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Toxic release consequence analysis tool (TORCAT) for inherently safer design plant

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ABSTRACT

Many major accidents due to toxic release in the past have caused many fatalities such as the tragedy of MIC release in Bhopal, India (1984). One of the approaches is to use inherently safer design technique that utilizes inherent safety principle to eliminate or minimize accidents rather than to control the hazard. This technique is best implemented in preliminary design stage where the consequence of toxic release can be evaluated and necessary design improvements can be implemented to eliminate or minimize the accidents to as low as reasonably practicable (ALARP) without resorting to costly protective system. However, currently there is no commercial tool available that has such capability. This paper reports on the preliminary findings on the development of a prototype tool for consequence analysis and design improvement via inherent safety principle by utilizing an integrated process design simulator with toxic release consequence analysis model. The consequence analysis based on the worst-case scenarios during process flowsheeting stage were conducted as case studies. The preliminary finding shows that toxic release consequences analysis tool (TORCAT) has capability to eliminate or minimize the potential toxic release accidents by adopting the inherent safety principle early in preliminary design stage.

1. Introduction

The application of inherent safety principle in process plant is a proactive approaches to minimize or eliminate potential accidents with a cost effective manner to as low as reasonably practicable (ALARP) [1]. Motivation on inherent safety application in process industries has been increased especially after many major accidents in the process plants. Some examples of toxic released accidents are at Seveso, Italy in 1976, in which over 250 reported cases of chloracne and the horrendous loss of thousand of life at Bhopal, India in 1984 and many more thereafter [2].

The conventional approaches in identifying hazard and assessing safety of process plant are performed at the later stages of process design when the operating conditions, vessel sizing and layout of major equipment have been determined. The hazard identification can be done using process hazard analysis tool such as HAZOP, What If and FMEA, whereby safety assessment can be performed by commercial safety softwares such as SAFETI, PHAST, FRED and SCOPE. The outcome of the assessment provides consequence and risk of the design. If the result is not acceptable, improvement can be done to reduce the consequence or risk. At this stage, only impact reduction strategies can be best implemented normally by the application of passive, active and procedural techniques. The application has proven to significantly improve the safety of the process plant. However, these additional protections could be expensive to install and maintain throughout the life of the process plant [3]. The outcome of this late safety analysis and design improvement even though is very important could prompt additional cost on extrinsic safety features.

A better technique is using inherent safety concept to reduce or eliminate the root causes of the hazards by modifying the process design such as raw materials, unit operations and operating conditions. The principles defining inherent safety as shown in Table 1 were formalized by Kletz [4]. These principles aim to reduce or eliminate hazards by modifying the design (using different chemicals, hardware, controls and operating conditions) of the plants itself. Plants that apply inherently safer design concepts are believed to be simpler in design, easier, more friendly to operate and more tolerant of errors [5]. However, a study by Mansfield et al. [6] stated that the lack of experience and understanding (field and "real world plant") of the design engineers who are applying these principles and the lack of documented methodology to review the agreement of different process alternatives according to the inherent safety principles are the critical problems to the implementation of this safety philosophy. They experienced that although many design engineers know the basic

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Table 1
General principle of inherent safety (Kletz [4]).

Principle	Definition
Minimize	Use smaller quantities of hazardous substances (also called intensification)
Substitute	Replace a material with a less hazardous substance
Moderate	Use less hazardous conditions, a less hazardous form of a material, or facilities that minimize the impact of a release of hazardous material or energy (also called attenuation and limitation)
Simplify	Design facilities which eliminate unnecessary complexity and make operating errors less likely, and which are forgiving of errors that are made (also called error tolerance)

principles of inherent safety, they are not always clear about how to apply them. There is also a general lack of familiarity with the specific advantages of adopting an inherently safer approach to process design. On the other hand, the aim to reduce the hazard/risk of a process is by adding protective barriers to mitigate impact as a conventional safety approach. Rushton et al. [7] highlighted the need for a computer aid that will perform comprehensive inherent safety analysis at each key decision point in the process life. The key benefits of automation are substantial reduction in time and effort, enhanced decision-making, improved documentation and better understanding of the process. Moore et al. [8] also stated that there is a need for more guidance especially in practical step-wise approaches to conduct inherently safer studies. The other reasons for lack of implementation of inherent safety in actual designs are summarized by Kletz [4] and shown in Fig. 1.

Purpose of inherent safety can lead to improve safety and lower capital and operating costs [9–11]. Khan and Amyotte [12] replicated similar findings in their works, which stated that considering the lifetime costs of a process and its operation, an inherently safer approach is a cost-optimal option. This is further validated by their work showing that inherent safety can be integrated at any stage of design and operation. However, its application at the earliest possible phase of process design gives in the best result (i.e., process selection and conceptual design). In term of cost, any re-design done after the detailed design of the process life cycle would be very expensive compared to alteration in the early stage i.e. during conceptual design stage [13]. Overton and King of Dow Chemical Company [14] prove several examples on the application of inherently safer design concept that result in lower capital cost and produced lower operating costs, greater reliability and faster start times for a new and existing plant. Referring to Crawley [15] and Warwick [16], the largest recompenses are attained by applying the inherent safety principle early in the process and engineering design stages. Inherently safer options are also economically and technically practicable for operation stage of the plant life cycle [17].

Various safety research groups have developed inherent safety tool with different approaches. One of the earlier methods is the inherent safety checklists developed by Bollinger et al. [18] and CCPS [19]. They provide wide-ranging questions related to inherent safety and also endow with guidance to implement inherent safety in process design. In addition, CCPS [20] suggested a set of checklists developed for specific types of process equipment such as heat transfer equipment, mass transfer equipment, etc. and the options are not only for inherent strategies but also for covering passive, active and procedural safety measures. There are also inherent safety-based checklists developed for incident based investigation and process safety management [21,22]. Another potential method is by using inherent safety indices. The pioneering index was proposed by Edwards and Lawrence [10] and Lawrence [23]. They

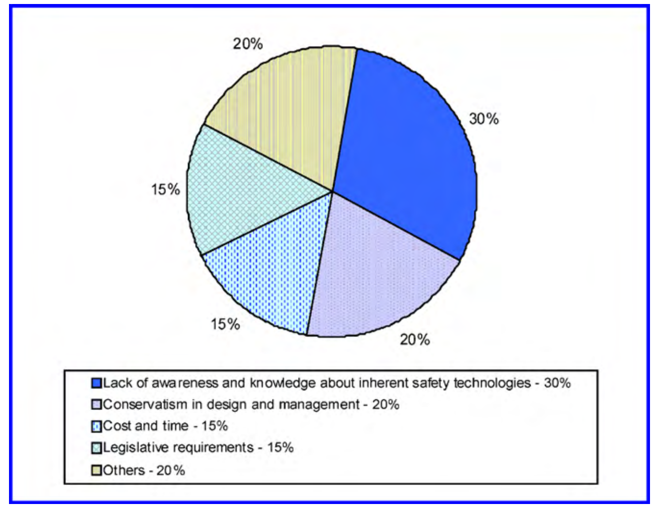


Fig. 1. Problems of implementing inherently safety (Kletz [4]).

were among the earliest researchers to propose the indices that are functions of pressure, temperature, composition, etc. Heikkila [24] improved the methods by including an additional aspect to the index system. The summary of the parameters used by the above researchers is given in Table 2. The parameters were then implemented by Palaniappan et al. [25] to develop an expert system for the application of inherent safety in chemical process design known as i-Safe. They also proposed three additional supplementary indices known as worst chemical index (WCI), worst reaction index (WRI) and total chemical index (TCI) to overcome shortcoming in earlier indices. Gentile et al. [26] have developed the fuzzy-based inherent safety index, which used fuzzy logic system to calculate inherent safety index based on if-then rules. Gupta and Edward [27] developed a graphical method to apply inherent safety index in evaluating six potential routes to produce methyl methacrylate (MMA) in an attempt to graphically show the comparison. Khan and Amyotte [28,29] proposed a new indexing technique which is intended to be applicable throughout the life cycle of process design. The index is known as integrated inherent safety index (I2SI) and has three sub-indices, i.e hazard index (HI), inherent safety potential index (ISPI) and inherent safety cost index (ISCI). The higher the value of I2SI, the more pronounced the inherent safety impact. In 2005, Rahman et al. [30] benchmarked the three pioneering inherent indices which are: Prototype Index of Inherent Safety (PIIS) developed by Edward and Lawrence [10], Inherent Safety Index (ISI) [24,31] and i-Safe [32,33] using the MMA processes and biased against expert opinion. The work summarized that inherent safety evaluation can be made in a reasonable accuracy with the above indices.

Table 2
Inherent safety index parameter (Heikkila [24]).

	Edwards and Lawrence [10]	Heikkila [24]
Inventory	x	x
Temperature	x	x
Pressure	x	x
Heat of main reaction	x	x
Heat of side reaction	–	x
Flammability	x	x
Explosiveness	x	x
Corrosiveness	–	x
Toxicity	x	x
Chemical interaction	–	x
Type of equipment	–	x
Safety of process structure	–	x

The present available indices also require tedious nature of manual data transfer of process information and parameters for inherent safety level calculation. The same issue was addressed by Mohd Shariff et al. [34] in which they have proposed the integrated risk estimation tool (iRET) that links the process design simulator, HYSYS with inherent safety index calculation. They have demonstrated the capability of the tool to extract data from HYSYS efficiently therefore eliminating manual data transfer and decrease data errors. Parallel approach is accepted by Leong and Shariff [46] in the development of Inherent Safety Index Module (ISIM). ISIM is an integrated safety index with HYSYS for simplicity of data transfer between the inherent safety tool based on Microsoft Excel spreadsheet to capitalize its calculation capability and also its ability to communicate with process design simulator, HYSYS via Visual Basic for Application (VBA) language as a prototype computer software tool. From the enhancement of ISIM, a new index known as the process route index (PRI) based on fundamental process parameter that influence the outcome of an explosion incident has been developed and furthermore from this approach, a preliminary inherent risk assessment (IRA) is carried out to evaluate the amount of risk which is inherent to the properties of the chemicals and process condition. IRA follows closely with the commonly used technique of quantitative risk assessment (QRA). Detail explanation of PRI and IRA are given by Leong and Shariff [13,35].

Recently, Tugnoli and Cozzani [36] proposed a new approach to assess inherent safety of process alternatives based on consequence estimation by using key performance indicator. Qualitative assessment for inherently safer design (QAISD) is the latest published work on inherent safety approach by Rusli and Mohd Shariff [5]. QAISD utilized a qualitative approach to assess potential application of inherent safety principles during preliminary design stage. A modified theory of inventive problem solving (TRIZ) [37] hazard review method invented by Altshuller [38] is used in this work to identify inherent hazards, whereby an extended inherent safety heuristic tool is developed based on established inherently safer design principle to create potential inherently safer design options.

Based on the tool developed for inherent safety application during preliminary design stage, iRET [34] shows potential to be further developed to include the consequences other than explosion. A new prototype tool from the evolution of iRET was developed using iCON process design simulator that integrated with toxic release consequence model built in MS-Excel. This new prototype tool known as toxic release consequences analysis tool (TORCAT) was used to assess the consequences of toxic release during the development of process flowsheeting at preliminary design stage. The design improvement can be done by the application of inherent safety principle to eliminate or minimize hazards to ALARP.

2. Framework of TORCAT

Consequence analysis assessment software is commonly used to predict the impact of incidents from identified hazardous cases in process plant. Typically well-known consequence analysis software such as Software for the Assessment of Flammable, Explosive and Toxic Impact (SAFETI) and Process Hazard Analysis Software Tool (PHAST) by Det Norske Veritas (DNV), and Fire, Release, Explosion and Dispersion (FRED) by Shell are used to generate consequence analysis result based on the probit methodology [39].

Chan [40] observed that none of the above mentioned software is connected to a process design simulator. At such the consequences analysis for varying operating conditions could not be done in a fast and efficient manner. In addition, when process plant modifications are required to minimize the consequence, the possibility of repeating a detail consequence analysis assessment would be relatively low due to time and cost constraints. In addition, some of the proposed modifications such as new operating conditions may change consequence levels related to the operations that may cause major revamp of the process plant. It is also a challenge to manually transfer the required data for the proposed modifications from process design simulator to the consequence analysis assessment software in the design stages, as there is no direct link between them. Therefore, study of effects due to changes of process conditions cannot be carried out efficiently. A new framework known as iRET was proposed by Mohd Shariff et al. [34] to overcome these limitations that integrate the process design simulator with consequence analysis assessment software. iRET allows design engineers to immediately analyze consequence levels at different process conditions efficiently since data on process conditions can easily be transferred to and from process design simulator. In addition, iRET provides the avenue to incorporate Inherent Safety features in early design stage that could eliminate or minimize the accidents.

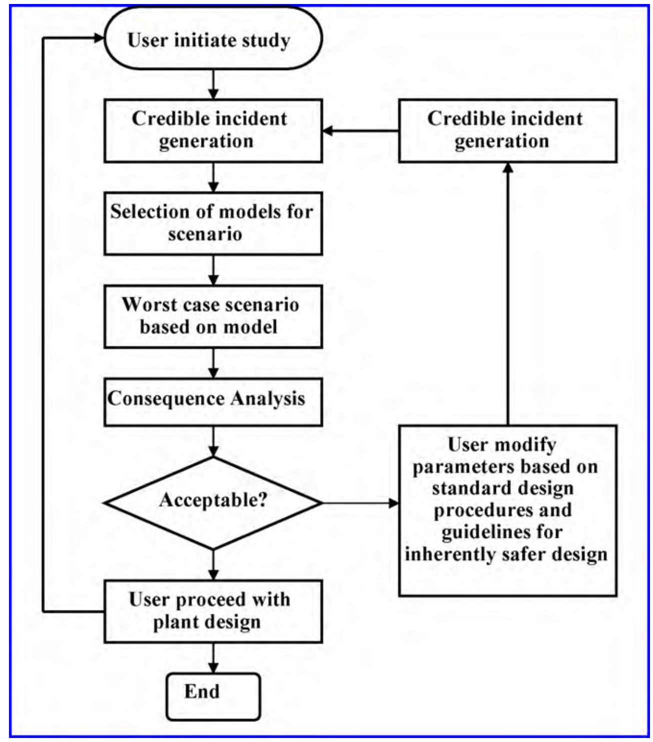


Fig. 2. Generic algorithm for integrated process simulator (Mohd Shariff et al. [34]).

A generic algorithm for iRET is given in Fig. 2. Process design simulator was linked with the consequence model developed in Microsoft Excel through an interface using object, linking and embedded (OLE) automation codes available in Microsoft Excel Visual Basic Application (VBA). Process data are extracted from HYSYS process design simulator for consequence analysis calculation in the model developed in Microsoft Excel. If the result is unacceptable, the improvement can be done by changing the process data based on the guidelines and standard design procedures. The case studies were demonstrated with the emphasis on the application of inherent safety concept to eliminate or improve the consequence due to explosion. It was successfully shown that the consequence due to explosion can be assessed and minimized during the initial design stage ensuring a safer plant. Thus, this paper presents an evolution of iRET dealing with toxic release. The framework for TORCAT is given in Fig. 3. TORCAT is used for consequence analysis of toxic

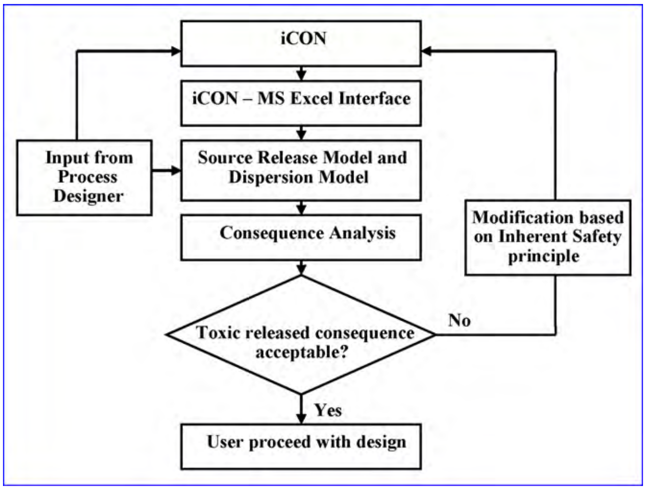


Fig. 3. Framework of TORCAT.

release and process design improvement at preliminary design stage using inherent safety principles.

The preliminary design of the process plant was done in iCON for the development of process flowsheeting based on process requirements. iCON is a new process simulation software developed in-house by PETRONAS for steady-state modeling tool for oil, gas and petrochemical industries. iCON can also be customized to specific plant requirements and the desired plant operation. The toxic release consequence assessment tool was developed in Microsoft Excel, manipulating Excel VBA as the programming code to avoid tedious data entry and transfer. In order to do so, Excel VBA was used to assist in the automation part. Automation, defined in its simplest form, is the ability to drive one application from another. It is desirable to use object linking and embedding (OLE) codes from Excel VBA to link the simulation in iCON for data transfer and analyze in MS-Excel spreadsheet. The assessment tool was designed such that it could generate outputs in the form of concentration level of toxic release and toxic effect from the source of release.

The consequence of the toxic gas release can be evaluated any time during the design stage as required by process designer. Basically the critical data required from iCON for the purpose of consequence analysis in MS-Excel are pressure, temperature, composition and heat capacities. Additional data must be provided by process designer such as duration of release, hole diameter and distance from point of release based on worst-case scenarios. The dispersion of the toxic release was calculated using toxic release consequence model recommended by Center for Chemical Process Safety (CCPS) [9]. The consequence analysis of toxic gas was determined using toxic effect gas model by Det Norske Veritas [41]. Similar models were adopted by many researchers for consequence analysis study such as by Pula et al. [39], Khan and Abbasi [42], and Crowl and Louvar [43]. Toxic effect model provides results of probit value and percent of fatalities. The process designer can make decision to proceed with the design in iCON if the consequence is considered acceptable. If the consequence is not acceptable, modifications can be made utilizing the concept of inherent safety principle. The proposed design modification needs to be simulated in iCON and then follows the same procedure again as proposed in the framework to check the acceptability of the release consequence based on the set criteria.

3. Source and dispersion models

Pipe ruptures are common problem that cause major accidents in process plant. The consequence of pipe rupture can be obtained by the application of source, dispersion and consequence modeling to quantify the release scenario. The first variable calculated by TORCAT is the release of toxic gas (mass/time). This paper reports on the choked-flow rupture from a pipeline as a case study. This scenario contributes to worst-case condition in the case of toxic release leading to choke flow and is common in real process industries [43]. When a rupture occurs, gas can exit as sonic velocity due to the 'choked' condition at exit. Choked flow or critical flow simply means that the gas is moving through the leak at its maximum possible speed, namely the speed of sound in the gas [9]. The pressure for choked or critical flow can be simply expressed [9] as:

$$\frac{P_{\text{choked}}}{P_1} = \left(\frac{2}{k+1}\right)^{k/k-1} \tag{1}$$

where P_1 is the pressure upstream of the hole (force/area); k is gas specific heat ratio (the heat capacity at constant pressure, C_p, divided by the heat capacity at constant volume, C_v).

For gas leaks to atmospheric conditions (P_{choked} = 14.7 psia), if the upstream pressure is greater than 13.1 psig, the flow will be choked and maximized through the leak [9]. If this choked flow condition is met, the gas release rate from the single end of a full-bore pipe rupture can be estimated using the widely recognized gas discharge equation [9,43] and will follow the critical flow relationship [44] which is independent of downstream pressure:

$$m_{\text{choked}} = C_{\text{D}} A P_1 \sqrt{\frac{k g_c M}{R_g T_1}\left(\frac{2}{k+1}\right)^{k+1/k-1}} \tag{2}$$

where C_{D} is the discharge coefficient (dimensionless); A is the area of the hole (length^2); P_1 is the pressure upstream of the hole (force/area); g_c is the gravitational constant (force/mass–acceleration); M is the molecular weight of the gas (mass/mol); k is the heat capacity ratio, C_p/C_v (unitless); R_g is the ideal gas constant (pressure–volume/mol-deg); T_1 is the initial upstream temperature of the gas (deg).

Dispersion model is used to estimate the concentration of toxic release once it is dispersed into the atmosphere. By knowing the amount of material release from the source model, design engineer can use the dispersion model to predict toxic release concentration at selected downwind receptor locations from a source of release. Various types of dispersion models have been developed to represent different types of release scenarios. The most commonly used models are based on continuous (plume) and instantaneous (puff) release Gaussian dispersion. These types of models are commonly used to simulate toxic release from industrial source. These models have undergone significant scientific analysis and rigorous testing using industrial case studies prior to real industrial application for assessing the consequence of toxic release [45].

For the worst-case rupture releases, it is acceptable to assume almost catastrophic of the process resulting in near instantaneous release of the entire process inventory or release over a short period of time [43]. Therefore, instantaneous release (puff) of the substance from a source that moves with the wind while it disperses into the atmosphere is included in TORCAT to evaluate the consequence of toxic gas release. The concentration can be estimated using the following equation [9]:

$$\langle C \rangle (x,y,z,t) = \frac{G^*}{(2\pi)^{2^{3/2}} \sigma_x \sigma_y \sigma_z} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \times \left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \tag{3}$$

where C is the time average concentration (mass/volume); G^* is the total mass of material released (mass); σ_x, σ_y, σ_z are dispersion

Input Data			
Composition		Chlorine	
Total Release	Q^*_m	1.0	kg
Molecular Weight	MW	70.8	
Ambient Temperature	T	298	K
Pressure	P	1	atm
Release Height	H	0	m
Distance Downwind	X	500	m
Distance Off Wind	Y	0	m
Distance Above Ground	Z	0	m

Result			
Stability Class		F	
Assumed wind speed μ:		2	m/s
Dispersion Coefficients:			
Sigma y:	σ_y	5.0	m
Sigma z:	σ_z	2.2	m
Downwind concentration:	C	2.31E-03	kg/m^3
		2310	mg/m^3
PPM:		797.85	ppm

Fig. 4. The data and results extracted from TORCAT dispersion model based on Example 5-2 of Crawl and Louvar [43].

Table 3
Dispersion coefficient $\sigma_x\,\sigma_y\,\sigma_z$ for instantaneous release (CCPS [9]).

Stability class	σ_x or σ_z (m)	σ_z (m)
A	$0.18x^{0.92}$	$0.60x^{0.75}$
B	$0.14x^{0.92}$	$0.53x^{0.73}$
C	$0.10x^{0.92}$	$0.34x^{0.71}$
D	$0.06x^{0.92}$	$0.15x^{0.70}$
E	$0.04x^{0.92}$	$0.10x^{0.65}$
F	$0.02x^{0.89}$	$0.05x^{0.61}$

coefficient in the x, y and z directions (length); x is the downwind direction (length); y is the cross-wind direction (length); z is the distance above the ground (length); H is the release height above the ground (length).

The dispersion coefficient $\sigma_x, \sigma_y, \sigma_z$ for the case of instantaneous can be calculated using the expression shown in Table 3.

4. Toxic release effect model

The toxic release effect model is used to estimate the fatalities due to the exposure to toxic concentration based on the set criteria by the authority. The consequence of the toxic release can be reduced during preliminary design stage by reducing the probit and percent of fatalities using inherent safety principle.

Probit (probability unit) is a term describing the probability of death, given by the following equation [9]:

$$Y = A + B\,\ln(c^n t) \tag{4}$$

where Y is the probit; c is the concentration in ppm by volume; t is the exposure time in minutes; A, B, n are constants depending on the substances.

For spreadsheet calculation, a more effective appearance for performing the conversion from probit to percentage of fatalities is given by [9]:

$$P = 50\left[1 + \frac{Y-5}{|Y-5|}\,erf\left(\frac{|Y-5|}{\sqrt{2}}\right)\right] \tag{5}$$

5. Validating of TORCAT

The source model and dispersion model in TORCAT is validated against the published data and results from Example 5-2 and Problem 5-18 of Crowl and Louvar [43]. The data and results from TORCAT as given in Figs. 4 and 5 are in agreement with Crowl and Louvar [43].

6. Applicability of TORCAT using case studies

To demonstrate the capability of the proposed consequence tool, two case studies were conducted using a typical ammonia purification plant. Case study 1 shows the capability of TORCAT to identify potential hazards from pipe ruptures and necessary moderation

Calculate	Import Data	
Pipe Diameter, D	0.493	inch
Temperature, T_o	540	°R
Pressure P_o	64.7	psia
Discharge Coefficient C_o	1	
Heat Capacity Ratio γ	1.33	
Molecular Weight M	70.8	lb$_m$/lb$_{mole}$
Q_m (choked)	0.434	lb$_m$/s

Fig. 5. The data and results extracted from TORCAT source model based on Problem 5-18 of Crawl and Louvar [43].

of process condition was implemented to ensure the consequence is within the accepted limit. Case study 2 shows how the proposed consequence tool was used to assess the consequence of toxic release. The consequence is reduced to ALARP by downsizing the size of the equipment by following the inherent safety principle.

6.1. Case study 1: identify potential hazards from selected streams

Fig. 6 shows a purification column in a typical ammonia production plant. The design engineer was interested to evaluate the

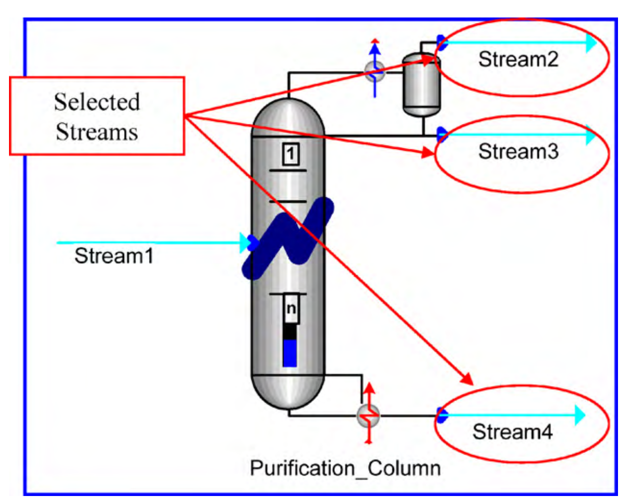
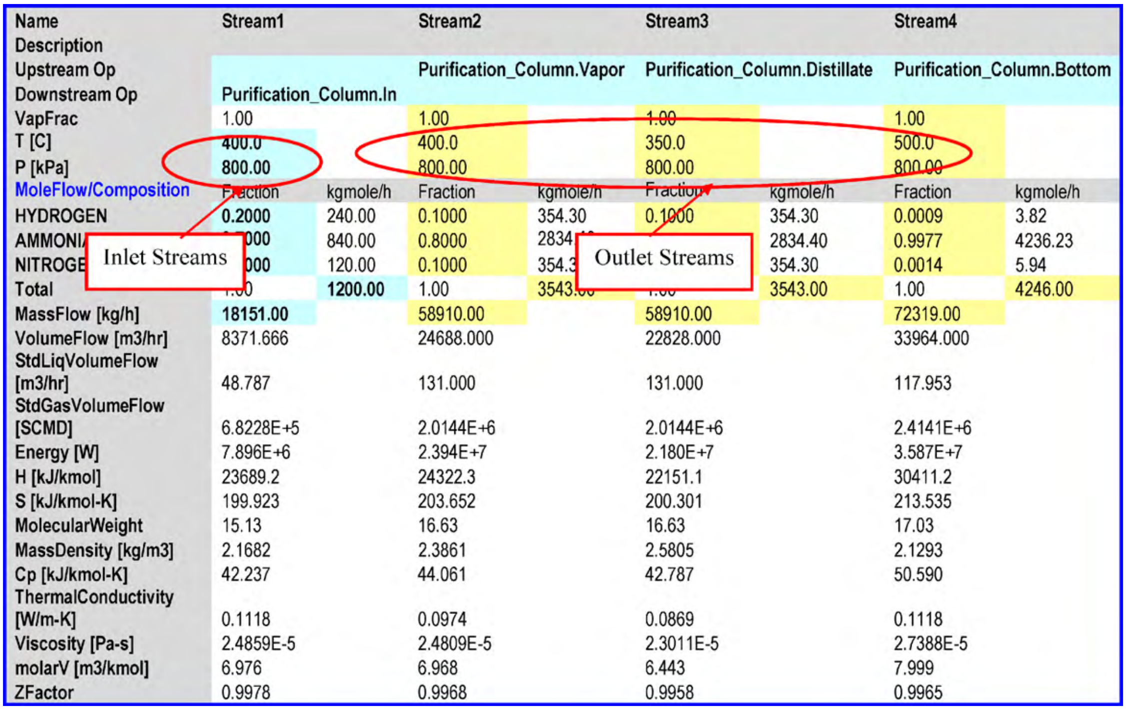


Fig. 6. Purification column from ammonia plant extracted from iCON.



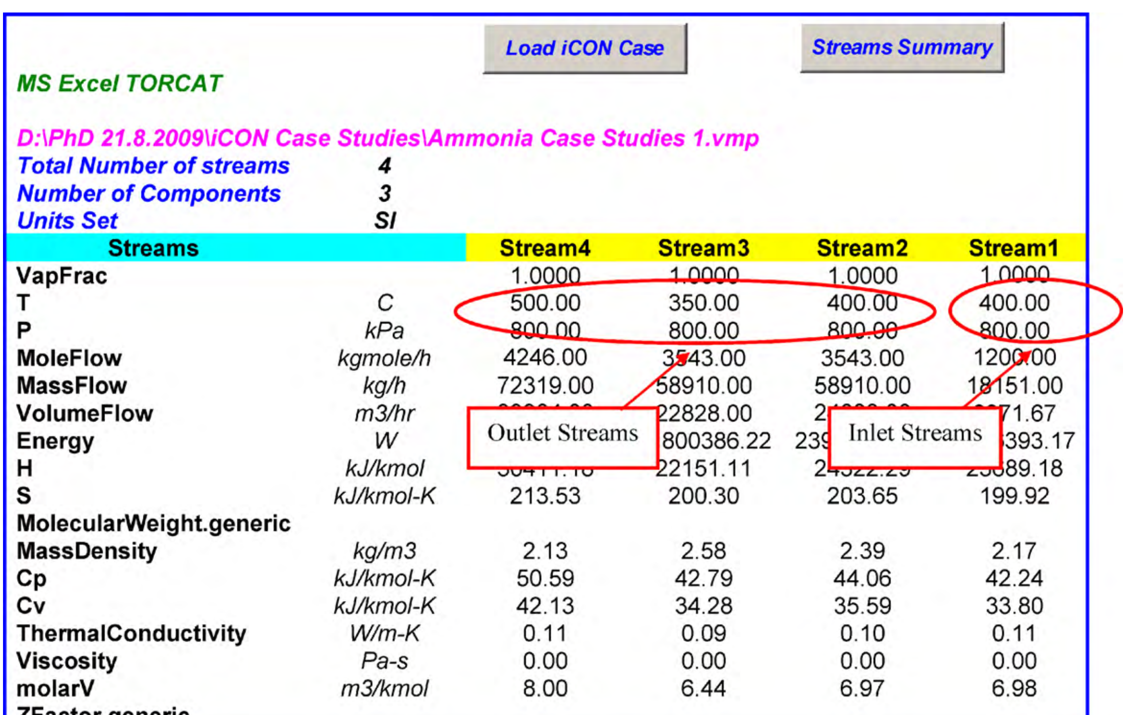
Name	Stream1		Stream2		Stream3		Stream4	
Description								
Upstream Op			Purification_Column.Vapor		Purification_Column.Distillate		Purification_Column.Bottom	
Downstream Op	Purification_Column.In							
VapFrac	1.00		1.00		1.00		1.00	
T [C]	400.0		400.0		350.0		500.0	
P [kPa]	800.00		800.00		800.00		800.00	
MoleFlow/Composition	Fraction	kgmole/h	Fraction	kgmole/h	Fraction	kgmole/h	Fraction	kgmole/h
HYDROGEN	0.2000	240.00	0.1000	354.30	0.1000	354.30	0.0009	3.82
AMMONI[illegible]	[illegible]000	840.00	0.8000	2834[illegible]	[illegible]	2834.40	0.9977	4236.23
NITROGE[illegible]	[illegible]000	120.00	0.1000	354.3[illegible]	[illegible]	354.30	0.0014	5.94
Total	[illegible]0	1200.00	1.00	3543.[illegible]	[illegible]	3543.00	1.00	4246.00
MassFlow [kg/h]	18151.00		58910.00		58910.00		72319.00	
VolumeFlow [m3/hr]	8371.666		24688.000		22828.000		33964.000	
StdLiqVolumeFlow [m3/hr]	48.787		131.000		131.000		117.953	
StdGasVolumeFlow [SCMD]	6.8228E+5		2.0144E+6		2.0144E+6		2.4141E+6	
Energy [W]	7.896E+6		2.394E+7		2.180E+7		3.587E+7	
H [kJ/kmol]	23689.2		24322.3		22151.1		30411.2	
S [kJ/kmol-K]	199.923		203.652		200.301		213.535	
MolecularWeight	15.13		16.63		16.63		17.03	
MassDensity [kg/m3]	2.1682		2.3861		2.5805		2.1293	
Cp [kJ/kmol-K]	42.237		44.061		42.787		50.590	
ThermalConductivity [W/m-K]	0.1118		0.0974		0.0869		0.1118	
Viscosity [Pa-s]	2.4859E-5		2.4809E-5		2.3011E-5		2.7388E-5	
molarV [m3/kmol]	6.976		6.968		6.443		7.999	
ZFactor	0.9978		0.9968		0.9958		0.9965	

Fig. 7. Example data from iCON simulation case for ammonia Purification Column.

worst-case scenario of potential toxic gas released if any of three outlet streams from the ammonia purification column are ruptured that produce instantaneous release.

The examples of original data from iCON for all three streams are given in Fig. 7. These data were extracted via OLE in Excel VBA into MS-Excel TORCAT as shown in Fig. 8. The example preliminary assessment of the streams identify that the pressures of the outlet streams are quite high that may cause high concentration of toxic gas release in the case of rupture. The release may produce potential fatalities if expose at very short duration of time. With respect to toxicity concept, exposure to high concentration will increase the severity of hazard consequence. In order to evaluate the hazards and minimize the impact, the consequence analysis was carried out using TORCAT.

It was assumed that a maximum concentration will occur at the center of the puff cloud and the release occurs in duration of 10 min



Streams		Stream4	Stream3	Stream2	Stream1
VapFrac		1.0000	1.0000	1.0000	1.0000
T	C	500.00	350.00	400.00	400.00
P	kPa	800.00	800.00	800.00	800.00
MoleFlow	kgmole/h	4246.00	3543.00	3543.00	1200.00
MassFlow	kg/h	72319.00	58910.00	58910.00	18151.00
VolumeFlow	m3/hr	[illegible]	22828.00	2[illegible]	[illegible]71.67
Energy	W	[illegible]	[illegible]800386.22	239[illegible]	[illegible]393.17
H	kJ/kmol	[illegible]	22151.11	2[illegible]	[illegible]89.18
S	kJ/kmol-K	213.53	200.30	203.65	199.92
MolecularWeight.generic					
MassDensity	kg/m3	2.13	2.58	2.39	2.17
Cp	kJ/kmol-K	50.59	42.79	44.06	42.24
Cv	kJ/kmol-K	42.13	34.28	35.59	33.80
ThermalConductivity	W/m-K	0.11	0.09	0.10	0.11
Viscosity	Pa-s	0.00	0.00	0.00	0.00
molarV	m3/kmol	8.00	6.44	6.97	6.98
ZFactor.generic					

Fig. 8. Example data in MS-Excel TORCAT.

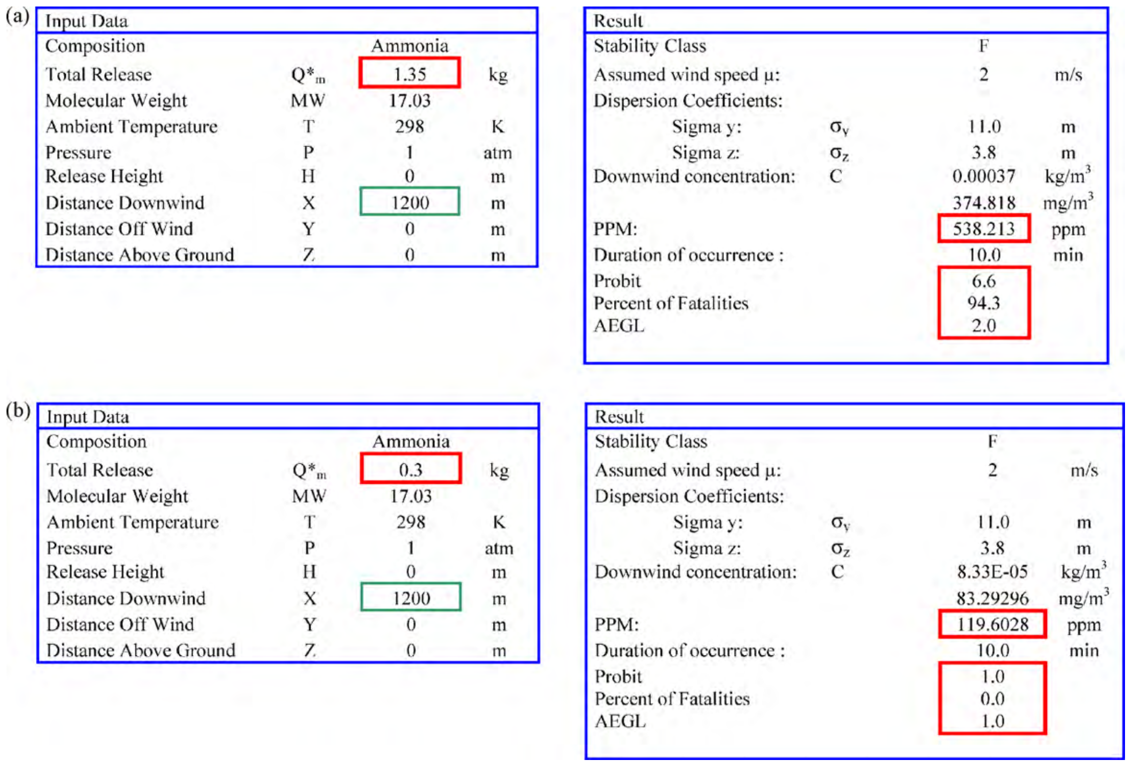


Fig. 9. (a) Data from TORCAT before lowering the inlet pressure *P*; (b) data from TORCAT after lowering the inlet pressure *P*.

[43]. The example result from TORCAT due the potential impact of ammonia exposure is given in Fig. 9(a). The calculated amount of ammonia released was estimated to be 1.35 kg and the percentage of fatalities for the people staying in the center of the puff cloud which is 1200 m from the plant is 94.3%. The design intension for this plant was to have 0% fatalities within 1200 m from the plant. One of the possible solutions for this case is to lower the pressure of stream 1 (inlet stream to purification column) to ALARP in order to achieve 0% fatalities as shown in Fig. 9(b). At this pressure, the calculated amount of the ammonia released was estimated to be 0.30 kg. Thus, the potential hazard due to toxic released is avoided at the distance within 1200 m from the ammonia plant.

This solution used concept of moderation in inherently safer design principle. Even though the result meets the design intention, however the design engineer must evaluate whether this simple changes will meet the overall design objectives such as the production target and demand. If not, other alternatives need to be considered in order to satisfy the overall design objectives.

This case study demonstrated the potential application of TORCAT to evaluate and reduce the severity of the consequence due to toxic release based on the stream operating conditions using moderation concept of inherent safety principle. If the consequence of toxic release is intolerable, other alternative of inherent safety principle can be applied such as using minimization, substitution and simplification techniques. This concept is further illustrated in the case study 2.

6.2. Case study 2: down sizing equipment to eliminate potential fatalities

The advantage of TORCAT can also be demonstrated by showing its capability to assess and reduce the consequence of toxic release using minimization concept of inherent safety principle during preliminary design stage without requirement to include additional protective system. In this case study, a supply line con-

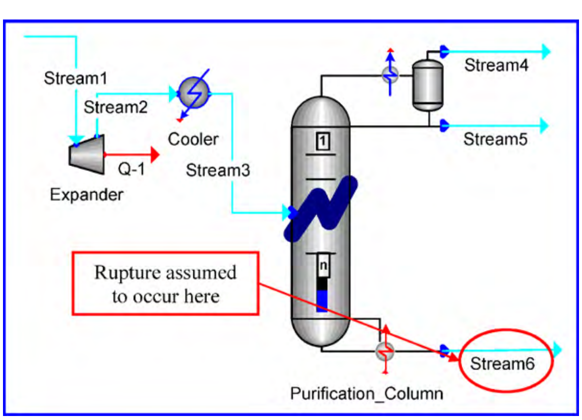


Fig. 10. Purification column system from the ammonia plant extracted from iCON.

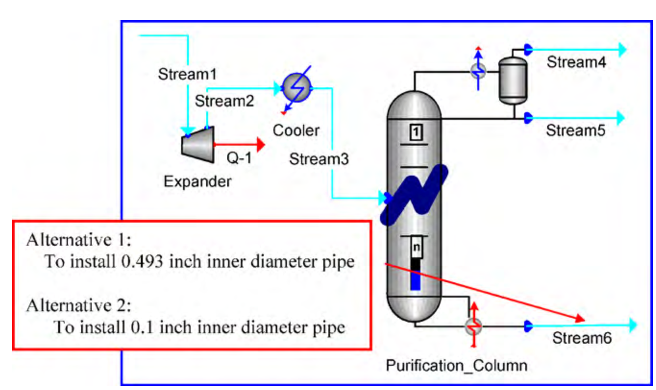


Fig. 11. Design modification alternative in stream 6.

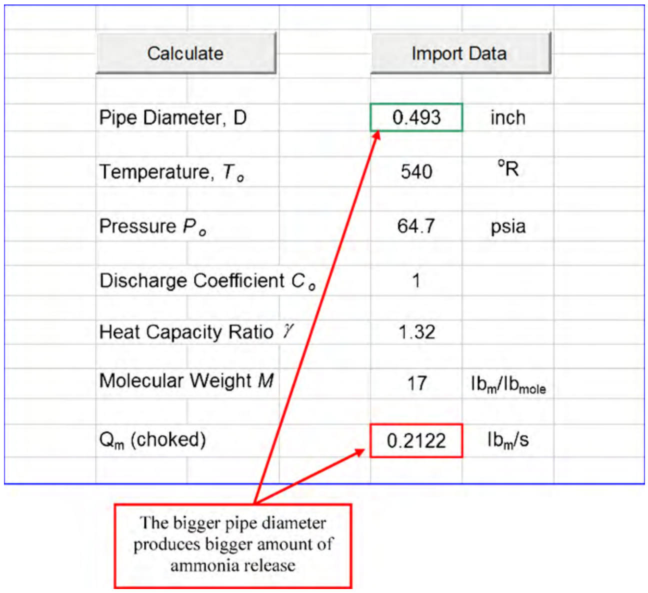


Fig. 12. Design modification alternative result from TORCAT by installing a bigger diameter pipeline in stream 6.

taining ammonia gas is piped from the column at 50 psig and a temperature of 80 °F. It was identified from preliminary hazard assessment that there is a possible rupture in case of accident at stream 6 of ammonia purification column as shown in Fig. 10. The design engineer had identified two possible alternatives in order to evaluate the impact of the release. The first alternative was to install 0.493 in. inner diameter pipe and the second alternative was to install 0.100 inch inner diameter pipe as a supply line. The proposed modifications are shown in Fig. 11 and the results from TORCAT are given in Figs. 12 and 13. The results showed that by installing a smaller inner diameter of the pipe (0.1 in.), the consequence of pipeline rupture was reduced to the acceptable limit required by the design. Therefore, the second alternative is finally chosen by the process designer.

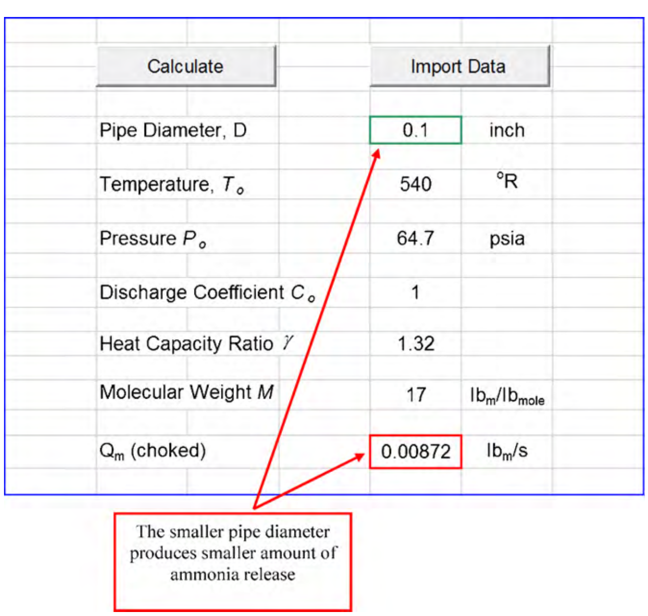


Fig. 13. Design modification alternative result from TORCAT by installing a smaller diameter pipeline in stream 6.

7. Conclusion

TORCAT is an evolution of prototype tool for consequence analysis of toxic release from the previous approach and the preliminary application in the case studies had successfully showed that it is capable to reduce the severity of the consequence to ALARP by using inherent safety principle during preliminary design stage. TORCAT eliminates the need to manually transfer the information from process design simulation into consequence analysis tool and therefore, saves time for transferring data and eliminates the possibility of data entry error. The modification of the design is easy since TORCAT provides direct link between process design simulation and the consequence model and it is validated and comparable to other published result. This will result in more efficient and cost effective decision-making on toxic release issues as early as in the preliminary design stage. The tool can also be used in the process life cycle of chemical plant.

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