	332

Table 10 – Comparison between Numerical Descriptive Inherent Safety Technique (NuDIST) and other methods in assessing MMA manufacturing routes.

Symbol	Route	NuDIST method	PIIS method	IBI method
R1	ACH	4	6	6
R2	C2/PA	6	5	4
R3	C2/MP	3	3	5
R4	C3	5	4	3
R5	i-C4	2	2	2
R6	TBA	1	1	1

routes followed by i-C4 based route. Table 10 also indicates that there are differences in the assessment results for the other four routes. The NuDIST method regarded C2/PA based route as the most hazardous route whereas the IBI method assessed ACH as the most hazardous route. Although both IBI and NuDIST methods eliminates the problem of subjective scaling in its assessment, there are several differences in the methods development and the parameters considered which resulted to different assessment results. IBI method uses NFPA rating value not only for reactivity evaluation but also flammability and toxicity while NuDIST method uses NFPA rating for reactivity evaluation and flash point and Threshold Limit Value (TLV) to assess flammability and toxicity. NFPA rates the parameters from 0 to 4 for reactivity, flammability and toxicity hazards, resulting to its own subjective assessment since a lot of chemicals do have the same NFPA rating value for one or more hazards parameter. It is difficult to distinguish which chemical is more hazardous than the other if both chemicals have the same rating value. Numerical Descriptive method provides a solution to this problem by assessing inherent safety using values which are exclusive to every chemicals (because the values are described by the chemical properties) which are flash point and Threshold Limit Value (TLV). As an example, IBI assessed carbon monoxide and methacrylic acid in C2/PA based route with the same toxicity rating value of 3 based on NFPA labelling. Meanwhile the NuDIST assessed both carbon monoxide and methacrylic acid with different toxicity value of 75 ppm and 60 ppm respectively. Based on this example, it is clearly shown that methacrylic acid is less hazardous than carbon monoxide in terms of toxicity and this proves the ability of NuDIST method to eliminate subjective evaluation problem.

5. Conclusion

The NuDIST was proposed in this paper as an alternative to the discrete scoring in index-based methods. A numerical scoring method assesses the score value for the evaluated parameter in a continuous range (compared with discretised values). This method uses logistic equations to evaluate parameters on continuum range, based on the worst case scenario, and can be applied to the assessment of safety parameters in the petrochemical industry. There are eight parameters involved in this technique. The first four parameters are flammability, explosiveness, toxicity and reactivity, and are grouped together as chemical safety parameters. The other four parameters are temperature, pressure, heat of reaction and process inventory and are grouped as process safety parameters. The parameters are evaluated under their respective groups before added together to yield the NuDIST Total Score. The calculation of the NuDIST Total Score is based on the worst case situation, which describes the riskiest possible situation. A lower value of the NuDIST Total Score indicates a less hazardous situation.

The application of the proposed method on six routes of the methyl methacrylate (MMA) manufacturing processes shows that C2/MP has the highest NuDIST Total Score, which indicates that the C2/MP route is the most hazardous route. Assessment methods using equations with simple scoring indicators and assuming the worst case scenario enables users to identify the most hazardous route, reaction step and chemical. In future works, these safety assessments will be integrated with the health and environmental assessments to provide a more comprehensive assessment for the petrochemical industry.

Although the NuDIST also gives some kind of index based results, this technique is unique due to the application of logistic function in score assignments for its inherent safety evaluations. Instead of using inherent safety assessment technique with complex multivariate statistical analysis NuDIST provides a simpler technique of eliminating the shortcoming of subjective scaling. Besides, this technique also provides the flexibility that is difficult to achieve with other methods by taking into account company's own historical chemical and process data.

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