Distillation column inherent safety index at preliminary design stage

Azmi Mohd Shariff[1,2,*]**, Muhammad Athar**[1,2]**, Azizul Buang**[1,2]**, Muhammad Ishaq Khan**[1,2]**, Heri Hermansyah**[3]

[1] Center for Advanced Process Safety (CAPS), Universiti Teknologi Petronas, 32610 Bandar Seri Iskandar, Perak Darul Ridzuan, Malaysia.
[2] Chemical Engineering Department, Universiti Teknologi Petronas, 32610 Bandar Seri Iskandar, Perak Darul Ridzuan, Malaysia.
[3] Industrial Bioprocess Engineering Laboratory, Department of Chemical Engineering, Faculty of Engineering, Universitas Indonesia, Kampus UI Depok, Depok 16424, Indonesia.

* azmish@utp.edu.my

Abstract. Distillation columns are widely used in many chemical process industries, especially in oil and gas processing. Accidents in the distillation columns have resulted in enormous loss of human lives and assets. Inadequate design of distillation columns is one of the vital reason for the failure, which can be enhanced through inherent safety concept. Therefore, this paper introduces a new indexing method for designing inherently safer distillation columns right from the preliminary design stage. Distillation Column Inherent Safety Index (DCISI) is based on three sub-indices; chemical index, process index and distillation index. These sub-indices are estimated through individual scores by considering various parameters in each category. For the unacceptable score, modification of process conditions is used to enhance safety level of the design. DCISI is estimated for all combination of conditions and lowest DCISI value indicates the inherently safer design of the distillation column.

1. Introduction

With the progressive development of the process industries, designers are focusing on safety as the most priority aspect, because of hazardous chemicals processing. Therefore, a number of guidelines and procedures have been developed and practiced over the last few decades in order to increase the safety level, as highlighted in Figure 1 [1].

In process industries, distillation columns are frequently used, because of cheap separation agent cost, to perform the separation of liquid components. Analysis of previous accidents has revealed that failure of the distillation column can be catastrophic. For example, accidents of Ojima Town, Gunma and Pascagoula, Mississippi have caused huge structural and human loss inside the facility and in the vicinity of the plant [2,3]. There are several reasons for failure for any process equipment which have been investigated by many authors. Among these reasons, design inadequacy has been identified as the most critical for any process equipment [4-6].

Most of the traditional safety studies are carried out once the process design is complete. At this stage, the risk is controlled rather than minimization or mitigation using passive, active and procedural

strategies of process safety [7]. At this stage, any modification in the process can cause extra investment in comparison to the design adjustments at the preliminary design stage [8].

Inherent safety concept proposed by Kletz can fulfill the objective of design modifications during early design phases. It emphasizes the reduction and elimination of the root cause of hazards associated with materials and operation. The key principles for inherent safety involve four major elements; as demonstrated in figure 2 [9].
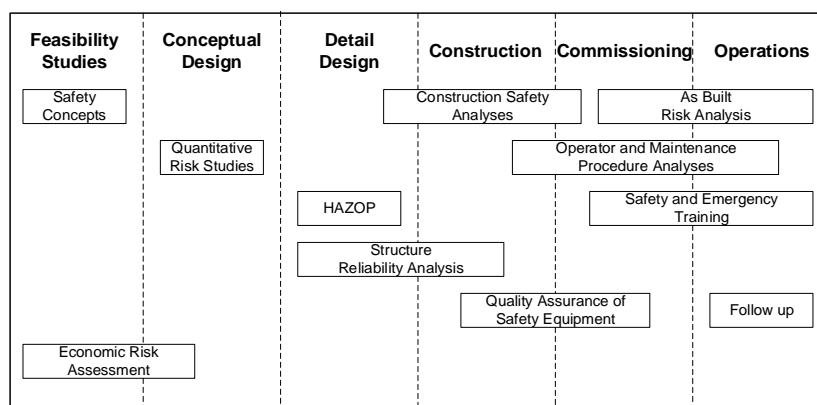
Figure 1. Safety analysis program [1].
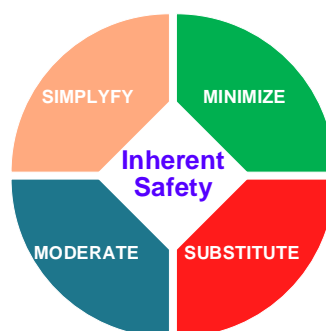
Figure 2. Inherent safety principles [9].

To evaluate numerous design options for a process, quantification of inherent safeness is the biggest challenge. To achieve this target, various inherent safety methods have been proposed. Majority of the methods use indexing technique for inherently safer process route selection [10]. These include inherent safety index (ISI), integrated inherent safety index (I2SI) and process route index (PRI) [10-13]. However, none of the technique is applicable to assess inherent safety level of the distillation column as the nature of individual equipment cannot be taken into account. Consequently, this paper intends to propose a new indexing method for the inherent safety assessment of the distillation column during the preliminary design stage. In the distillation column inherent safety index (DCISI), different design options for the distillation column are proposed and prioritized to identify the inherently safer design for the distillation column. This index would help to identify the safer and cost-effective design for the distillation column at the early design phase.

2. Methodology

A systematic framework to design an inherently safer distillation column at the preliminary design stage is provided in Figure 3. There are various factors, which have a major contribution in distillation column design and are divided into three categories namely chemical, process, and distillation, outlined in Table 1.

Table 1. Parameters for DCISI

Category	Parameters
Chemical	Auto-ignition temperature, flammability, explosiveness
Process	Operating pressure, temperature
Distillation	Reflux ratio, relative volatility

The higher the score for a parameter, the more hazardous is the category. Initially, the factors for distillation column design are analyzed and then merged to provide the value of the distillation column inherent safety index (DCISI). The scoring values for these factors are explained in Table 2. Finally, the ranking of DCISI values identifies the inherently safer design.

Table 2. Score for DCISI

Score	Description
1	Recommended
2	Sound engineering practice
3	Probably unsafe
4	Minor accident
5	Major accident

In next subsections, the contributing factors for safe distillation column design are described. The scoring of all the parameters is provided in table 3.
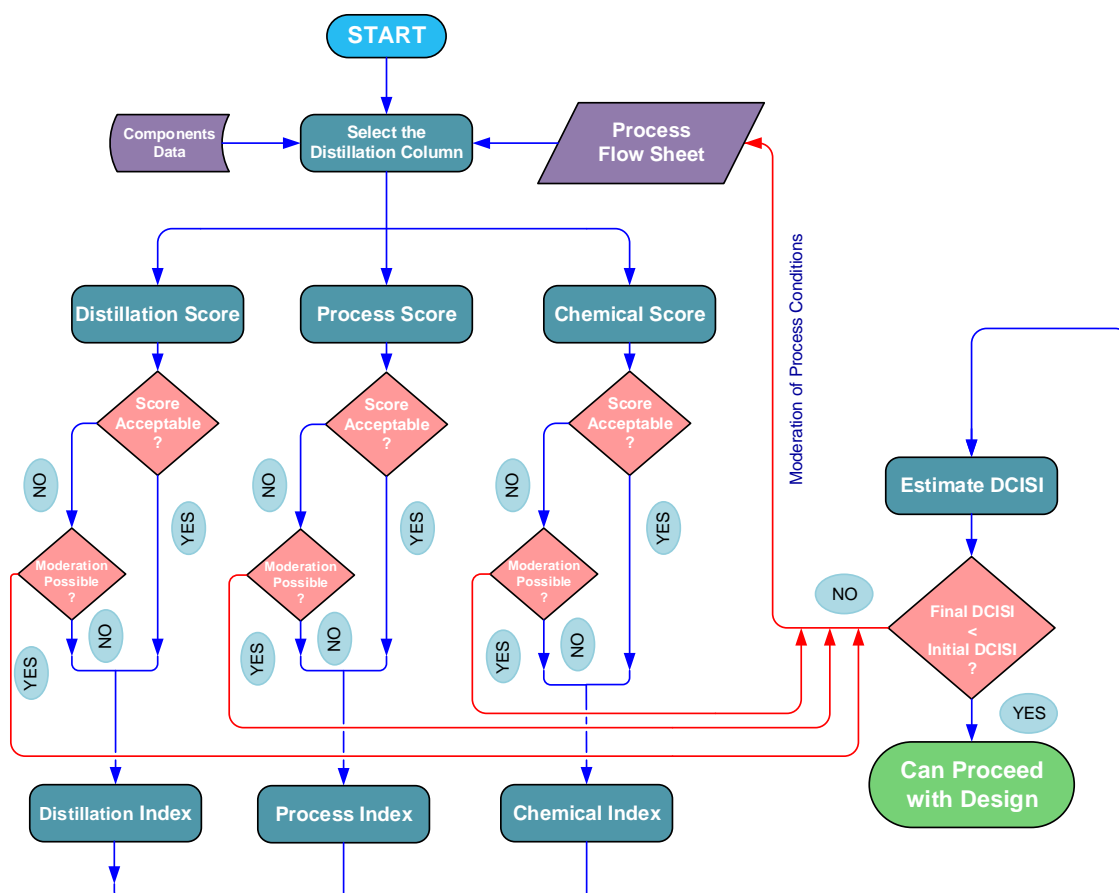
Figure 3. Framework for the distillation column inherent safety index (DCISI).

Chemical Score (CS)

The overall chemical score (CS) is a combination of autoignition temperature score, flammability score, and explosiveness score expressed:

$$CS = CS_{AIT} + CS_{FM} + CS_{EX} \tag{1}$$

Auto Ignition Temperature Score (CS$_{AIT}$). Auto-ignition temperature (AIT) of the fluid is a key factor to identify the safer scenario for a distillation column. Temperature greater than the AIT enhances the chances of fire and explosion and vice versa. The score in table 3 is based on the comparison of distillation column temperature and autoignition temperature.

Flammability Score (CS$_{FM}$). Flammability is the capability of any chemical to ignite, which can cause major fire or explosion in the process industry. The score for flammability is described in table 3 which is adapted and modified from ISI [11].

Explosiveness Score (CS$_{EX}$). Explosiveness is the chemical mixture composition which can convert to the explosion and can be estimated by the difference between lower flammability limit (LFL) and upper flammability limit (UFL) of a mixture. Like flammability, the explosiveness score is adapted from ISI and described in table 3 [11].

Process Score (PS)

The operating conditions of the distillation column are the major elements to define the process score. This score can be estimated by:

$$PS = PS_P + PS_T \tag{2}$$

Pressure Score (PS$_P$). The pressure of the distillation column is one of the critical factors to define the safety level of the column. The leak chances are increased due to greater forces created by high pressure. The score for pressure is adapted from ISI method and furnished in table 3 [11].

Temperature Score (PS$_T$). Temperature is an indication of heat energy in any process. The higher the heat energy, the more are the chances for the process to get out of control. Also, the higher heat energy decreases the vessel material strength, especially in case of thermal shocks. The temperature scoring values are adapted from ISI method and outlined in table 3 [11].

Distillation Score (DS)

The distillation specific characteristics also contribute to deciding the safety level of the distillation column. The distillation score is a function of reflux ratio and relative volatility and can be estimated as follows:

$$DS = DS_R + DS_\alpha \tag{3}$$

Reflux Ratio Score (DS$_R$). Reflux ratio is defined as the ratio between the liquid returning back to the distillation column to the distillate collected. Although, increasing the reflux ratio enhances the distillate quality [14, 15], however, the increasing flow rates would increase the inventory in the column and duty requirements of distillation column. Therefore, the smaller the reflux ratio the safer is the column, and the relevant scoring is described in Table 3.

Relative Volatility Score (RS$_\alpha$). Relative volatility is the comparison of vapor pressures in a liquid chemical mixture. For a multicomponent mixture, the relative volatility is measured between light key comment and heavy key component [14,15]. The higher the relative volatility, the easier is the separation and safe. However, for lower relative volatility, the separation becomes difficult, and distillation column is operating under risky conditions. The scoring values are explained in table 3.

Evaluation of Scores

The score for each category is obtained from equations (1) - (3), and score value describes the safety level of the distillation column. The safety criteria are defined as if any category score for distillation column design option is more than the half of the maximum category score, the design is considered as unsafe. However, if the score is less than the half of maximum category score, the design is safe. For example, the maximum score for the process category is 10, and for a design option, if the process score is > 5, the design is unsafe.

2.1. Estimation of distillation column inherent safety index (DCISI)

The score values are converted to the indexing value for each category and can be estimated by:

$$CI = \frac{CS}{15} \tag{4}$$

$$PI = \frac{PS}{10} \tag{5}$$

$$DI = \frac{DS}{10} \tag{6}$$

The overall value of DCISI is obtained by the summation of the chemical index, process index, and distillation index, as follows:

$$DCISI = CI + PI + DI \tag{7}$$

Distillation column design option with lower DCISI value is preferable in terms of safety in comparison and vice versa.

Table 3. Parameters scoring description for DCISI

| Score	Chemical			Process		Distillation	
	Auto-ignition temperature	Flammability	Explosiveness (%)	Operating Pressure (bar)	Temperature (°C)	Reflux Ratio	Relative volatility
1	Column temperature < Auto ignition temperature	Non-flammable	Non explosive	0.5-5	0-70	R ≤1.5	$\alpha > 1.1$
2	-	Combustible (flash point > 55°C)	0-20	6-25	< 0 & 71-150	R ≤ 2.5	-
3	-	Flammable (flash point < 55°C)	21-45	26-50	151-300	R ≤ 3.5	-
4	-	Easily flammable (flash point < 21°C)	46-70	51-200	301-600	R < 5	-
5	Column temperature > Auto ignition temperature	Very flammable (flash point < 0°C & boiling point < 35°C)	71-100	201-1000	> 600	R ≥ 5	$\alpha \leq 1.1$

3. Results and Discussions

The design of distillation column (C-4501) in methanol production process is used to demonstrate the capability of DCISI for the safety assessment of distillation column during the preliminary design stage. Four different design options are considered to design C-4501, which are organized in Table 4.

The simulation of methanol process is available in Figure 4 [16], which has been simulated using the PRSV equations of state due to extended capabilities. Industrially the methanol is produced by synthesis gas in the catalytic environment. Cooling is used for removing the additional heat and the methanol separation from the reaction mixture is achieved by exploiting the thermodynamic characteristics followed by the distillation process. The methanol is obtained as distillate from distillation column, while the vapor separated through phase separation are recycled to increase the process efficiency.

Table 4. Design options for C-4501

Parameter	Design 1	Design 2	Design 3	Design 4
Operating Pressure (bar)	5.00	1.50	1.01	1.01
Operating temperature (°C)	109.2	87.34	78.75	78.05
Reflux Ratio	4	3.5	3	2.5
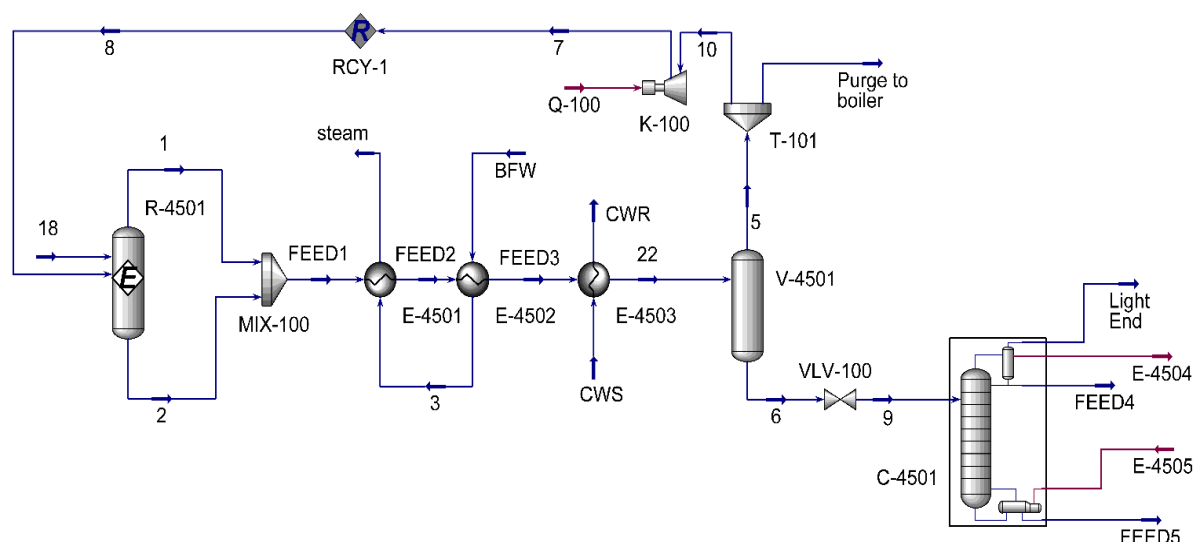
Figure 4. Process simulation of methanol process [16].

The DCISI concept has been applied to the distillation column, C-4501. Initially, process information for the design 1 is extracted from HYSYS and transferred to MS Excel program through VBA coding. The components data is obtained from literature and introduced in the spreadsheet tool using input interface. Scores for the process, chemical and distillation categories are estimated as per equations (1) - (3), presented in table 5. By analyzing the scores, it is recognized that chemical and distillation scores are acceptable, while process score is unacceptable. To minimize these scores, the process conditions for the operation of C-4501 are moderated as design 2, 3 and 4 available in table 4. The calculations of chemical, process and distillation scores are performed one by one for each design option and summarized in Table 5. Although, the moderated process design has not affected the chemical and process scores, however a positive effect on the distillation score is observed. Conclusively, for all modified designs, each category score is in the acceptable range. However, no change in the process and chemical scores are observed, while the distillation score is gradually changing, for the reason of small changes in process conditions, which have created a minute effect on the distillation score. Although, the chemical characteristics are slightly changed, however, the chemical score remains same due to the ranges defined in table 3. For all design options, the DCISI

has been estimated using equations (4) to (7), and a slight change in the index value is witnessed. From the score and index values, design 4 is considered as the best design option for the distillation column, C-4501.

Additionally, the effect of changes in the design has been examined in the process to identify the benefits of inherent safety employment in the chemical process design. The safety criteria in this work are the lower value of DCISI, which is achieved through moderation of process conditions and changing the reflux ratio. These moderated conditions have a positive effect on the process efficiency, which is defined in terms of lesser distillation column duty and improved product purity from the distillation column. By moderating the process conditions and reflux ratio, the duty of distillation column is considerably reduced, i.e., 21%. However, the product quality is slightly compromised, around 3%. Conclusively, the design for distillation column can be considered as inherently safer and improved in terms of process characteristics. The effect of moderated design on the performance of the distillation column is depicted in Figure 5.

Table 5. Parameters scores and DCISI for different designs of C-4501

Parameter	Score Value	Design 1	Design 2	Design 3	Design 4
Chemical Aspect					
Auto ignition temperature	1 or 5	1	1	1	1
Flammability	1 - 5	3	3	3	3
Explosiveness	1 - 5	4	4	4	4
Chemical Score		8	8	8	8
Chemical Index		0.533	0.533	0.533	0.533
Process Aspect					
Pressure	1 - 5	1	1	1	1
Temperature	1 or 5	2	2	2	2
Process Score		3	3	3	3
Process Index		0.3	0.3	0.3	0.3
Distillation Aspect					
Reflux Ratio	1 - 5	4	3	3	2
Relative Volatility	1 or 5	1	1	1	1
Distillation Score		5	4	4	3
Distillation Index		0.5	0.4	0.4	0.3
Distillation Column Inherent safety Index (DCISI)		1.333	1.233	1.233	1.133
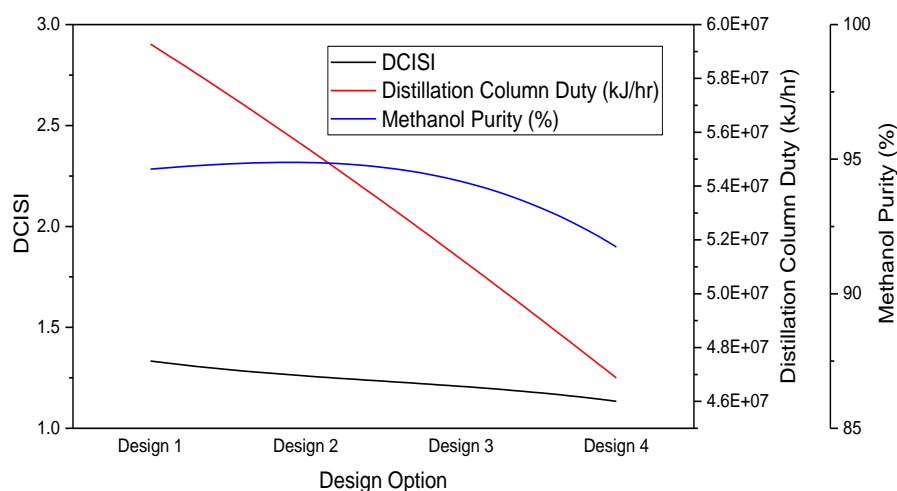
Figure 5. DCISI effect on the performance of C-4501.

For future work, more case studies can be investigated for improvement of the presented indexing method by the inclusion of further significant characteristics of distillation to define the safety level of the column. Furthermore, the type of the internals for columns can be investigated to design an inherently safer distillation from the very early design stages.

4. Conclusion

To achieve the objective of inherently safer distillation column during the early design phase, a new indexing method is proposed in this paper. Distillation column inherently safety index (DCISI) compares different design options of the distillation column focusing the chemical, process and distillation characteristics. The index is estimated by summation of individual indices, which are obtained by converting the score values. DCISI value of all design options are estimated and ranking of DCISI values can identify the inherently safer design. A low DCISI value indicates the design as safe and vice versa. Modification of conditions in distillation column can help to achieve a safer design.

References

[1]   Taylor J R 2003 *Risk Analysis for Process Plant, Pipelines and Transport*, CRC Press
[2]   U.S. Chemical Safety and Hazard Investigation Board 2003 Investigation Report, Vapor cloud deflagration and fire at BLSR Operating LTD
[3]   Koseki H, Kobayashi M, and Masamitsu T 2017 Explosion and Fire of Hydroxylamine
[4]   Jalani J A, Kidam K, Shahlan S S, Kamarden H, Hassan O and Hashim H 2015 An analysis of major accident in the US chemical safety board (CSB) database *J. Tek.* **75** pp 53-60
[5]   Kidam K and Hurme M 2012 Design as a contributor to chemical process accidents, *J. Loss Prev.   Proc. Indus.* **25** pp 655-666
[6]   Kidam K, Sahak H A, Hassim M H, Shahlan S S and Hurme M 2016 Inherently safer design review and their timing during chemical process development and design *J. Loss Prev. Proc. Indus.* **42** pp 47-58
[7]   Shariff A M and Zaini D 2010 Toxic release consequence analysis tool (TORCAT) for inherently   safer design plant *J. Hazard. Mater.* **182** pp 394-402
[8]   Ashford N A and Zwetsloot G 2000 Encouraging inherently safer production in European firms: a report from the field *J. Hazard. Mater.* **78** pp 123-144
[9]   CCPS, Center for Chemical Process Safety 2010 *Inherently Safer Chemical Processes: A Life Cycle Approach* (Wiley)
[10]   Leong C and Shariff A M 2009 Process route index (PRI) to assess level of explosiveness for inherent safety quantification *J. Loss Prev. Proc. Indus.* **22** pp 216-221
[11]   Heikkilä A 1999 *Inherent safety in process plant design: an index-based approach* (VTT Technical Research Centre of Finland)
[12]   Khan F and Amyotte P 2004 Integrated inherent safety index (I2SI): a tool for inherent safety evaluation *Process Saf. Prog.* **23** pp 136-148
[13]   Khan F and Amyotte 2005 P I2SI: a comprehensive quantitative tool for inherent safety and cost evaluation *J. Loss Prev. Proc. Indus.* **18** pp 310-326
[14]   Coulson J, Richardson J, Backhurst J and Harker J 1996 *Coulson & Richardson's Chemical Engineering: Particle technology and separation processes. 5th ed* (Butterworth-Heinemann)
[15]   Kister H 1992 *Distillation Design* (McGraw-Hill Education)
[16]   Nian C W and You F 2013 Design of Methanol Plant *EURECHA Student Contest Problem Competition ESCAPE-23 Symp.* (Finland, p 25)