

**DEVELOPMENT OF A FRIENDLIER CHEMICAL PROCESS  
FRAMEWORK USING THE INHERENT SAFETY CONCEPT**

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USING THE INHERENT SAFETY CONCEPT

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# **DEVELOPMENT OF A FRIENDLIER CHEMICAL PROCESS FRAMEWORK USING THE INHERENT SAFETY CONCEPT**

## **ABSTRACT**

To date, inherent safety concept has been regarded as the most robust solution for risk management and loss prevention in chemical processes. Its proactive interventions of building safety measures into the process design schemes can avoid adding extensive end-of-pipe protections when the processes evolve to the operation stage. In practice, numerous frameworks have been presented to develop inherently safer process routes. Together with the inherent Safety (S) framework, various dedicated assessment tools for designing inherent Health (H) and Environmentally (E) benign chemical process routes have been proposed to eliminate or minimize the SHE risks at the design stage. However, the dedicated inherent SHE assessment tools give limited attention to the weights and uncertainties of the component indicators. Also, whether the incremental costs of implementing "inherent" principles can distort the overall process friendliness is yet to be demonstrated. To bridge the gaps, this study weighted and reconciled the separate inherent SHE metrics with cost indices considering the risk uncertainties, thus developing a novel Reconciled Friendly Process Framework (RFPF) to realize inherently Friendlier Chemical Processes (FCP). The FCP are characterized to be inherently safer, healthier, and more environmentally benign with tradeoff considerations on the incremental costs of design modifications. To develop the RFPF and realize the FCP, the pioneering Inherent Safety Index (ISI), Inherent Occupational

Health Index (IOHI), Inherent Environmental Toxicity Hazard (IETH), and Inherent Safety Implementation Cost (ISIC) were selected and adapted to indicate the inherent friendliness features. Subsequently, the selected inherent friendliness indicators were weighted using Analytic Hierarchy Process (AHP) method and reconciled using the fuzzy logic and Bayesian Networks (BN). Lastly, the newly developed RFPPF was validated by a case study of biodiesel production processes. The results show that the inherent friendliness of the Baseline Design Processing Option (BDPO) was estimated as Moderate (M) level (inherent friendliness  $\approx 3.05$ ), while it improved to Relatively Friendly (RF) level (inherent friendliness  $\approx 2.28$ ) after implementing inherently friendlier modifications. The significant improvement of the inherent friendliness implies that the Modified Design Processing Option (MDPO), compared with the BDPO, can be a more reliable option with fewer built-in SHE risks under the incorporated incremental costs. The newly developed RFPPF synthesized the conflicting factors of SHE and cost indices with weights and normalized risk scores to develop inherently FCP during the process design stage, which can be expected to use as a more realistic tool to proactively, fundamentally, and economically reduce the SHE risks at their sources.

**Keywords:** Inherent safety, Inherent health, Environmental protection, Incremental cost, Chemical process design

# **PEMBANGUNAN RANGKA KERJA PROSES KIMIA YANG MESRA DENGAN MENGGUNAKAN KONSEP KESELAMATAN TERWUJUD**

## **Abstrack**

Sehingga kini, konsep keselamatan terwujud (atau inherent safety) yang wujud telah dianggap sebagai penyelesaian yang paling kukuh dalam pengurusan risiko dan pencegahan kerugian dalam proses kimia. Kaedah pencegahan proaktif dalam skema reka bentuk proses keselamatan bangunan dapat mengelakkan penambahan perlindungan hujung paip skala besar apabila proses berkembang ke peringkat operasi. Secara lazimnya, pelbagai rangka kerja telah dibentangkan untuk membangunkan laluan proses terwujud yang lebih selamat. Setara dengan rangka kerja Keselamatan (Safety atau S) terwujud, pelbagai kaedah penilaian khusus untuk merancang Kesihatan (Health atau H) terwujud dan laluan proses kimia lebih mesra Alam (Environmentally atau E) telah dibangunkan untuk menghapus atau mengurangkan risiko SHE pada peringkat reka bentuk. Walau bagaimanapun, kaedah penilaian SHE terwujud yang sedia ada hanya memberikan perhatian terhad kepada beban dan ketidakpastian penunjuk komponen. Di samping itu, kebarangkalian kemerosotan kadar kemesraan keseluruhan proses yang wujud daripada pertambahan kos untuk melaksanakan prinsip "terwujud" masih belum ditunjukkan. Untuk merapatkan jurang, kajian ini menekankan dan menyelaraskan metrik SHE yang sedia ada dengan kos indeks yang mempertimbangkan ketidakpastian risiko, sekali gus membangunkan alat penilaian baru yang dinamakan

Rangka Kerja Proses Mesra Bersatu (Reconciled Friendly Process Framework atau RFPF) untuk merealisasikan Proses Kimia Mesra (Friendlier Chemical Process atau FCP) terwujud. FCP dicirikan sebagai lebih selamat, lebih sihat, dan lebih mesra alam dengan mempertimbangkan kos tambahan pengubahsuaian reka bentuk. Untuk membangunkan RFPF dan merealisasikan FCP, Indeks Keselamatan Terwujud (Inherent Safety Index atau ISI), Indeks Kesihatan Pekerjaan Terwujud (Inherent Occupational Health Index atau IOHI), Bahaya Ketoksikan Alam Sekitar Terwujud (Inherent Environmental Toxicity Hazard atau IETH), dan Kos Pelaksanaan Keselamatan Terwujud (Inherent Safety Implementation Cost atau ISIC) telah dipilih dan digunakan untuk menunjukkan sifat kemesraan terwujud. Seterusnya, metrik yang dipilih telah ditimbang menggunakan kaedah Proses Hierarki Analitik (Analytic Hierarchy Process atau AHP) dan diselaraskan dengan menggunakan logik tidak jelas dan Rangkaian Bayesian (Bayesian Network atau BN). Akhir sekali, RFPF yang baru dibangunkan telah disahkan melalui kajian kes proses pengeluaran biodiesel. Keputusan menunjukkan bahawa kemesraan terwujud bagi Pilihan Pemprosesan Reka Bentuk Dasar (Baseline Design Processing Option atau BDPO) dianggarkan sebagai tahap Sederhana (Medium atau M) (kemesraan terwujud  $\approx 3.05$ ), namun meningkat kepada tahap Mesra Relatif (RF) (kemesraan terwujud  $\approx 2.28$ ) selepas melaksanakan pengubahsuaian yang lebih mesra. Peningkatan ketara dalam kemesraan yang wujud menunjukkan bahawa Pilihan Pemprosesan Reka Bentuk Bolehubah (Modified Design Processing Option atau MDPO), berbanding dengan BDPO, boleh menjadi pilihan yang lebih memuaskan dengan risiko SHE yang lebih rendah di bawah pertambahan kos. RFPF yang baru dibangunkan menghasilkan faktor percanggahan SHE dan kos indeks

dengan beban dan skor risiko yang dinormalkan untuk membangunkan FCP terwujud pada peringkat reka bentuk proses, dan boleh dijangka sebagai alat yang lebih realistik untuk mengurangkan sumber risiko SHE secara proaktif, asas dan ekonomik.

**Kata kunci:** Keselamatan terwujud, Kesihatan terwujud, Perlindungan alam sekitar, Kos pertambahan, Reka bentuk proses kimia

Universiti Malaysia



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## **List of Symbols and Abbreviations**

5M1E	Man, Machine, Material, Method, Measurement, and Environment
AHP	Analytic Hierarchy Process
ALARP	As Low As Reasonably Practicable
BDPO	Baseline Design Processing Option
BE	Basic Engineering
BLEVE	Boiling Liquid Expanding Vapor Explosion
BN	Bayesian Networks
CI	Consistency Index
CR	Consistency Ratio
CR	Environment
E1	Explosiveness
EC	Economic Concern
ED	Early Design
EP	Economic Performance
F	Flammability
F&EI	Fire and Explosion Index
FCP	Friendlier Chemical Processes
FMEA	Failure Mode Effects Analysis
FTA	Fault Tree Analysis
HAZOP	Hazard and Operability Analysis
H	Health

HF	Human Factor
HQI	Health Quotient Index
I	Inventory
I2SI	Integrated Inherent Safety Index
IETH	Inherent Environmental Toxicity Hazard
IOHI	Inherent Occupational Health Index
ISD	Inherently Safer Design
ISI	Inherent Safety Index
ISIC	Inherent Safety Implementation Cost
ISM	Inherently Safer Modifications
ISM <sub>s</sub>	Inherent Safety Metrics
LPA	Layer of Protection Analysis
M	Moderate
MDPO	Modified Design Processing Option
MMA	Methyl Methacrylate
OEL	Occupational Exposure Limit
OHI	Occupational Health Index
P	Pressure
PCA	Principal Components Analysis
PE	Preliminary Engineering
PFD	Process Flow Diagram
PN	Petri Nets
PIDs	Piping and Instrumentation Diagrams

PIs	Primary Indicators
PIIS	Prototype Index for Inherent Safety
PRHI	Process Route Healthiness Index
PS	Process Stage
QRA	Quantitative Risk Analysis
R&D	Research and Development
RF	Relatively Friendly
RFPF	Reconciled Friendly Process Framework
RH	Relatively Hostile
RI	Random Index
SC	Special Concern
SHEC	Safety, Health, Environment, and Cost
SIS	Systematic Inherent Safety
SIIs	Secondary Indicators
T1	Temperature
T2	Toxicity
TIs	Ternary Indicators
TORCAT	Toxic Release Consequence Analysis Tool
VF	Very Friendly
VH	Very Hostile
Y	Yield

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## **CHAPTER 1: INTRODUCTION**

### **1.1 Background**

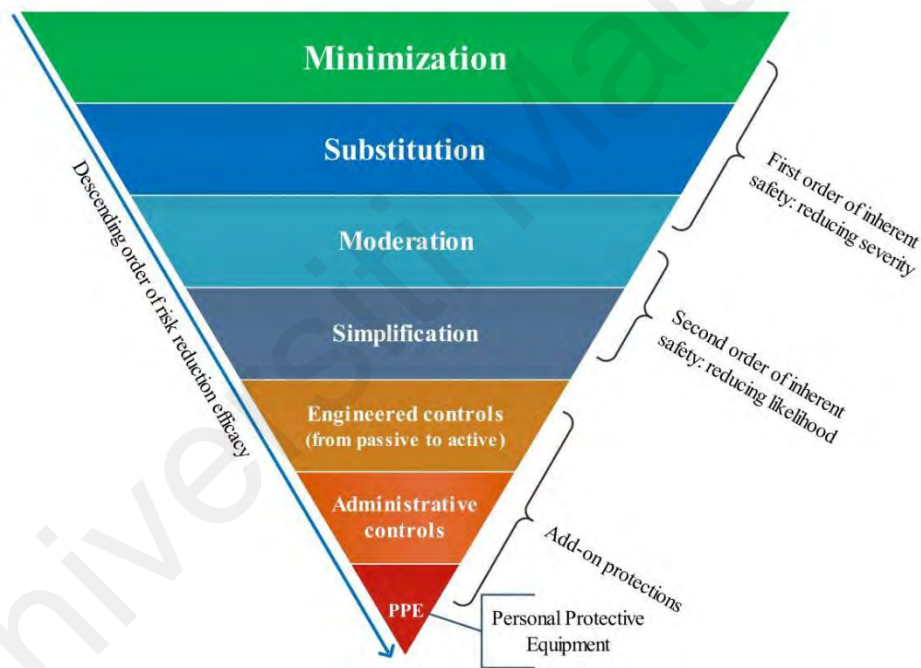
The chemical process industries are perceived as accident-prone promises due to the intrinsic and diverse safety risks from the chemical toxicity, flammability, explosiveness, corrosiveness, the high operating temperature and pressure, and the complex equipment and processes (Stoessel, 2020). The negative perception has been further enhanced by various high-profile chemical industry accidents around the world, such as the Flixborough disaster (1974, UK), the Beek explosion and fire accident (1975, Netherlands), the Seveso disaster (1976, Italy), the Bhopal disaster (1984, India), the Piper Alpha disaster (1988, UK), . To date, despite the increasingly comfortable safety conditions arising from the advances in materials and engineering technology (Tao et al., 2020), the occurrences and consequences of chemical process accidents have not yet been substantially reduced (Khan et al., 2015). Also, the further expanded chemical industries, both in plant size, location, and process complexity, reinforce the need of handling hazardous substances involved in the resultant enlarged storage, inventory, operation, and transportation units (Athar, Shariff, & Buang, 2019; Rajagopalan et al., 2019). Worldwide, the scale of the chemical industry keeps growing (exceeded US\$5 trillion in 2017 and is expected to double by 2030) (United Nations Environment Programme, 2019), which in turn intensifies chemical accidents with huge casualties over the last decade. Statistically, approximately 65,000 deaths were caused by

technological chemical incidents between 2009 to 2018 around the world (World Health Organization, 2021), implying that there remain endeavors to explore the chemical process safety problems.

To cope with the increased safety requirements, various remedial measures, as is often the case, are added for safety risk mitigation. Ironically, these kinds of add-on safety barriers are always advanced by tragic events or compulsory corrective actions (Kidam et al., 2016). By that time, it may be too late or too practically constrained to make changes over the processes in commission. Also, the add-on protections appear to be costlier than inherent safety (Khan & Amyotte, 2002) and do not perform any fundamental functions until a process upset occurs (Amyotte, Goraya, et al., 2007). To develop proactive safety measures and reduce the lifetime costs as a cohesive part of process operation, the risk components are addressed in the design stage, which led to the early conception of inherent safety. Formally, the prototype and implementation of inherent safety were first proposed by Kletz (1978, 1985) based on the fact that the best way to prevent leak accidents is to avoid the use or storage of large quantities of hazardous materials.

Since the inception, inherent safety has received considerable accomplishments in risk management and loss prevention, which can be summarized as follows: 1) its philosophical methodology has been becoming a well-accepted concept even common practice for process safety researchers and practitioners (Edwards et al., 2015), 2) a good number of assessment tools, dedicated for various process stages and hazards, have been developed and improved (Zainal Abidin et al., 2018), and 3) inherent safety

concept has been incorporated into a more inclusive scope for proactive risk management (CCPS, 2019). As shown in Figure 1.1, in contrast with the passive, active, and procedural safeguards that respectively need to be inspected, tested, and audited regularly, inherent safety has been regarded as the top hierarchy in the cycle of risk management (Athar, Shariff, & Buang, 2019). This is analogous to the Layer of Protection Analysis (LPA), where inherent safety is positioned as the central to indicate its most straightforward, robust, and reliable attributes to accident and loss prevention (Amyotte & Khan, 2021).



**Figure 1.1: The overall safety risk management strategies**

Thus far, inherent safety has been employed as a preferable safeguard to unearth fundamental, permanent, and economical choices to eliminate or significantly reduce risks at their sources without relying on too many end-of-pipe (i.e., engineered and procedural) protections (Amyotte & Khan, 2021). Over the intervening years, inherent safety has been recognized and promoted by many process safety researchers and



practitioners in the light of Professor Trevor Kletz (1922–2013) (Amyotte, 2020), who is regarded as the father of inherent safety. In this regard, the productive pioneers and their cooperation networks have been presented via a bibliometric analysis together with country distribution and keyword density visualization (Athar, Shariff, & Buang, 2019). In current practice, the inherent safety concept has been used as an inclusive way for developing friendly chemical plants (Kletz, 1989; Kletz, 1990; Kletz, 1991; Kletz & Amyotte, 2010), which can be largely characterized by the proactive enhancements in safety performance, environmental protection, industrial hygiene, and waste disposal (Khan & Amyotte, 2002; Kletz & Amyotte, 2010). By way of explanation, the concept of inherent safety can be well-illustrated through the adage: prevention is better than cure (Khan & Abbasi, 1998a). This proactive concept makes inherent safety function harmoniously with other cleaner technologies like pollution prevention and green chemistry in achieving sustainable societies (Khan & Amyotte, 2003), verified by their highly related and intertwined implementation principles (Anastas & Eghbali, 2010; Kletz & Amyotte, 2010). More specifically, inherent safety attempts to prevent risks that pose not only immediate dangers but also chronic environmental contamination. As such, the synergies of inherent safety, pollution prevention, and green chemistry present the common goals in pursuing 1) less manufacturing wastes, 2) molecules with less Persistent, Bio-accumulative, and Toxic substances (PBTs), and 3) processes with less built-in hazards (Mulholland et al., 2000). In practice, inherent safety concept, besides the chemical process industries where it was proposed, has been extended and incorporated into many other fields, including offshore operations (Khan & Amyotte,

2002), nuclear operations (Sofu, 2015), dust explosion prevention and mitigation (Amyotte, Pegg, et al., 2007), process safety management (Amyotte, Goraya, et al., 2007), human error reduction (Wahab et al., 2016), risk-based process plant design (Rathnayaka et al., 2014), inherent occupational health (Hassim & Edwards, 2006), inherent environmental friendliness (Gunasekera & Edwards, 2006), and inherent SHE (Safety, Health and Environment) (Anuradha et al., 2020).

## **1.2 Problem statement**

The inherent safety concept based chemical process design has a primary focus on the loss prevention and risk management from the Safety (S) side, a secondary focus on the occupational Health (H) improvement, and a directly linked benefit to the Environmental (E) protection (Khan & Amyotte, 2004) and the lifetime Cost (C) reduction (Khan & Amyotte, 2002). With this perception, it has been an established fact that implementing inherent safety concept can create inherently Friendlier Chemical Processes (FCP) (Kletz, 1989; Kletz, 1990; Kletz, 1991; Kletz & Amyotte, 2010) with integrated SHEC benefits. However, there is still a need of developing a holistic framework that can inclusively reconcile the separate SHEC dimensions for indicating and generating inherently FCP. The existing associated studies give little attention to the weights and dimensions of the risk factors. Without considering the risk weights, the minor risk factors are equally treated with the major. Without considering the risk dimensions, the risk scores with different units are directly added together to derive an overall score. These problems have puzzled researchers and practitioners for years and

can make the risk assessment results less realistic. Besides, the existing associated studies lack sufficient consideration of the incremental costs of implementing the "inherent" principles for modifying the baseline design, which cannot reveal whether the incremental costs can conceal or twist the overall inherent friendliness. To overcome these problems, this study is going to develop a more realistic framework to indicate and generate the inherently FCP during the design stage.

### **1.3 Research questions**

The relevant research questions going to be addressed in this study are defined as follows:

- 1) What are the existing solutions to demonstrate the inherent friendliness of chemical processes?
- 2) What are the limitations of the existing solutions that consider SHE components in demonstrating the inherent friendliness of chemical processes?
- 3) Are there any implications to incremental cost for carrying out inherent SHE oriented design modifications?
- 4) Can a reconciled framework with incremental cost considerations be developed for modifying baseline process routes towards inherent SHE options?
- 5) Can the proposed framework be implemented successfully for a selected case study at the design stage?

## **1.4 Aim and objectives**

This study aims to develop a dedicated framework to indicate and generate inherently Friendlier Chemical Processes (FCP) by "inherent" principles based design modifications for safety, health, environment, and related cost problems at the design stage. Accordingly, five stepwise objectives are defined to realize the aim.

- 1) To apply the "inherent" methods to develop inherently Friendlier Chemical Processes (FCP) with SHE elements.
- 2) To develop a reconciled SHE framework to compute the inherent friendliness of chemical process routes based on the currently available metrics.
- 3) To incorporate incremental cost elements into the SHE framework.
- 4) To apply the newly developed inherent friendliness framework with a selected chemical process for case study.
- 5) To generalize the procedures of implementing the newly developed inherent friendliness framework.

## **1.5 Scope of the study**

The focus of this study is the development of the dedicated inherent Safety, Health, Environment, and Cost (SHEC) framework to indicate and generate inherently Friendlier Chemical Processes (FCP) based on inherent safety concept during design stages. The scope of this study is limited to 1) chemical processes, 2) design stage, 3) process safety, 4) occupational health and environmental protection, and 5) incremental

cost. It is pertinent to note that this study used and adapted the data from the published literatures since the core novelty of this study lies in the development of the inherent Safety, Health, Environment, and Cost (SHEC) framework. As such, testing and validating the published data fall outside the scope of this study.

## **1.6 Novelties**

As per the problem statement, research questions, and the aim and objectives, the novelty of this study lies in the development of a dedicated framework to indicate and generate inherently Friendlier Chemical Processes (FCP) based on Safety, Health, Environment, and Cost (SHEC) dimensions. The newly developed measurement tool will incorporate the weighting solutions of the conflicting sub-indices of the selected Safety, Health, Environment, and Cost (SHEC) indices, the normalizations of risk scores with different units, the integration of incremental costs of implementing "inherent" principles based design modifications, and the comprehensive models to hierarchically reconcile the selected Safety, Health, Environment, and Cost (SHEC) indices.

## **1.7 Thesis outline**

### **1.7.1 Chapter 1: Introduction**

The introduction chapter depicts the epitome of the whole study. Firstly, the background of this study, including the safety situations of chemical process industries, the overall

safety management strategies, and a brief state of the art regarding inherent safety was described, and then the existing problems in using inherent safety concept to develop inherently Friendlier Chemical Processes (FCP) were stated. Subsequently, based on the problem statement, the research questions, aim and objectives, scope and novelties of this study were clarified.

### **1.7.2 Chapter 2: Literature review**

This section reviewed the literatures associated with inherent safety and its concept based explorations. Firstly, the origin and early development, implementation principles, implementation stages, implementation benefits of inherent safety were investigated, and then the Inherently Safer Design (ISD) principles and their implementation spectrum were analyzed. Subsequently, various Inherent Safety Metrics (ISMs) including cost metrics were compared. Then, the prominent industrial applications of inherent safety in offshore industries, nuclear industries, dust explosion prevention, and risk-based safety interventions were presented. Lastly, a synopsis was offered to succinctly present the purposes, methods, and main findings of the literature review on the inherent safety concept and its extended applications.

### **1.7.3 Chapter 3: Methodology**

This section includes the methods to realizing the aim and objectives. Firstly, the inherent SHEC metrics were selected, and then the risk weights and scores of the conflicting factors in the selected Safety, Health, Environment, and Cost (SHEC)

metrics were addressed using and Analytic Hierarchy Process (AHP) and fuzzy logics. Subsequently, Bayesian Networks (BN) were adopted to hierarchically integrate the selected Safety, Health, Environment, and Cost (SHEC) metrics to thus develop a Reconciled Friendly Process Framework (RFPF) for generating inherently Friendlier Chemical Processes (FCP). This section also includes the quality control measures, inherently friendlier modification dimensions, and case study information.

#### **1.7.4 Chapter 4: Results and discussion**

The results of developing Reconciled Friendly Process Framework (RFPF) and its demonstration and validation in the biodiesel production process were presented and discussed in this section based on the obtained information from the Baseline Design Processing Option (BDPO) to the Modified Design Processing Option (MDPO). In the BDPO, the results of the selected Safety, Health, Environment, and Cost (SHEC) metric weights and risk score normalization were first discussed, and then the RFPF values were concluded for indicating the inherent friendliness. In the MDPO, the "inherent" interventions and RFPF results were analyzed. Meanwhile, RFPF was also compared with the existing studies used for proactively incorporating SHEC considerations in chemical process design. Besides, the implications of the graphical inherent friendliness assessment tools, incremental cost, design modification manners, hybrid inherent safety concept, and application guidelines were also discussed.

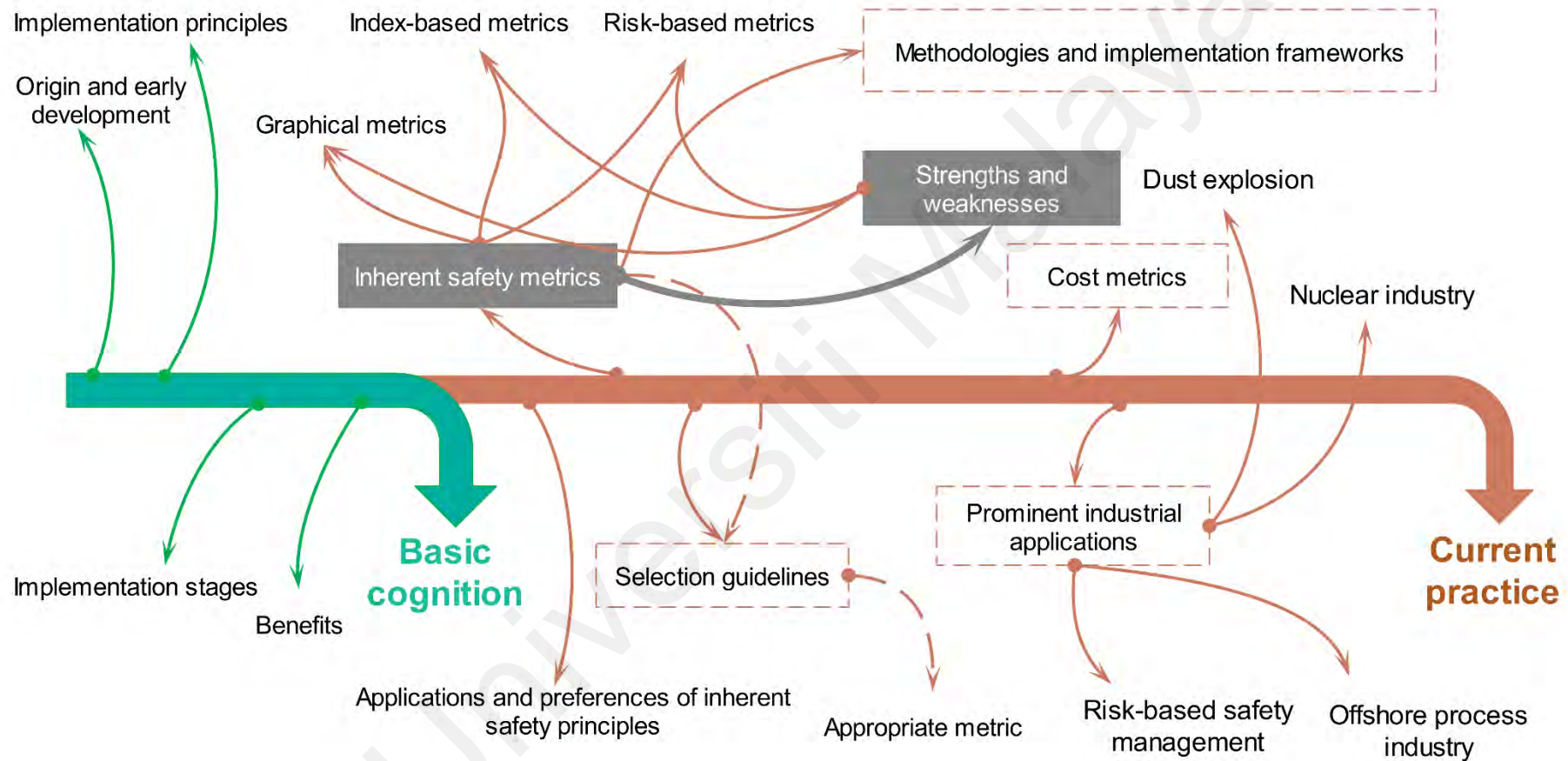
### **1.7.5 Chapter 5: Conclusion and recommendation**

This section reviewed the key points of the aim and novelties, stated the answers to the main research questions, and reflected the implications of the development of the Reconciled Friendly Process Framework (RFPF) to measure and compare the inherent friendliness of the chemical processing options. This section also described the knowledge contributions, clarified the limitations of the study, and presented some research recommendations as the ways forward.



## CHAPTER 2: LITERATURE REVIEW

Since the inception of inherent safety in the 1970s, significant progress has been made in using it to develop FCP which is largely characterized by proactive and simultaneous augmentation in safety, health, environment, and economic performance. This section investigated the development spectrum of inherent safety with a primary focus on the ISMs in chemical processes. Firstly, the basic cognition for inherent safety was encapsulated from its origin, early development, principles, implementation stages, and benefits. Subsequently, its current practice for creating FCP was highlighted via synthesizing the applications and preferences of inherent safety principles. With particular focus, the numerous ISMs were categorized into index-based, risk-based, graphical, and SHE-based to compare their development methodologies, typical implementation frameworks, and strengths and weaknesses. For selecting appropriate ISMs, a brief guideline was presented considering the inherent friendliness index preferences, implementation stages, case study concerns, and citation strengths. Considering the cost implication is the essential component of the inherent friendliness, the cost issues were reviewed. To demonstrate some real practice, the prominent industrial applications of inherent safety in the offshore process industry, nuclear industry, dust explosion prevention, and risk-based safety management were also presented. The overview of the literature review is presented in Figure 2.1.



**Figure 2.1: The overview of the literature review**

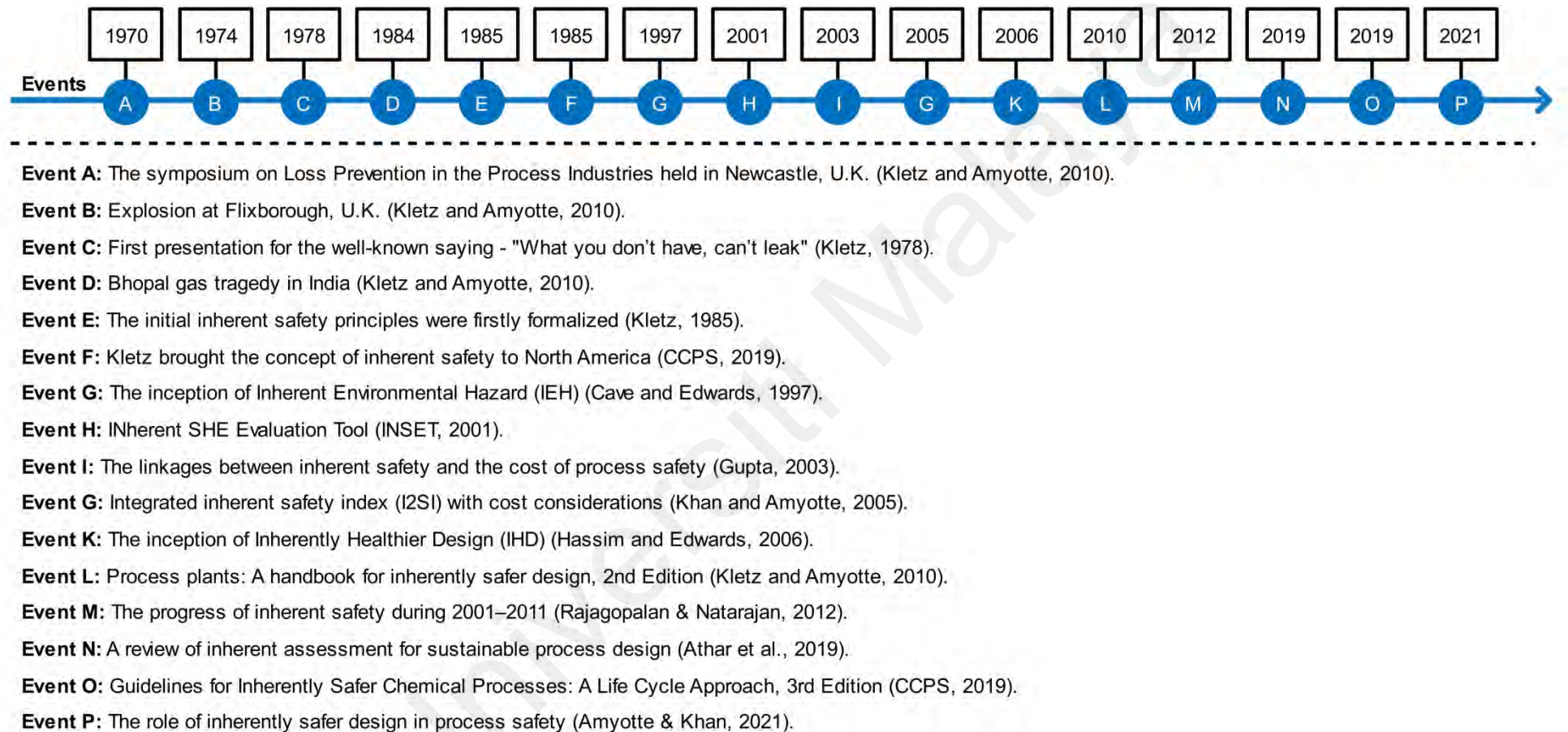
## **2.1 The basic cognition for inherent safety**

In this section, the basic cognition for inherent safety is introduced to illustrate the "inherent" concept. Accordingly, the established knowledge including the origin and early development, implementation principles, implementation stages, and implementation benefits was presented to understand the inherent safety and its concepts.

### **2.1.1 The origin and early development of inherent safety**

Inherent safety, with its varied terms such as ISD, Intrinsic Safety (IS), Inherently Safer Principles (ISP), Inherently Safer Technology (IST), and Inherently Safer Chemistry (ISC), is a modern concept with age-old applications that can date back to prehistoric times. For example, building sheep pens where there are no wolves is better than protecting them through fences (add-on passive engineered protections). The inherent safety concept was first formalized by Professor Trevor Kletz (Amyotte, 2020) in the 1970s. In the subsequent years, the accidents of the Flixborough explosion (1974, U.K.) and the Beek explosion (1975, Netherlands) boosted inherent safety growth. After that, a famous paper titled "What you do not have, cannot leak" was presented (Kletz, 1978). This presentation is deemed as the initial formal introduction for inherent safety (Khan et al., 2020), and it also laid the foundation for its subsequent development in the process industries (Rajagopalan & Natarajan, 2012). In 1985, the initial inherent safety principles were first formalized as substitution, intensification, attenuation, and

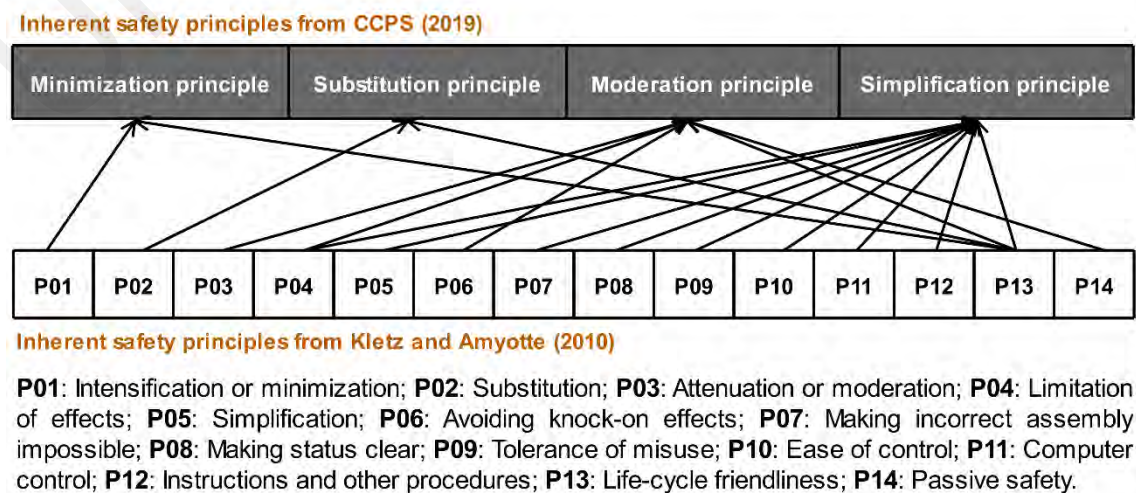
simplification (Kletz, 1985). When the time comes to the early 1990s, inherent safety interest picks up speed due to a spate of chemical catastrophes (e.g., Bhopal, Mexico City, Piper-alfa, Philips Petroleum incidents) during this period (Khan et al., 2020). With the development of inherent safety towards a conscious and optimal risk management strategy, its engineering education has been taken into the agenda. In this regard, Gupta and Edwards (2002) identified the insufficient awareness of using the ISD concept among scientists, engineers, managers and regulators, and proposed corresponding solutions by teaching students, conducting short courses, and publishing case studies. Likewise, Edwards et al. (2015) and CCPS (2019) initiated ISD teaching in undergraduate chemistry, chemical engineering, and related disciplines for reserving talents. More specifically, from inherent to procedural safety interventions, a recent study (Gunasekera et al., 2020) exemplified an engineering curricula framework for teaching safety protocols through reactor design. To date, impressive accomplishments in using inherent safety for loss prevention have been achieved, benefiting from its well-recognized proactive solution. In line with the temporal achievements, the scientific milestones with the development of inherent safety concept are encapsulated, as shown in Figure 2.2.



**Figure 2.2: The scientific milestones of the development of inherent safety concept**

### 2.1.2 The implementation principles of inherent safety

Generally, inherent safety can be done by a cohesive set of implementation principles. Kletz (1985) first formulated the initial inherent safety principles as substitution, intensification, attenuation, and simplification. Then, the concept of inherent safety was extended in various ways with its increasing recognition and awareness among safety researchers and practitioners, thus forming various inherent safety principles. In this regard, examples may include hybridization and stabilization used for respectively transferring risks and ensuring dynamic stability (Edwards, 2009), and segregation used for limiting hazard penetration and escalation through distance, barriers, or other pro-protective measures (INSET, 2001). Holistically, Kletz and Amyotte (2010) elucidated and compared the various strategies and formalized a cohesive set of fourteen implementation inherent safety principles. Furthermore, CCPS (2019) compared the fourteen principles and grouped them into four major ISD principles, as shown in Figure 2.3.



**Figure 2.3: The cohesive relationship of inherent safety principles**

As can be seen from Figure 2.3, the four ISD principles formed a set of representative protocols by which various inherent safety principles are encompassed. Of the ISD principles, minimization is preferable to substitution as it can save more in process capital investment. As the alternatives of the substitution, the moderation and simplification aim to make reaction conditions less extreme and easier to operate (Kletz & Amyotte, 2010). Besides, the minimization, substitution, and moderation are generally used to reduce the risk severity, whereas simplification is preferably employed to minimize the risk likelihood (INSET, 2001).

### **2.1.3 The implementation stages of inherent safety**

Process safety design is a complex activity that needs to suffice for the features of various process stages. This implies that the indices, weights, reconciliation strategies, and other possible implications should be tailored when developing inherently safer solutions. For instance, during the route selection stage, the main safety objective is to ascertain and isolate the hazards that are from the reactions and chemicals involved in the available process routes. Accordingly, an expert system was developed according to the data availability in this stage (Palaniappan, Rajagopalan, et al., 2002a). Then, this expert system was further adapted to the safety objective in the later flowsheet development stage (Palaniappan, Rajagopalan, et al., 2002b). Based on the data availability and safety objective on the various phases of the design and early engineering stage, inherently healthier design was successively conducted for process Research and Development (R&D) stage (Hassim & Hurme, 2010c), Basic Engineering

(BE) stage (Hassim & Hurme, 2010a), and Preliminary Engineering (PE) stage (Hassim & Hurme, 2010b). Likewise, inherent SHE design and cost assessment were customized to the R&D stage (Liew et al., 2014), BE stage (Liew et al., 2016), and PE stage (Liew et al., 2015).

In practice, the above three successive phases, together with the idea phase, constitute the best timing for implementing inherent safety. Notably, there are still a limited number of items (e.g., selection of substances/materials, quantities, and operations) that can be considered to incorporate the ISD concept during the phases before PE. Subsequently, most major decisions will be made, and most of the process information will be available. When it comes to the PE stage, it will be the last step when inherent safety can be incorporated at a moderate cost (Hurme & Rahman, 2005). As such, the Early Design (ED) stages (Rajagopalan & Nhan, 2008), generally consisting of the idea, R&D, and BE phases, were often used for the sake of easier and cheaper inherent safety interventions. Other similar terms may include the initial design stage (Khan & Amyotte, 2003), conceptual design stage (Ruiz-Femenia et al., 2017), and preliminary design stage (Athar, Shariff, Buang, Shaikh, et al., 2019).

More inclusively, CCPS (2019) demonstrated the potentials of iteratively integrating inherent safety concept with the entire footprint of a process Life Cycle (LC), though its application during the early phases of process design stage would be easier and cheaper. From the ED stage to the decommissioning stage, the researchers and regulatory authorities (CCPS, 2019; Hurme & Rahman, 2005; Kidam et al., 2016; Rathnayaka et



al., 2014) presented multiple classifications for the timing of implementing inherent safety. Based on these classifications, the progressions of a process lifetime with reiterated inherent safety opportunities are specified into four representative stages: 1) process development and design stage, 2) construction stage, 3) operation, maintenance, and modification stage, and 4) decommissioning stage. The corresponding potentials of applying inherent safety are briefly discussed as follows.

In the process design stage (mainly comprising the ED phase), the key objective is to generate and compare process options with promising benefits in SHE and cost dimensions. Meanwhile, the designers have the greatest opportunity to implement inherent safety principles by, for example, selecting process routes with less hazardous raw materials and intensified layout based on the available information from Process Flow Diagram (PFD) and feasibility study. In this regard, Castillo-Landero et al. (2019) developed a trade-off methodology for different levels of process intensification with simultaneous considerations on inherent safety, economic, and sustainability for minimizing the number of equipment pieces. As the process proceeds to the construction stage from the BE phase, the main task is to complete the whole process according to the Piping and Instrumentation Diagrams (PIDs) and plot plan. In the interim, the primary considerations for incorporating inherent safety are moderating the mechanical design, checking equipment installation, testing processing facilities, and training operators. When the process evolves to the third stage, enhancing operation skills (e.g., vocational training and work permit) can protect against the decay of inherently safer features implemented and documented in the former two stages. In

addition, the periodical process maintenance, modifications, and safety re-validations would reassign new opportunities to consolidate the inherently safer level through updating more reliable and robust equipment or adopting more effective and less hazardous reaction materials, though no changes are welcomed in this stage. In the final stage, the ISD concept and principles can do a better service for facilitating equipment dismantling, site reuse, and environmental clean-up, thus promoting cleaner processes of closure and post-closure activities. As a case in point, an inherently safer closure can be accomplished by eliminating or reducing the volume of hazardous substances to be removed from the surrounding production environment.

#### **2.1.4 The benefits of implementing inherent safety concept**

Implementing inherent safety concept has been recognized with a primary focus on loss prevention and risk management from the safety side, a secondary focus on occupational health improvement, and a directly linked benefit to environmental protection (Khan & Amyotte, 2004). Besides, inherent safety based chemical process design option is proved to be cheaper than that with extensive end-of-pipe protections considering the lifetime costs (Khan & Amyotte, 2005). This implies that the principal benefits of implementing inherent safety concept can be positive to the SHE enhancement and lifetime cost reduction.

##### **2.1.4.1 Safety, Health and Environmental (SHE) enhancement**

In practice, there has been an increased recognition for this benefit afforded by various

paradigms within SHE fields (see Table 2.1). Also, many efforts have been made to incorporate inherent SHE as an integral part of process design (Shah et al., 2003) concerning their strong correlations among SHE indices (Hassim et al., 2008). Especially, inherent SHE-based synthesis route selection during the various phases of the process design stage has been given great attention (Anuradha et al., 2020), in which the safety, health, and environmental considerations can be synergistic for ranking and selecting inherently friendlier process options.

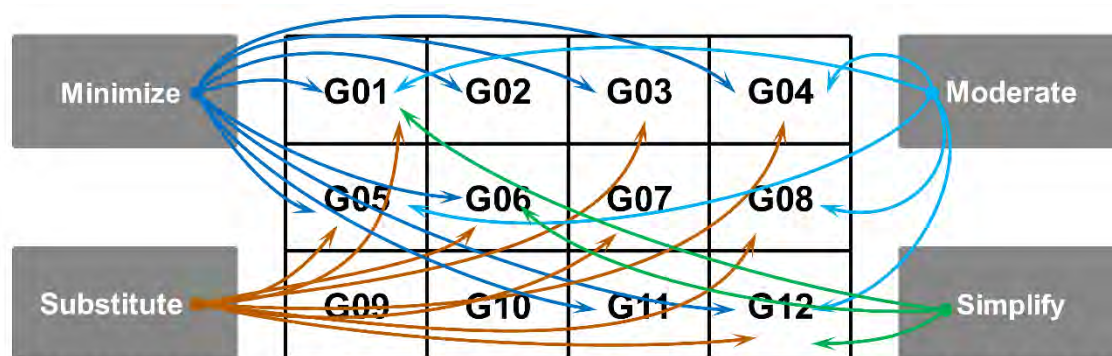
**Table 2.1: Paradigms available for integration within a SHE framework**

Paradigm	Safety	Health	Environment
Inherent safety	a	b	c
Pollution prevention		c	a
Green chemistry	b	c	a
Green technology	c		a
Design for the environment		c	a

a: primary focus, b: secondary focus, c: directly linked benefit.

As shown in Table 2.1, the inherent safety concept and its practice are useful for enhancing occupational health and environmental protection, though tackling the safety risks at the earliest process design stages is the original and primary focus. Particularly, the tangible and intangible benefits for SHE can be well-illustrated with the green chemistry principles (Anastas & Eghbali, 2010), where the inherent safety concept can match its various implementation principles, as shown in Figure 2.4. For example, of the twelve green chemistry principles (Anastas & Eghbali, 2010), the third principle - design less hazardous chemical syntheses - aims to use and generate substances with little or no toxicity to either humans or the environment; the fifth principle - use safer solvents and reaction conditions - aims to select less hazardous solvents, separation

agents, or other auxiliary chemicals if inevitable; the twelfth principle - inherently safer chemistry for accident prevention - aims to eliminate the potentials of chemical accidents. As evident, the implementation principles of ISD and green chemistry share the concept of fundamentally reducing or eliminating the use and generation of hazardous substances and processes. Besides the obvious connections as presented in Figure 2.4, the latent associations between the principles of ISD and green chemistry could be perceived as neither ISD nor green chemistry principles are defined with sharp boundaries (Anastas & Eghbali, 2010; Kletz & Amyotte, 2010). In practice, guided by their principles, ISD and green chemistry could complement each other and synergize in attaining sustainable societies. In this regard, various real ISD applications have been reported for embracing green chemistry. For example, Patel et al. (2010) adopted Computer Aided Molecular Design (CAMD) to select inherently safer solvent substitutes for liquid extraction of acetic acid-water mixture. Likewise, Medina-Herrera, Grossmann, et al. (2014) developed a multi-objective optimization approach to proactively identify safer and cheaper solvents. Furthermore, Guillen-Cuevas et al. (2018) developed a Safety And Sustainability Weighted Return On Investment Metric (SASWROIM) during the process preliminary design stage to assess the comprehensive impacts of inherent safety, sustainability, and economic viability.



G01: Prevention (waste); G02: Atom economy; G03: Less hazardous chemical syntheses; G04: Designing safer chemicals; G05: Safer solvents and auxiliaries; G06: Design for energy efficiency; G07: Use of renewable feedstocks; G08: Reduce derivatives; G09: Catalysis; G10: Design for degradation; G11: Real-time analysis for pollution prevention; G12: Inherently safer chemistry for accident prevention.

**Figure 2.4: Approximate matching of inherent safety principles with green chemistry principles**

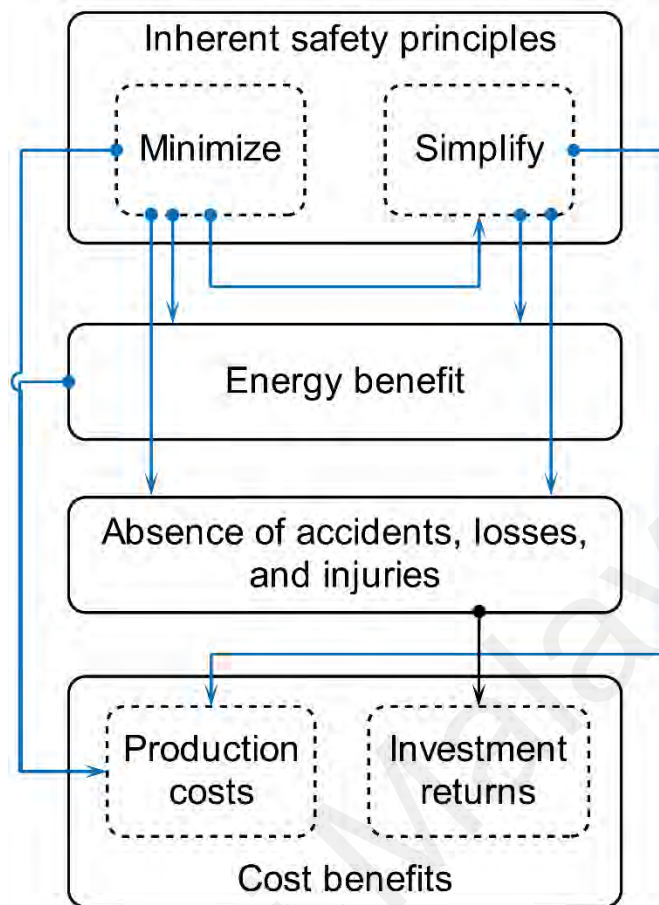
#### 2.1.4.2 Cost reduction of inherent safety based processes

Numerous pioneering researches (Gupta et al., 2003; Hendershot, 1997; Khan & Amyotte, 2005; Kletz & Amyotte, 2010) have demonstrated that the life time costs (both fixed costs from supporting facilities and dependent costs from operations, maintenance, modifications, decommissioning, etc.) of developing inherently safer processes are much cheaper than the total costs of major accidents (Khan & Amyotte, 2005). In terms of the fixed costs, the conventional processes or plants may be cheaper; however, they would turn out to be costlier once including the other costs from the latter maintenance, modifications, and the losses of life, property, business interruption, etc. (Srinivasan & Iqbal, 2018). Notably, incorporating inherent safety strategies during the earliest phase of the process design stage would produce the maximum efficacy for cost savings. In contrast, the costs of fixing safety problems would explode by 1,000 times at the post-incident stage (see Table 2.2) (Kletz & Amyotte, 2010). Generally, the cost savings, both for production costs and investment returns, stem from the proactively

reduced hazardous materials and simplified equipment operations (Kletz & Amyotte, 2010). This implies that, of the ISD principles, minimize and simplify could be endowed with the major expectations for economic friendliness as shown in Figure 2.5. More specifically, the minimized (or intensified) and simplified processes can reduce the capital and operating costs by cutting down purchasing, testing, monitoring, and maintaining add-on protective equipment (Edwards, 2005). On the other hand, if the inventories can be reduced, another noticeable cost saving will come from the land use due to resultant reduction in the size of pipework, structures, and foundations (Kletz & Amyotte, 2010). Also, as a free ride, the recycles of unconverted raw materials can be reduced without pushing them repetitively throughout the processes, thus leading to cheaper material conveying with simple and energy-efficient operations. It is pertinent to note that the process design, as well as the later operation and maintenance, could be outsourced to different entities; therefore, it would need a specialized team for the whole lifetime to follow and to assess inherent safeness to thus assure the envisaged cost reduction.

**Table 2.2: Relative cost of fixing safety problems at different process stages**

Stages	Relative cost
R&D stage	1
Process flowsheet stage	10
Final decision stage	100
Production stage	1000
Post-incident stage	10000



**Figure 2.5: Cost-benefiting routes of implementing inherent safety**

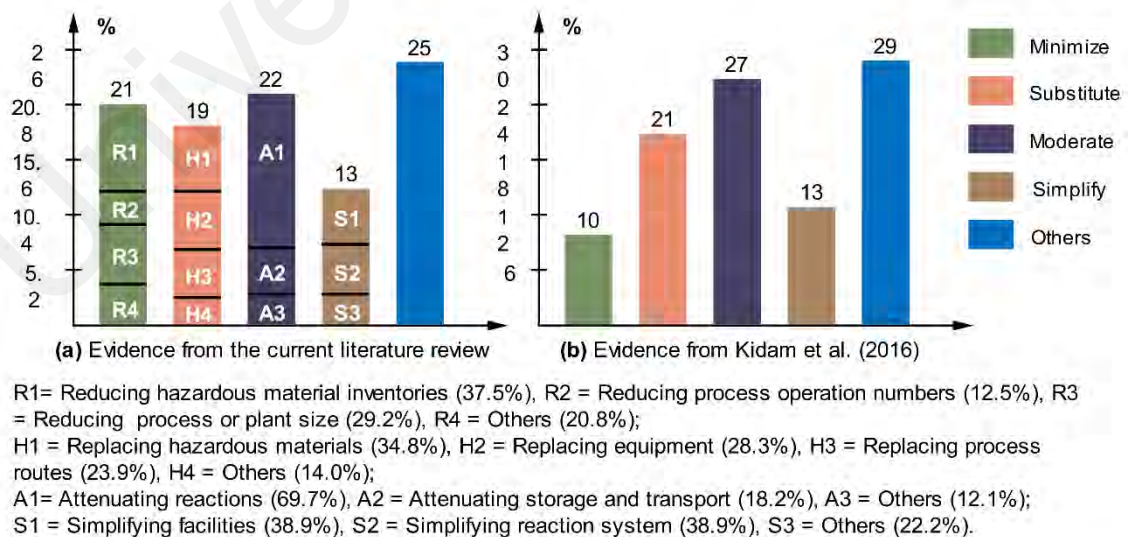
In this section, the established knowledge was presented to introduce inherent safety and its concepts. The inception of inherent safety was first encapsulated from the perspectives of time, location, person, and event with some milestones of the inherent safety development. Then, the fourteen elucidated inherent safety principles were illustrated and compared with the four main inherent safety principles. Subsequently, based on the fact that inherent safety is applicable during the entire process life cycle, the implementation opportunities were discussed successively from the R&D, BE, PE stages to the construction, operation, maintenance, modification, and decommissioning stages. Lastly, the prominent benefits of implementing inherent safety concept were analyzed from the SHE enhancement and the cost reduction effects.

## 2.2 Applications and preferences of inherent safety principles

FCP can be achieved and consolidated through implementing inherent safety concept throughout process lifetime. Wherein, the ISD principles are usually regarded as the most general and therefore widely applicable approaches as inherently safe processes or plants are rare in practice (Khan & Amyotte, 2002), enabling the popularity of using the comparative term (inherently safer). Various inherent safety principles can be used to develop FCP in the design stages or retrofit existing processes during the operation stage. It is pertinent to note that the published evidence also presented a welcoming trend toward using ISD terminology (Amyotte et al., 2018). With a primary focus on the ISD practice, this work systematically reviewed the preferences, level of applications, and gaps in using the fourteen inherent safety principles (Kletz & Amyotte, 2010) and figured out a relative frequency spectrum, as shown in Figure 2.6 (a). The application preferences for using the minimize principle implies that reducing the hazardous material and the size of process or plant account for approximately 67%, and relatively less attention is given to the reduction of process operation numbers; the spectrum for using the substitute principle reveals that replacing hazardous materials, equipment, and process routes consumes the major proportion (87%); the application preferences for using the moderate principle denotes that moderating chemical reactions is largely preferable (approximately 70%) compared with moderating transportation, storage, and other possible units; the application preferences for using the simplify principle discloses that nearly equal attention is devoted for simplifying process facilities and reaction systems, and other possible simplifications account for a relatively lower



percentage (approximately 22%). Similarly, Kidam et al. (2016) investigated Inherently Safer Modifications (ISM) based on 124 corrective actions documented in online databases and accordingly concluded the potentials of ISD principles for curing accidents, as shown in Figure 2.6 (b). As evident, there presented relatively consistent favorites in using the ISD principles. The only significant deviation on using the minimize principle may result from their research scope regarding process stages (i.e., the former focused on the lifetime inherent solutions, while the latter mainly examined the post-accident rectifications). Overall, FCP can be achieved through design and consolidated through retrofitting using inherent safety principles throughout the process lifetime. Of the fourteen principles, the four ISD principles are regarded as the most general and therefore widely applicable approaches since inherently safe processes or plants are rare in practice (Khan & Amyotte, 2002), enabling the popularity of using the comparative term (inherently safer).



**Figure 2.6: The application preferences of inherent safety principles**

### 2.3 Inherent Safety Metrics (ISMs)

ISMs have been proliferated over the past decades to compare and select inherently safer process options. The numerous ISMs have been classified into several categories, as shown in Table 2.3. As evident, index-based ISMs were recognized by Zainal Abidin et al. (2018) and Athar, Shariff and Buang (2019); risk-based ISMs were recognized by Zainal Abidin et al. (2018), Jafari et al. (2018), Athar, Shariff and Buang (2019), and Park et al. (2020); graphical metrics were recognized by Jafari et al. (2018) and Athar, Shariff and Buang (2019). On the other hand, with much literature, SHE-based metrics recently represent a welcoming trend in using inherent solutions. For these considerations, the index-based, risk-based, graphical, and SHE-based ISMs were selected to elaborate their methodologies, typical implementation frameworks, selection guidelines, and cost implications. It deserves noting that the four categories are not defined with sharp boundaries and the ISMs without clear abbreviations are re-named for facilitating the later drawing. Besides, the literature investigation mainly used the "snow ball" method (Greenhalgh & Peacock, 2005) – Firstly, the literatures from Professor Trevor Kletz, the father of inherent safety, were first reviewed; then, the associated review articles and literatures from the various pioneers as reported by Athar, Shariff and Buang (2019) were reviewed; lastly, the recently published literatures absent in the previous ISMs classifications were included in the present classifications.

**Table 2.3: The classifications for inherent safety metrics (ISMs)**

Categories	References
1) overall approach; 2) individual approach	Kidam et al. (2016)
1) index-based approach; 2) risk-based approach; 3) consequence-based approach	Zainal Abidin et al. (2018)
1) relative ranking approach; 2) advanced mathematical approach; 3) risk-based approach; 4) graphical approach; 5) hybrid approach; 6) equation-based approach	Jafari et al. (2018)
1) indexing method; 2) consequence and risk-based method; 3) graphical output method; 4) numerical output method; 5) computer aided tool; 6) optimization scheme; 7) experimental method	Athar, Shariff and Buang (2019)
1) hazard-based assessment tool; 2) risk-based assessment tool; 3) cost optimal assessment tool	Park et al. (2020)

### 2.3.1 Index-based inherent safety metrics

Like the Accident Hazard Index (AHI) (Khan & Abbasi, 1997) using a standard 1 - 10 scale, index-based ISMs are to establish and aggregate a set of numerical scales used to compare process routes (Park et al., 2020). In this respect, a good number of inherent safety indices were developed for comparing and identifying inherently safer process options; their coverage, however, may vary depending on the process stages, process flow sheets, production features, company interests, etc. In this context, this work mainly used the credible safety parameters (i.e., inventory, temperature, pressure, yield, toxicity, flammability, and explosiveness) (Edwards and Lawrence, 1993) as the benchmark to demonstrate and compare the research scopes regarding the metric indicators, which has not been presented by the previous review articles. Also, the economic concerns, special concerns, and implementation stages of the metrics are yet to clearly presented by the previous review articles. On the other hand, the occupational

health and environmental concerns are also incorporated considering its essential components in FCP, as shown in Table 2.4. Where, I: Inventory, T1: Temperature, P: Pressure, Y: Yield, T2: Toxicity, F: Flammability, E1: Explosiveness, EC: Economic Concern, H: Health, E: Environment, SC: Special Concern, PS: Process Stage (R&D, BE, PE, ED, LC).

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**Table 2.4: Index-based metrics for assessing inherent safety**

Terms	Metric indicators												PS	References
	I	T1	P	Y	T2	F	E1	EC	H	E	SC			
Prototype index for inherent safety, PIIS	√	√	√	√	√	√	√	√					ED	Edwards and Lawrence (1993)
Inherent safety index, ISI	√	√	√		√	√	√	√					ED	Heikkilä et al. (1996)
Fuzzy logic-based inherent safety index, FLISI		√	√		√	√	√						ED	Gentile et al. (2003b)
iSafe route index, iRI		√	√	√	√	√	√						ED	Palaniappan et al. (2004)
Integrated inherent safety index, I2SI		√	√		√	√	√	√		√			LC	Khan and Amyotte (2005)
Inherent safety index calculation, ISIC	√	√	√	√	√	√	√					√	ED	Abedi (2005)
Inherent safety index module, ISIM		√	√				√						PE	Leong and Shariff (2008)
Two-tier inherent safety index, 2TISI		√	√				√	√				√	PE	Leong and Shariff (2009)
Qualitative assessment for ISD, QAISD	√	√	√										PE	Rusli and Shariff (2010)
Enhanced inherent safety index (1), EISI-1	√	√	√		√	√	√			√			ED	Li et al. (2011)
Inherent safety index for explosion, ISIE		√	√			√	√					√	LC	Salzano and Di Benedetto (2012)
Process stream index, PSI			√			√	√					√	PE	Shariff et al. (2012)
Inherent safety key performance indicators, IS-KPIs	√											√	ED	Tugnoli et al. (2012)
Comprehensive inherent safety index, CISI	√	√	√		√	√	√		√				ED	Gangadharan et al. (2013)
Overall FLISI, OFLISI												√	ED	Tadic et al. (2014)
3-tier inherent safety quantification, 3TISQ			√		√							√	PE	Zaini et al. (2014)
Simplified I2SI, SI2SI		√	√		√	√							LC	Hua et al. (2018)
Inherent safety performance index, ISPI	√	√	√		√	√	√						PE	Song et al. (2018)
Optimizable fuzzy inherent safety index, OFISI	√	√	√			√			√				ED	Vázquez et al. (2019)
Inherent safety assessment for process equipment, ISAPE		√	√									√	PE	Athar, Shariff, Buang, Nazir, et al. (2019)
Extended inherent safety index (2), EISI-2	√	√	√		√	√	√					√	ED	Ee et al. (2019)
Extended process route index, EPRI	√	√	√			√	√					√	PE	Athar et al. (2020)
Multi-target inherent safety indices, MISI	√											√	ED	Crivellari et al. (2021)

### 2.3.1.1 Methodologies of the index-based inherent safety metrics

The PIIS, consisting of seven typical safety indices as exhibited in Table 2.4 is one of the pioneering inherent safety assessment tools. In the PIIS, each of the indices is divided into ten sub-categories assigned with numerical scores based on the Dow fire and explosion index, Mond index, and empirical judgments. The PIIS is two-fold by process scores and chemical scores, respectively for measuring the group of I, F, T2, E1 and the group of P, T1, Y. Eventually, the two scores will be added together to derive an overall score (the lower, the safer) based on the worst-case scenario for indicating the safety performance of a process route (Edwards & Lawrence, 1993). The PIIS covers most typical chemical hazards and offers an easy-to-use procedure for selecting inherently safer synthesis paths yet lacks sufficient considerations for the sources of process risks. In this regard, the ISI, an extension of the PIIS, further incorporated other risk sources (i.e., the heat of main and side reaction, corrosiveness, chemical interaction, equipment safety, process structure safety), offering a relatively wider range of factors affecting inherent safety assessment (Heikkilä et al., 1996). However, the ISI did not consider the interactions of the various indicators and the volume of chemicals and equipment used. These gaps were bridged by the ISIC (Abedi, 2005), the PSI (Shariff et al., 2012), the EISI-1 (Li et al., 2011), and the CISI (Gangadharan et al., 2013) which incorporated the number of chemical materials, the amount of equipment, the mixture properties, the compounding effect of materials and equipment. Based on the ISI, a recently developed EISI-2 (Ee et al., 2019) offers a comprehensive chemical, physical, and biological hazard analysis with the additional biological inherent safety index.

Among the index-based metrics, various fuzzy logic-based tools were explored to address the uncertainties, subjectivities, and sudden scoring jumps in the conventional the ISI procedures. For example, Gentile et al. (2003a) developed the FLISI based on fuzzy logic to assess the same process with the same input conditions of ISI, and the results demonstrated its advantages concerning complex chemical plants. Interestingly, the methodology of the FLISI was further extended to an overall FLISI for food inherent safety evaluation with special concerns on microbiological, chemical, and physical hazards (Tadic et al., 2014). In recent studies, a new fuzzy logic-based index called ISPI introduced supplemental hazard index apart from the two-fold indices (i.e., chemical hazard index and process hazard index) in the conventional PIIS and ISI, thus integrating more inclusive input parameters like process safeness, complexity, and operability (Song et al., 2018). Furthermore, the OFISI, another newly developed fuzzy logic-based index, presented a systematic methodology to optimize the safety level besides the function of inherent safety assessment (Vázquez et al., 2019). In contrast with the advantages of using fuzzy logic to address the uncertainties, the resultant mathematical knowledge-intensive implementation procedures may discourage potential users in practical applications. This problem can be well addressed using Monte Carlo Simulation (MCS) which is essentially math-free for solving complex mathematical equations (Ma et al., 2018). Accordingly, Ortiz-Espinoza et al. (2021) developed MCS-based uncertainty solutions to generate wide-ranging design variables for implementing safety metrics more extensively.

Generally, most index-based metrics focus on process route selection, while there often

lack sufficient considerations for selecting inherently safer mechanical materials, equipment characteristics, and economic performance evaluation. The former two deficiencies were respectively addressed in the ISAPE (Athar, Shariff, Buang, Nazir, et al., 2019) and the EPRI (Athar et al., 2020) by embracing process, chemical, and equipment aspects to design and build inherently safer equipment. The latter deficiency was improved by an extensively cited index called I2SI (Khan & Amyotte, 2004, 2005). The I2SI, built upon a framework like the HAZOP procedure, can simultaneously measure the hazards and costs for each option using inherent safety penitential index and inherent safety cost index, respectively. Based on the insightful two-fold considerations, the I2SI framework is further expanded with more inclusive functions (e.g., risk-based safety management) by the subsequent studies (Hua et al., 2018; Rathnayaka et al., 2014; Rusli et al., 2013). Besides, the I2SI can involve data-intensive procedures, which can be moderated using automated indexing tools like the iSafe (Palaniappan et al., 2004). The iSafe is an intelligent expert system by automating hazard analysis based on the safety objectives and data availability during the different phases of chemical process design.

Most of the initial indices are constrained by the process data absence during the process design stages. To address this limitation, a process simulator (i.e., HYSYS) was integrated into the ISIM for process safety assessment and ISD interventions (Leong & Shariff, 2008). As an evolution of the ISIM, the 2TISI presented a systematic approach for assessing inherent safety in two stages: 1) comparing and ranking various routes using process route index, and 2) conducting a preliminary inherent risk assessment

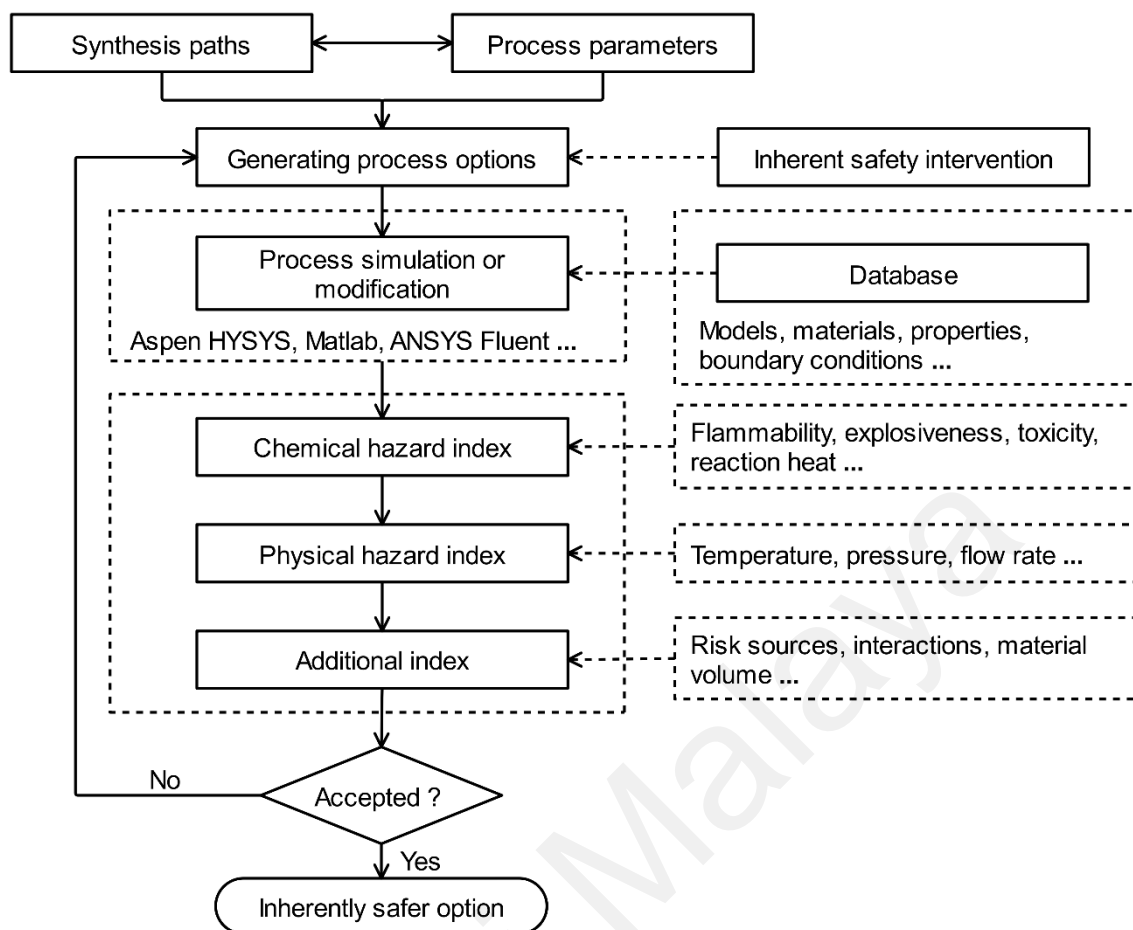


(Leong & Shariff, 2009). Likewise, the QAISD methodology consists of two stages (i.e., hazard identification and ISD option generation) and offers some clear tabulated ISD options (Rusli & Shariff, 2010). Afterward, the 2TISI was further extended as the 3TISI with special concern on toxic release assessment (Zaini et al., 2014). Despite the profound insight on explosiveness assessment, the 2TISI does not distinguish different explosion scenarios, and this defect could be overcome by the ISIE (Salzano & Di Benedetto, 2012) which includes considerations on unconfined and partially confined gas and vapor cloud explosion, confined gas, and vapor explosion, and confined dust explosion. In this respect, the PSI (Shariff et al., 2012) also offers an insightful assessment approach with special concern on explosion risks. It is worth noting that most of the index-based metrics focused much on the safety risks while gave limited attention to the security risks. In this respect, the IS-KPIs (Tugnoli et al., 2012) were developed as inclusive hazard identification and safety evaluation procedure with simultaneous consideration of external threats like malicious acts, external attacks, extreme weather conditions. More inclusively, the IS-KPIs were advanced as multi-target inherent safety indices (Crivellari et al., 2021) with extra concerns on human, assets, and environmental contributors to the safety profile of the offshore oil & gas production system.

#### **2.3.1.2 Typical implementation framework of the index-based inherent safety metrics**

Like the steps in Optimal Risk Analysis (ORA) (Khan & Abbasi, 2001), the typical implementation procedures of index-based ISMs comprise risk identification,

assessment, quantification, and estimation. In practice, the index-based ISMs furnished in Table 2.4 have expanded vigorously from the initial PIIS by integrating more hazard indicators. For example, supplemental hazard indices including process safeness, complexity, and operability were integrated with the conventional indices (i.e., chemical hazard index and process hazard index) to produce an aggregated index (i.e., ISPI) for better characterizing inherently safer process options. This implies that the risk assessment procedures of using the index-based ISMs could be more targeted by adding the risk considerations from, for example, the policy of a company or the goals of safety issues in hand. Accordingly, a typical indexing procedure (see Figure 2.7) could be represented by three steps: 1) finding and generating alternatives according to synthesis paths and process parameters, 2) conducting process simulation or data collection to characterize the alternatives, and 3) aggregating indices and ranking the alternatives with specific safety concerns. It is pertinent to note that inherent safety is a preferable but not stand-alone risk management strategy. For making reasonable safety strategies, inherent safety often works in concert with appropriate add-on safeguards (Amyotte & Khan, 2021).



**Figure 2.7: Typical implementation framework of the index-based metrics**

### 2.3.1.3 Strengths and weaknesses of the index-based inherent safety metrics

The major advantages of index-based metrics for measuring inherent safety lie in the ease of use in early process design stages, where the information on synthesis paths and operation parameters is still limited. Besides, the index-based metrics can merge various safety risks into an overall quantitative indicator for demonstrating safety performance, thus facilitating the selection of process alternatives without conflicts for balancing risk contributors. However, some evident disadvantages are also apparent with the personal judgments in determining index ranges, scoring index parameters, aggregating disparate sub-indices; on the other hand, the indexing procedures are often criticized due to the limited coverage of potential loss contributors, the missing data during process design

phases, and the unclear granularity of overall index value (Gupta & Edwards, 2003; Rajagopalan & Nhan, 2008). Furthermore, the index-based metrics might neglect, including the risk considerations from multiple entities with different preferences (National Research Council, 2012). This limitation was demonstrated using the I2SI (Khan & Amyotte, 2004), one of the extensively cited inherent safety metrics. Specifically, the I2SI, as well as most index-based metrics, offers a single numerical result that cannot be used to indicate the willingness of different process participants regarding risk acceptance (or tolerance). For example, the company owner may choose a process route with higher yield performance and be willing to tolerate a minor risk of fugitive chemical emissions, whereas the on-site employees always disagree with this trade-off concerning their occupational health.

In addition, the index-based risk assessment tools are often practically constrained due to subjective weights on various indices (Rajagopalan & Nhan, 2008). To address this problem, the weighting process is always needed for the synthesis of various indicators to reconcile the conflicting factors with considerations on their contribution to the comprehensive impacts. In this regard, the inherent safety indicators based on the power, temperature, and pressure were weighted during the development of the instability severity index (Ni et al., 2016). The weighting solution is based on the AHP method. The AHP, first precisely described by Saaty (1977), is one of the most popular methods for weighting conflicting factors in various fields (Ishizaka & Labib, 2011). The AHP has been extensively studied and used in nearly all domains of multiple criteria decision making (Ho & Ma, 2018) owing to its simplicities, flexibilities, and standard

implementation procedures. In practice, the AHP solutions have formed a systemic procedure, generally consisting of 1) establishing hierarchical structure mode, 2) constructing a set of pairwise comparison matrix, and 3) calculating weight vectors and consistency test (Leccese et al., 2020; Saaty, 2008). The essence of the AHP solutions lies in establishing and resolving pairwise comparisons to sort out the individual importance of competing entities, which can be used to determine the weights of the safety indicators. By the pairwise comparisons, the relative importance of the inherent safety indicators can be determined and incorporated into the development of the index-based ISMs.

### **2.3.2 Risk-based inherent safety metrics**

The process safety risk is defined as a function for indicating the severity of consequence and the likelihood of occurrence for an accident scenario (CCPS, 2019; Khan & Abbasi, 1998b). Guided by this definition, the hazard and consequence-based tools used for assessing inherent safety were collected and compared. In chemical processes, the types of risks can vary due to the characteristics and categories of chemical substances in use or manufacturing. Nevertheless, the risks could be largely represented by the indices in the PIIS due to its relatively complete spectrum for chemical safety risks. For this reason, the risks in the PIIS are employed as the main indicators to synthesize the features of risk-based ISMs, as shown in Table 2.5.

**Table 2.5: Risk-based metrics for assessing inherent safety**

Terms	Metric indicators												PS	References
	I	T1	P	Y	T2	F	E1	EC	H	E	SC			
Rapid risk analysis based design, RRABD	√	√	√				√	√				ED	Khan and Abbasi (1998a)	
Integrated risk estimation tool, iRET			√			√	√					ED	Shariff et al. (2006)	
Likely-loss fire and explosion index, LL-FEI							√					ED	Jensen and Jørgensen (2007)	
Key performance indicator, KPIs	√		√		√	√						ED	Tugnoli et al. (2009)	
Inherent risk assessment, IRA							√					PE	Shariff and Leong (2009)	
Toxic release consequence analysis tool, TORCAT		√	√				√				√	PE	Shariff and Zaini (2010)	
Inherent fire consequence estimation tool 1), IFCET-1						√					√	PE	Shariff and Wahab (2013)	
Toxic release inherent risk assessment, TRIRA						√						PE	Shariff and Zaini (2013a)	
Integrated TORCAT, ITORCAT		√	√				√				√	PE	Shariff and Zaini (2013b)	
Risk-based inherent safety index, RISI	√	√	√		√	√	√					LC	Rathnayaka et al. (2014)	
Quantitative index of inherently safer design, QI2SD	√	√	√				√					PE	Rusli et al. (2013)	
Inherently safer distillation system assessment, ISDSA					√	√	√	√				ED	Medina-Herrera, Jiménez-Gutiérrez, et al. (2014)	
Inherent safety index for shell and tube heat exchanger, ISISTHE			√			√	√				√	ED	Zaini et al. (2016)	
Inherent fire consequence estimation tool 2), IFCET-2			√			√	√				√	PE	Shariff et al. (2016)	
Inherent safety intra-equipment index, IaEI	√	√	√		√	√	√				√	PE	Athar, Shariff, Buang, Nazir, et al. (2019)	
Process stream characteristic index, PSCI		√	√			√					√	PE	Athar, Shariff, Buang, Shaikh, et al. (2019)	

### **2.3.2.1 Methodologies of the risk-based inherent safety metrics**

The risk-based metrics focus on assessing the envisaged main accident scenarios regarding their severity of consequence or likelihood of occurrence (Jafari et al., 2018). For example, the RRABD (Khan & Abbasi, 1998a) was developed for assessing the accident scenarios of Boiling Liquid Expanding Vapor Explosion (BLEVE) and Confined Vapor Cloud Explosion (CVCE) in manufacturing glycol and polyol. Briefly, the TRRABD encompasses generating accident scenarios, defining acceptance criteria, proposing design or modification solutions, performing deterministic calculations, and evaluating the results of the eventually accepted scenario. Similarly, with the explosion scenario-based ISD, the iRET was developed for mitigating the potential explosion risks in piping systems (Shariff et al., 2006). Unlike the deterministic manual calculations in the TRRABD, the iRET adopted a simulator (HYSYS) to extract more evaluation data, thus relieving many risk assessment difficulties because of data absence for the assumed accidents. The iRET was initially limited for measuring the consequences of explosion risk, and its scope was extended thereafter for measuring the risk in heat exchanger networks (Zaini et al., 2016).

Furthermore, the TORCAT, evolved from the iRET, was adapted as a more inclusive metric with special concerns on the toxic release consequences when selecting inherently safer alternatives (Shariff & Zaini, 2010, 2013a, 2013b). The methodology of the TORCAT can be described as three main steps: 1) generating alternative, 2) using the iCON (simulator) to obtain evaluation data based on source release model and dispersion model, and 3) modifying the alternative using ISD principles until the results

meet the design intention. Subsequently, using a similar procedure and same simulator, the TORCAT was expanded as the IFCET-1 (Shariff & Wahab, 2013) and the IFCET-2 (Shariff et al., 2016) respectively tailored for pool fire and BLEVE risks. In addition, the jet fire risk was also demonstrated by the PSCI (Athar, Shariff, Buang, Shaikh, et al., 2019) in selecting a less dangerous process stream.

As a holistic approach, the RISI (Rathnayaka et al., 2014) was developed for assessing the major chemical process safety risks (i.e., fire, explosion, and toxic release); as the most prominent advancement, it realized risk reduction rather than hazard reduction through modifying the I2SI procedures (Khan & Amyotte, 2004, 2005). However, the RISI did not merge the cost metric of the I2SI, concealing the potentials in selecting both safer and cheaper process alternatives. Comparatively, as a semi-holistic approach, the LL-FEI (Jensen & Jørgensen, 2007) presented a novel method for measuring the damage factor used in the Dow Fire and Explosion Index, where the fire and explosion risks were exemplified (Jensen & Jørgensen, 2007). The IRA (Shariff & Leong, 2009), using similar procedures of Quantitative Risk Analysis (QRA), demonstrated its efficacy when measuring the inherent risks in conditioned process industries. In addition, the KPIs proposed a consequence-based method for assessing inherent safety of alternatives. Interestingly, this method incorporated human targets and domino accident escalation in the assessing procedures (Tugnoli et al., 2009). However, relatively limited attention was given regarding potential conflicts when generating ISD alternatives. This challenge was addressed by the QI2SD by three main steps: 1) quantifying inherent hazards, 2) assessing the conflicts in ISD alternatives, and 3) ranking the ISD

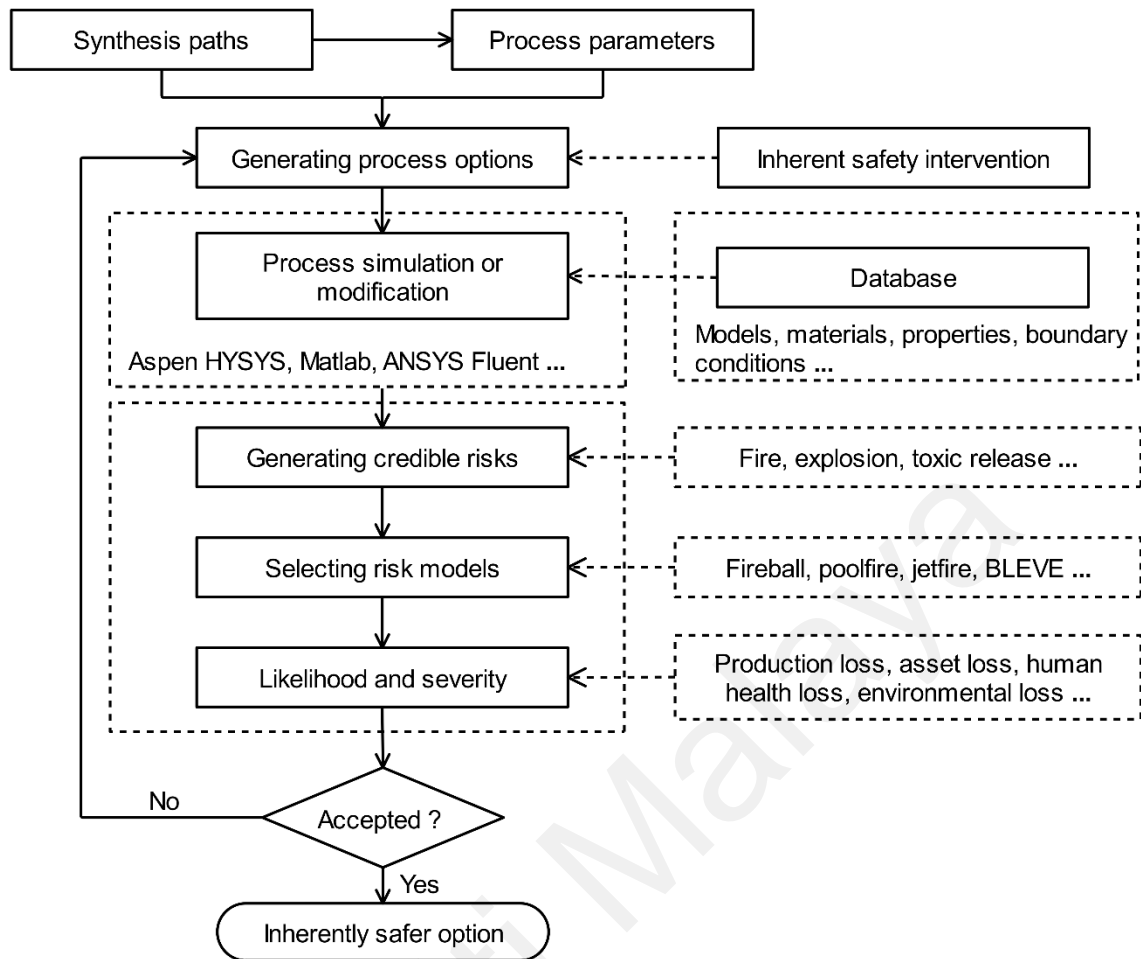


alternatives (Rusli et al., 2013). It is worth noting that, with different concerns on the risk forms, the indicators can vary when developing and using the risk-based metrics. For example, to design inherently safer distillation systems, four special indices (i.e., societal risk, individual risk, total annual cost, and product purity) were considered to do risk quantification (Medina-Herrera, Jiménez-Gutiérrez, et al., 2014). This technical consensus was also demonstrated by the IaEI (Athar, Shariff, Buang, Nazir, et al., 2019) in reconciling the on-demand sub-indices of distance concerning the process equipment, nature of process equipment, and equipment failure rates.

#### **2.3.2.2 Typical implementation framework of the risk-based inherent safety metrics**

Like the index-based metrics, the risk-based metrics aim to rank and select the optimal process option during the design stage. However, a variety of additional risk contributors like process stream, layout, and equipment were included (or separated) apart from the most credible chemical hazards (i.e., fire, explosion, and toxic release) in the risk-based metrics for inherent safety intervention, making the risk-based metrics more realistic and targeted in managing the anticipated accident scenarios and assigning inherent safety principles accordingly. Typically, the risk-based metrics could be implemented by generating credible risk scenarios, selecting risk models, and calculating risk likelihoods and severities based on the various process options, as depicted in Figure 2.8. It is pertinent to note that the typical implementation procedures to rank and select inherently safer options among various synthesis paths using ISMs. However, in some cases, especially for existing processes, the synthesis path is already

fixed. On this occasion, the risk-based metrics could function via ISM based on the fixed baseline processing scenario. During the modifications, inherent safety could be adopted with priority to address the process hazards guided by ISD principles. As the last resort, other realistic risk management strategies like passive, active, and procedural safeguards would be added to thus generate inherently safer options. A good example of using this research route to implement inherent safety can be found in this literature (Rathnayaka et al., 2014). In addition, when using the risk-based metrics, only considerable differences between the options should be deemed significant as risk determinations depend on many variables with much-involved uncertainty. As a case in point, the dominating wind direction could be an accident contributor to the downwind facilities, but in turn, it could be a safety contributor to preventing the local aggregation of flammable and explosive gases.



**Figure 2.8: Typical implementation framework of risk-based metrics**

### 2.3.2.3 Strengths and weaknesses of the risk-based inherent safety metrics

Risk-based metrics highlight the contribution of certain hazards to the most credible accident scenario in comparing various process alternatives. This endeavor makes inherently safer interventions more realistic and reliable in managing targeted risk factors posed by specific process units. For instance, the jet fire risk in the critical process stream was envisaged as the main characteristic for the process piping design (Athar, Shariff, Buang, Shaikh, et al., 2019), by which the inherent fire risk can be targeted and mitigated based on As Low As Reasonably Practicable (ALARP) principle. However, the weaknesses might arise in subjectively determining the loss potentials of

various accident scenarios. As the above example, although the jet fire could be induced in the pipework by an accidental release with a higher risk likelihood, it will tell nothing on the severity if the fugitive emission was considered. This further implies that the dangerous accident scenario has no absolute advantage over the hazardous accident scenario. In addition, the subjective judgment could be inevitably factored into accident scenarios' envisaging since it is always challenging or twice subjective for benchmarking with the past case studies or unit vulnerabilities. Furthermore, the risk analysis is generally conducted according to the worst case, while it is insufficient to confirm the same risk level regarding the average case or additive case (Hassim & Hurme, 2010c). Another clear weakness is the lack of considering human factors induced safeness degradation because human factors has been implicated in approximately 80% of chemical accidents (Kariuki & Löwe, 2007).

### **2.3.3 Graphical inherent safety metrics**

Unlike the index-based metrics and risk-based metrics which always yield an aggregated numerical result, graphical metrics can intuitively and visually display the assessment results using easy-to-understand and straightforward graphics, enabling the comparison and selection of inherently safer solutions via differentiating each synthesis step of each process option. Here, the risks in PIIS are also used as the main indicators of graphical metrics, as shown in Table 2.6.

**Table 2.6: Graphical metrics for assessing inherent safety**

Terms	Metric indicators												PS	References
	I	T1	P	Y	T2	F	E1	EC	H	E	SC			
Inherent safety evaluation of synthesis routes, ISESR	√	√	√	√	√	√	√				√	R&D	Palaniappan, Rajagopalan, et al. (2002a)	
Inherent safety expert system, iSafe	√	√	√	√	√	√	√				√	ED	Palaniappan, Rajagopalan, et al. (2002b)	
Simple graphical method, SGM		√	√		√	√	√					ED	Gupta and Edwards (2003)	
SREST hierarchical assessment, SRESTHA					√		√		√	√		ED	Shah et al. (2003)	
Petri Nets based inherent safety assessment, PNISA		√	√									LC	Moradi and Bahri (2008)	
Extended simple graphical method, ESGM		√	√						√			R&D	Hassim et al. (2013)	
Descriptive technique for inherent safety assessment, GRAND					√	√	√					R&D	Ahmad et al. (2015)	
2-Dimensional Graphical Rating, 2DGR	√	√	√		√	√	√					R&D	Ahmad et al. (2016)	
Three-stage ISD matrix, TIM	√								√			ED	Zainal Abidin et al. (2016)	
Bayesian network based inherent safety intervention, BNISI		√	√		√	√	√			√		LC	Abimbola et al. (2016)	
Process route and stream indices, PRSI			√				√	√	√		√	ED	Ortiz-Espinoza et al. (2017)	
Graphical inherent safety assessment technique, GISAT					√	√	√					PE	Ahmad et al. (2019)	

### 2.3.3.1 Methodologies of the graphical inherent safety metrics

Based on the reaction network used in the ISESR (Palaniappan, Rajagopalan, et al., 2002a) and the iSafe (Palaniappan, Rajagopalan, et al., 2002b), a graphical method (Gupta & Edwards, 2003) was proposed by plotting the parameters associated with inherent safety concerns for each step of each process option. This graphical method has a major advantage of presenting a relatively thorough assessment without requiring intensive mathematical operations and incorporating the cost, regulatory, pollution control, occupational health factors, etc. In this respect, Hassim et al. (2013) further adapted it as a new assessment tool (i.e., the ESGM) for indicating health risk both for the overall process routes and their sub-processes. The graphical metrics highlighted the contributions of individual hazards to the safety and health performance of various process alternatives. Also, no addition for disparate hazard values is suggested to derive an overall index value, which is often criticized due to its dimensionless mathematical operations. However, the graphical methods may lack enough hierarchical concerns on the various plant layers, making them deficient in highlighting the potential risks in different process sections. This deficiency could be addressed by the SREST (Shah et al., 2003) which consists of hierarchical assessments on substance layer, reactivity layer, equipment layer, and safety-technology layer. More inclusively, the SREST graphically demonstrated integrated evaluation results concerning SHE parameters.

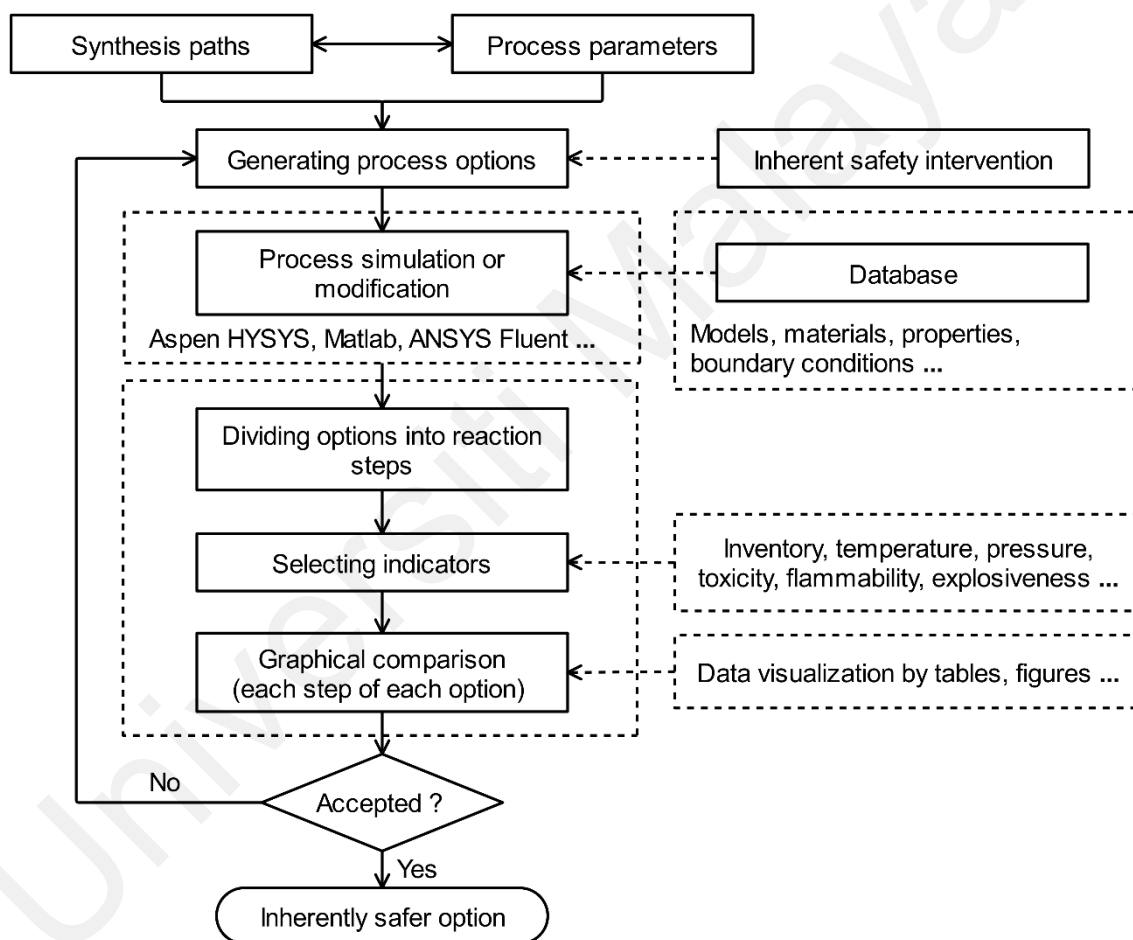
Another two graphical tools, called PNISA (Moradi & Bahri, 2008) and BNISI (Abimbola et al., 2016), were respectively developed based on the Petri Nets (PN) and the BN. The PNISA aligns with the I2SI indexing system and thus presents a graphical

metric with cost considerations in assessing process options. Comparatively, the salient feature of BNISI lies in its capability for identifying key contributors to failure scenarios via the BN diagnostic analysis. Likewise, the 2-DGR (Ahmad et al., 2016) was also developed with the capability of investigating the critical hazardous parameters based on logistic function. Evolving from the GRAND (Ahmad et al., 2015) that presented both aggregated total scores of process routes and detailed data of the chemical and operational properties, the 2DGR was then extended to the GISAT (Ahmad et al., 2019) from the R&D stage to the PE stage, where more information on flammability, explosiveness, and toxicity has been available. Moreover, the TIM (Zainal Abidin et al., 2016) was developed to graphically illustrate ISD principles, ISD indicators, and ISD variables in tabular forms. Compared to the former tools, the TIM, via a graphical trade-off approach, incorporated economic comparison based on capital and operating costs for resolving the conflicts of inherent safety implementation towards the overall processing aim. Furthermore, a trade-off mechanism of inherent safety with economic and environmental performance was also developed through a graphical comparison for the process route level and process stream level (Ortiz-Espinoza et al., 2017).

#### **2.3.3.2 Typical implementation framework of the Graphical inherent safety metrics**

The graphical metric aims to exhibit the safety level through data visualization techniques via, for example, easy-to-understand tables and figures. Unlike the preceding inherent safety assessment tools, the graphical metrics focus more on the individual

performance of each hazard form, which necessitates dividing process routes into different steps for global comparison. This also necessitates selecting corresponding hazard parameters in each step of each route for exhibiting the safety level through data visualization techniques via, for example, easy-to-understand tables and figures. Accordingly, a typical implementation framework of graphical metrics for assessing inherent safety is illustrated in Figure 2.9.



**Figure 2.9: The typical implementation framework of the graphical metrics**

### 2.3.3.3 Strengths and weaknesses of the graphical inherent safety metrics

In contrast with index-based and risk-based metrics using a proverbial black box to produce a single dimensionless number for measuring inherent safety across the



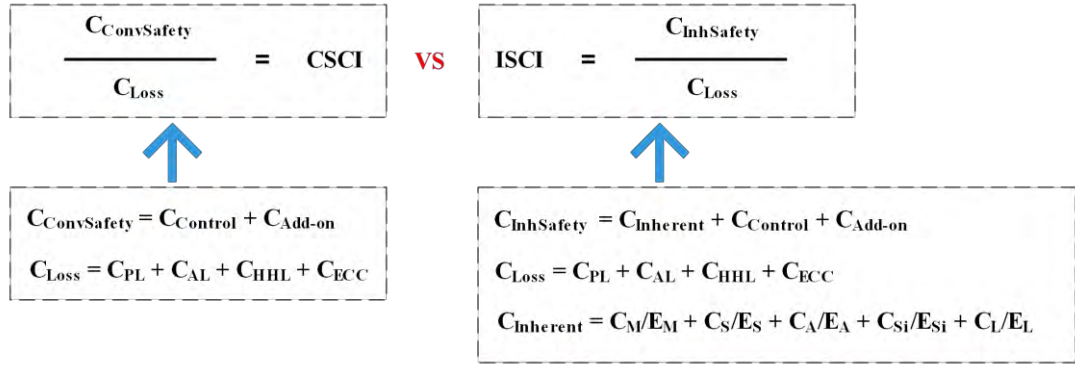
competing process alternatives, graphical metrics are advantageous in the global visual comparison without hiding the effects of different input parameters. This advantage also enables easier benchmarking analysis for different process alternatives by less mathematical operations. Moreover, by comparing the same metric indicators, such an approach is helpful to understand the exact causes of safeness degradation and encourage efforts for their early prevention when developing a new process (Hassim et al., 2013). However, the weaknesses also arose mainly due to the lack of a convincing equivalency for multi-dimensional parameter comparison. For example, in the six process routes for manufacturing methyl methacrylate (Gupta & Edwards, 2003), the inventory was largely characterized by the material volume while gave little attention to the compositions of raw materials and intermediates. In addition, graphical metrics may care little about the weights when comparing the same parameters. For example, in the first route of the above case (Gupta & Edwards, 2003), the minimum and maximum temperatures are respectively 29 °C and 1200 °C in its six reaction steps, while it cannot indicate with certainty that the 1200 °C reaction step is the most hazardous since it may be inconsistent with the heat flux in this step. It is pertinent to note that the heat flux is only an illustrative component for determining the temperature weight. Other parameters may have similar problems in both reaction steps and process routes.

Over the past decades, there has been a proliferation for the development of the ISMs for measuring, ranking, and selecting inherently safer process alternatives. Despite the great efforts in this regard, there has yet to be a unified metric for assessing inherent safety due to its wide scope in the SHE concerns, applicability in various process stages, and other assorted possible principles besides the key principles. Nevertheless, the

numerous ISMs have been classified into several established groups. In this section, the cross-used groups (i.e., index-based, risk-based, graphical, and SHE-based metrics) were gleaned to analyze their development and implementation methodologies, typical implementation frameworks, and strengths and weaknesses. It is worth noting the inherent safety concept is expanded to the occupational health and environmental protection fields. In practice, the expanded explorations share the same outlooks to develop proactive and fundamental solutions to eliminating or reducing the SHE risks by Prevention through Design (PtD) strategies.

#### **2.3.4 Cost metrics of implementing inherent safety**

Although inherent safety has been proven to be economically attractive (Rusli et al., 2013), the cost metric is sporadically studied. To exemplify the most accepted cost metric for measuring the implementation of inherent safety, the most-cited study which involves economic evaluation was selected. Accordingly, the cost metric in the I2SI (Khan & Amyotte, 2005), whose TC equal 161, was extracted to analyze its methodology for quantifying the financial aspects of implementing inherent safety. The cost indexing procedure in the I2SI is composed of two sub-indices, and the detailed computation processes are shown in Figure 2.10.



CSCI = Conventional safety cost index; ISCI = Inherent safety cost index;  $C_{ConvSafety}$  = The sum of the costs of process control measures ( $C_{Control}$ ), and add-on safety measures ( $C_{Add-on}$ );  $C_{InhSafety}$  = The sum of the costs of inherent safety implementation ( $C_{Inherent}$ ), process control measures ( $C_{Control}$ ), and add-on safety measures ( $C_{Add-on}$ );  $C_{Loss}$  = Cost of losses;  $C_{PL}$  = Cost of production loss;  $C_{AL}$  = Cost of asset loss;  $C_{HHL}$  = Cost of human health loss;  $C_{ECC}$  = Cost of environmental cleanup.

$C_M$ ,  $C_S$ ,  $C_A$ ,  $C_{Si}$ , and  $C_L$  represent the costs of minimization, substitution, attenuation, simplification, and limitation of effects, respectively.

$E_M$ ,  $E_S$ ,  $E_A$ ,  $E_{Si}$ , and  $E_L$  are the extent of applicability of the respective inherent safety principles.

**Figure 2.10: Cost indexing procedures in Integrated Inherent Safety Index (I2SI)**

In the I2SI cost indexing procedures, guidelines consisting of ten grades and ten respective scores were developed to obtain the extent of applicability of inherent safety principles. Subsequently, index values with various ranges of applicability for the key inherent safety principles were determined through corresponding scales. According to the implementing processes in Figure 2.10, the obtained final values of the CSCI and ISCI are used for comparison to find cheaper options (the lower value, the cheaper process). This cost metric offers a heuristic indexing methodology for cost estimation when conducting inherent safety modifications on a baseline design. However, during the ED stage, the baseline design could be ill-specified when comparing various process alternatives from the PFD and PIDs. This situation could pale the principle-based cost indexing method since the principles on the various alternatives are latent without a benchmark or baseline design.

Apart from the inherent safety principles based cost indexing solutions, economic implications can be integrated into the modules of ISMs. For example, Edwards and

Lawrence (1993) and Heikkilä et al. (1996) incorporated product yields as an independent indicator for ranking and selecting inherently safer and cheaper process alternatives. On the other hand, the economic concerns when developing inherent solutions can be tailored to the successive phases of process design stage to thus suffice for the available items. Specifically, during the R&D phase, Liew et al. (2014) used annual operating costs from 1) raw materials ( $C_{\text{raw}}$ ) and 2) electricity energy consumption ( $C_{\text{ele}}$ ) together with the Annual Revenues (AR) from the selling price of products to evaluate the Economic Performance (EP) of a certain chemical synthesis pathway, as shown in Equation 2.1 (Liew et al., 2014). During the PE phase, with more detailed considerations on process flow rate, unit price, and annual operating time, Equation 2.1 was enriched as Equation 2.2 (Liew et al., 2015). For the BE phase, the specifics of capital investment and utility expense have been sufficient, and the EP measurement focuses on the assembly of piping components such as pipes, fittings, flanges, valves, bolts, gaskets, and other associated piping specials. Accordingly, Liew et al. (2016) developed a Total Annualized Cost (TAC) method based on utility cost and incurred capital investment, as shown in Equation 2.3 (Liew et al., 2016).

$$EP = AR - (C_{\text{raw}} + C_{\text{ele}}) \quad (2.1)$$

$$EP = \left[ \sum_n F_n^{\text{Prod}} C_n^{\text{Prod}} - \left( \sum_m F_m^{\text{Feed}} C_m^{\text{Feed}} + \sum_l P_l C_l^{\text{Uti}} \right) \right] \times AOH \quad (2.2)$$

Where,  $F_n^{\text{Prod}}$  = flow rate of product n,  $C_n^{\text{Prod}}$  = unit price of product n,  $F_m^{\text{Feed}}$  = flow rate of feedstock m,  $C_m^{\text{Feed}}$  = unit cost of feedstock m,  $P_l$  = power consumption of process module l,  $C_l^{\text{Uti}}$  = unit cost of energy utility, AOH = Annual Operating Hours.

$$TAC = COST^{Util-Pip} + AF \times COST^{TCI-Pipe} \quad (2.3)$$

Where,  $COST^{Util-Pip}$  = utility cost associated with pipe size,  $COST^{TCI-Pipe}$  = capital investment associated with piping fittings,  $AF$  = annualized factor used for determining equal annual payments.

Aside from the tangible inclusion of economic indicators, the inherently economic friendliness can intangibly work in concert with other proactive interventions in the design stage. For example, Guillen-Cuevas et al. (2018) developed the SASWROIM with simultaneous considerations on inherent safety and sustainability at the conceptual design stage. Wherein, the economic implications are included in the sustainability issues based on an extended Return On Investment (ROI) analysis. Despite the endeavors for incorporating tangible and intangible cost issues, a cost benefit metric capable of indicating a full spectrum of lifetime economic friendliness is yet to be presented. Specifically, the existing cost metrics mainly addressed the safety conflicts concerning production costs and investment returns, while with few concerns on the cost savings, such as the Maximum Probable Days Outage (MPDO), Maximum Probable Property Damage (MPPD), and Business Interruption (BI) (Dow, 1994), from the resultant absence of accidents, injuries, and losses.

## **2.4 Prominent industrial applications**

### **2.4.1 Inherent safety in offshore process industry**

Inherent safety-based offshore process risk management came to be recognized after it was introduced by Mansfield et al. (1996). The authors presented a pilot study using the

two key inherent safety principles of minimization and simplification to respectively develop lower inventories and less active protections. The "minimum" inventories and facilities could reduce the topside weights, as well as the operation and maintenance procedures, and therefore could bring a win-win situation for improving the economic and safety performance. In the subsequent years, Khan and Amyotte (2002) elucidated the applicability and availability of inherent safety in offshore activities for designing and operating various facilities, including wellhead locations relative to platform location, subsea manifolding, and accommodation module location. Meanwhile, the main targets for inherently safer interventions were identified from process facility layout, separation processes, heat exchangers, multiphase pumping and metering, compressors, subsea installations, and structural integrity. Moreover, Abimbola et al. (2016) investigated the influencing factors of well integrity failures during casing and cementing operations, and recognized the critical contributors as managed pressure drilling system, logging tool, slurry formulation, casing design, casing handling and running method, surge and swab pressures. The critical failure contributors then were addressed using potential safety measures guided by inherent safety principles. Like comparing and selecting inherently safer process alternatives in onshore chemical industries, Crivellari et al. (2021) developed a novel assessment tool with human, asset, and marine environmental concerns, to indicate the potential accident scenarios in offshore oil & gas installations in the ED stage. This proactive assessment could relieve the complexity and cost implications of weight, space, and maintenance requirements, making inherent safety an appealing solution for hazard management in the design of offshore installations (Khan & Amyotte, 2002). However, in a recent study (Tam, 2020),

the practical applications were found to be patchy due to the lack of effective, efficient, and consistent implementation procedures. Accordingly, the improvement strategies were concluded with four main aspects, i.e., 1) including design safety in all design stages, 2) instigating appropriate ISD goals at different process stages, 3) avoiding over-reliance on detailed quantified risk assessment, and 4) understanding and managing major hazards.

#### **2.4.2 Inherent safety in nuclear industry**

The current inherent safety practice in the nuclear industry concentrates on developing ample safety margins for normal operations and postulated accidents (Sofu, 2015), conforming with the conventional inherent safety principles of limitation of effects, tolerance of misuse, and passive safety. In breeder reactors, the inherently safer features, relying on less engineered safeguards, could ease a moderate shut down and remove the decay heat principally by 1) keeping the elevated temperature below damaging limit and 2) ensuring the asymptotic state temperature against inducing creep failures (Sathiyasheela et al., 2013). Especially, removing decay heat with inherent safety concept has received extensive attention recently. For example, Wang et al. (2020) developed a passive decay heat removal system in case of emergency heat removal transients. This system is designed with a primary heat exchanger in a reactor pressure vessel, a secondary heat exchanger in a dry cooling tower, and a fail-open valve, by which the shutdown was done without any external power sources and operator actions. This inherent safety capability is likely helpful in developing a cheaper reaction system and offering more confidence to the reactor designers and operators. In the

contemporary nuclear industry, an initiative for adopting inherent safety as a new paradigm for safety management is being made, aiming to inoculate the reactors and the fuel cycles with a guaranteed risk-free immunity (Adamov et al., 2015).

#### **2.4.3 Inherent safety for preventing dust explosion**

Generally, dust explosion prevention can be done by avoiding explosive dust clouds and ignition sources (Eckhoff, 2009). In the two regards, the potential and efficacy of inherent safety principles were well demonstrated. For example, processing explosive materials under less hazardous operating forms by mixing solid inert agents or water vapor could decrease its reactivity (Amyotte, Pegg, et al., 2007), corresponding to the ISD principle of attenuation. Holistically, the utilities of the remaining ISD principles were also demonstrated for dust explosion prevention (Amyotte et al., 2009). The representative cases are encapsulated as the follows: 1) by the minimization principle, the airborne dust concentrations can be reduced below the Minimum Explosible Concentration (MEC), and as such, the fuel component of the fire triangle can be removed to realize explosion prevention; 2) by the substitution principle, the bucket elevators and other mechanical conveying systems can be replaced with dense-phase pneumatic transport for limiting dust dispersion; 3) by the simplification principle, the process or plant could be further intensified to limit the generation of explosive dust clouds. Furthermore, a conceptual framework (Abuswer et al., 2013) for dust explosion risk management was proposed. This framework offered a criticality-based dust explosion risk reduction strategy based on hierarchical controls starting from inherent safety principles.



#### **2.4.4 Inherent safety for developing risk-based safeguards**

Risk-based safety measures strive to allocate corresponding and straightforward safety measures if the QRA results exceed the threshold level after comparing to acceptance criteria (Khan et al., 2002). For instance, Yuan et al. (2015) identified the critical contributing factors to a dust explosion scenario and accordingly assigned the potentially optimal safety interventions. Likewise, Abimbola et al. (2016) identified the critical contributors to the casing and cementing failure scenarios during well integrity, and allocated appropriate safety measures with a primary focus on inherently safer solutions. More explicitly, Rathnayaka et al. (2014) developed a risk-based inherent safety metric (i.e., RISI) for implementing inherent safety. The RISI was first used for estimating the risk level of baseline design, and then, key risk factors identified were addressed using inherent safety principles to generate various design alternatives. Lastly, the RISI would be re-employed to estimate the safety performance to thus select the inherently safer alternative. Overall, under limited labor, time, or financial resources, the risk-based inherent safety interventions could be more efficient and more fundamental to cope with the major risks with priority according to a threshold value to tolerate or accept the residual risks.

With the awareness of inherent safety in practice, its concepts are applied into various industries with the prominent explorations of safety management in the offshore process industry, nuclear industry, dust explosion prevention, and risk-based risk reduction. In the offshore process industry, inherent safety is generally used to comfort critically risky facilities, but its applications remain patchy because of the lack of effective, efficient,

and consistent implementation procedures. In the nuclear industry, inherent safety concept is generally used to build ample safety margins to limit the postulated accident effects, and there also presents an initiative of using it as a paradigm to conduct nuclear safety management. For preventing dust explosion prevention and developing risk-based safeguards, inherent safety principles are used to limit the dust explosion conditions and make efficient safety decisions considering risk criticalities.

It is pertinent to note that the BN has been extensively used for conducting risk-based inherently safer design or modifications. In practice, the BN have been regarded as the most widely adopted mathematical tool in risk assessment researches due to the prominent capabilities of integrating multi-state variables, updating new evidence, and representing node uncertainties (Khan et al., 2020). The BN, proposed by Pearl (1985) based on the Bayes' theorem, are recognized as robust techniques for various kinds of risk assessment due to their salient capabilities of integrating conditional dependencies with probabilistic relationships among the variables with multiple states (Khakzad & Khan, 2021). The BN represent the structural and numerical relationships of the variables using the Directed Acyclic Graph (DAG) and Conditional Probability Tables (CPTs), respectively (Khakzad et al., 2011). The DAG is to indicate the directed impacts with no closed loops (i.e., no vertex can reach itself via a nontrivial path). The CPTs are to demonstrate the conditional probabilities of discrete and mutually dependent random variables to others. The DAG and CPTs constitute the main information of the BN input data.

Generally, the BN is used for probabilistic risk inferences based on discrete probabilities and CPTs (Khakzad et al., 2013). Continuous variables represented by simultaneous

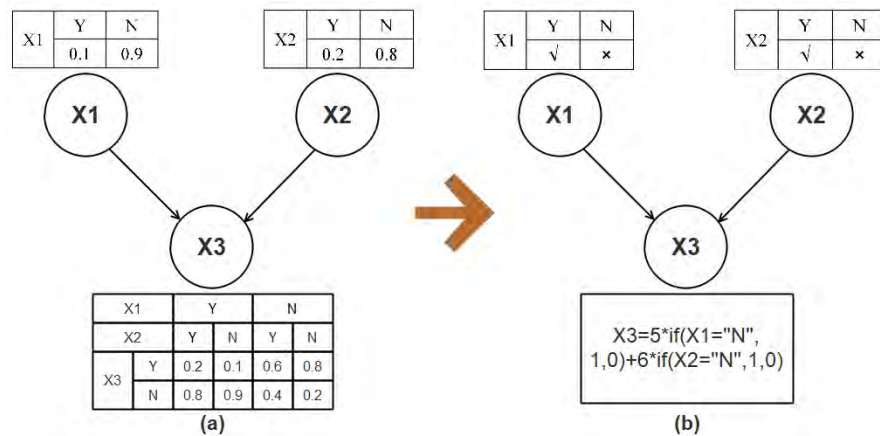
structural equations are close relatives with the discrete values in the BN inferences. For illustrative purposes, the BN fundamentals were briefly revisited as follows.

Bayesian theorem (also known as Bayesian law or Bayesian rule) describes the probability of an event according to its conditions and the corresponding prior knowledge, which is formally represented in Equation 2.4.

$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{\sum_j P(B|A_j)P(A_j)} \quad (2.4)$$

Where  $P(A_i)$  represents marginal probabilities of observing event  $A_i$ ;  $P(A|B)$  and  $P(B|A)$  respectively represent conditional probabilities of event A occurrence given event B and event B occurrence given event A; the denominator represents a formula of total probabilities via several distinct events of  $A_j$ .

Based on the Bayesian theorem, the BN was first developed by Pearl (1985) to make uncertainty inferences by simulating causalities. The network topology is represented by the DAG with random variables (or nodes) and CPTs, as shown in Figure 2.11 (a), where X1 and X2 are parent (or root) nodes of child node X3. Also, the conventional numerical prior probabilities and CPTs can be respectively adapted as deterministic nodes and equation-based (or continuous) representations, as shown in Figure 2.11 (b).



**Figure 2.11: The transition of CPT-based BN to equation-based BN.**

Based on the deductive reasoning of the BN based modeling, the risk-based inherently safer design or modifications can be used for ranking the contribution degrees of the causal factors to the potential accidents. With this deductive reasoning, Abimbola et al. (2016) and Yuan et al. (2015) investigated the key contributors to the failure of cementing operations and the vulnerable parts touching off aluminum dust explosions and then addressed them using inherent safety and appropriate add-on protections. Similarly, Yuan et al. (2013) and Ding et al. (2020) examined the influential basic events of wool dust explosions and storage fire hazards, and based on the influential basic events, they proposed inherent safety interventions for risk avoidance, prevention, control, and mitigation, together with complementary engineered safety barriers and administrative controls.

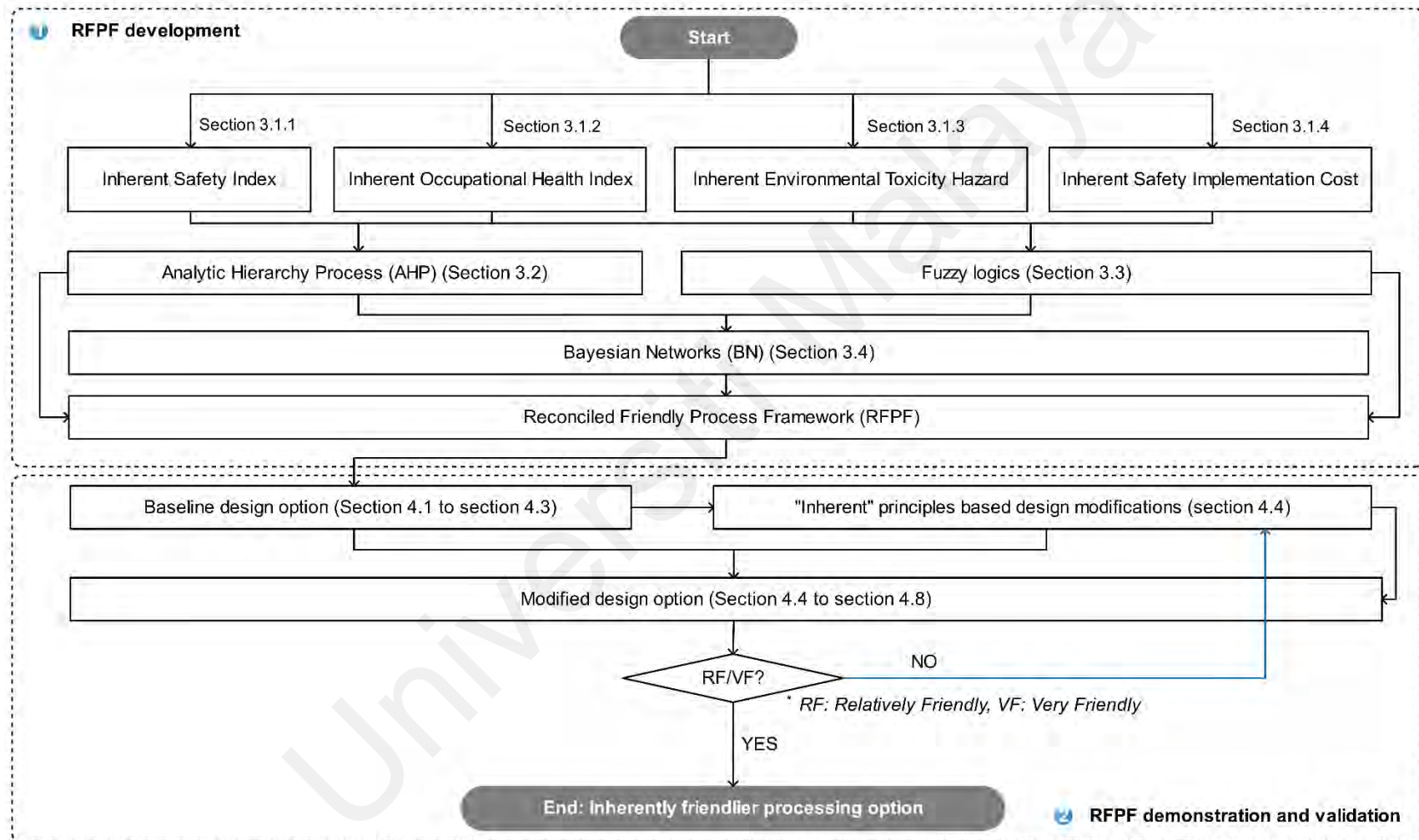
## **2.5 Summary of the literature review**

Since the inception of inherent safety in the 1970s, significant progress has been made in using it to develop and consolidate the FCP, which is largely characterized by the proactive and simultaneous augmentation in safety, health, environment, and economic performance. In this section, a comprehensive review on the temporal accomplishments of inherent safety over the past four decades was presented. Firstly, the basic cognition for inherent safety was encapsulated from its origin, early development, implementation principles, stages, and benefits. Subsequently, its current practice for creating the FCP was highlighted via synthesizing the application and preference of inherent safety principles, the development methodologies, implementation frameworks, strengths and weaknesses, and selection guidelines of the ISMs. Lastly, the cost metrics of

implementing inherent safety and the prominent industrial applications in the offshore process industry, nuclear industry, dust explosion prevention, and risk-based safety interventions were presented. In general, this section presents a complete picture of the most concerning contents of inherent safety. The literature review found that, as a proactive safeguard, inherent safety has achieved significant performance in loss prevention and risk management over the past four decades. In practice, the researchers and practitioners are continuing to develop tailored ISMs to suffice for different process stages and different risk forms. In the various existing metrics, there demonstrates a trend towards inherently healthier and more environmentally benign process design together or separately with inherent safety. These efforts also reflect that the "inherent" concept can be generic for proactively minimizing the SHE problems during the process design stage, which is consistent with the concept of inherently friendlier processes and plants striving to reduce the wastes, hazards, losses, injuries, and other process problems proactively and fundamentally. However, a holistic and inclusive framework that can reconcile the SHE components is yet to be presented. Also, how to incorporate the incremental costs to generate inherently cheaper processes remains to be further elucidated.

### CHAPTER 3: METHODOLOGY

As per the aim of developing a dedicated framework to indicate and generate inherently FCP, the prestigious inherent SHEC metrics consisting of the ISI, IOHI, IETH, and ISIC were selected and adapted as the inherent friendliness indicators. The weights of the inherent friendliness indicators were determined using the AHP and assigned to the primary, secondary, and ternary factors derived from the inherent SHEC metrics. Then, the risk values are normalized using the triangular membership functions. After obtaining the indicator weights and the normalized values, the BN were used to reconcile the components to figure out the RFPF. The reconciliation means the integration of the selected inherent friendliness indicators with weights and risk values, thus forming the RFPF used for generating inherently FCP via "inherent" principles based design modifications. Overall, the technical research routes and the cohesive roles of the adopted methods are two-fold as shown in Figure 3.1. The first step is the development of the RFPF, and the second step is the demonstration and validation of the RFPF. The developed RFPF was firstly implemented in the baseline design to check whether its inherent friendliness is satisfactory. If not, the "inherent" principles based design modifications would be implemented until the inherent friendliness of the modified design is rated as Relatively Friendly (RF) or Very Friendly (VF).



**Figure 3.1: Overview of the technical research routes and the cohesive roles of the adopted methods**

### 3.1 Indicators for the inherently Friendlier Chemical Processes (FCP) features

As the inherent friendliness is characterized by the synthesis of inherent safety, health, environmental concerns as well as the incremental costs, the indicators in the renowned inherent SHEC metrics were extracted to constitute the RFPPF.

#### 3.1.1 Safety indicators

Impressive accomplishments of inherent safety metrics have been reported (Athar, Shariff, & Buang, 2019). This work adopted the ISI earlier developed by Heikkilä (1999) considering its clear modular structures for easing the RFPPF construction. ISI is evolved from the pioneering PIIS (Edwards & Lawrence, 1993), comprising Chemical Inherent Safety Index ( $I_{CI}$ ) and Process Inherent Safety Index ( $I_{PI}$ ).  $I_{CI}$  consists of chemical factors that may affect inherent safety, and  $I_{PI}$  expresses the inherent safety of the process itself. Their values can be obtained via the sum of their sub-indices using Equation 3.1 and Equation 3.2, respectively.

$$I_{CI} = I_{RM,max} + I_{RS,max} + I_{INT,max} + \max(I_{FL} + I_{EX} + I_{TOX}) + I_{COR,max} \quad (3.1)$$

$$I_{PI} = I_I + I_{T,max} + I_{P,max} + I_{EQ,max} + I_{ST,max} \quad (3.2)$$

Where the symbol meanings and their range are furnished in Table 3.1.



**Table 3.1: The symbols and range in the Inherent Safety Index (ISI)**

Symbols	Meanings	Range
$I_{RM, \max}$	Maximum of main reaction heat	0 - 4
$I_{RS, \max}$	Maximum of side reaction heat	0 - 4
$I_{INT, \max}$	Maximum of chemical interaction	0 - 4
$I_{CI}$	$I_{FL}$ Flammability	0 - 4
	$I_{EX}$ Explosiveness	0 - 4
	$I_{TOX}$ Toxic exposure	0 - 6
	$I_{COR, \max}$ Maximum of corrosiveness	0 - 2
	$I_I$ Inventory	0 - 5
	$I_{T, \max}$ Maximum of process temperature	0 - 4
$I_{PI}$	$I_{P, \max}$ Maximum of process pressure	0 - 4
	$I_{EQ, \max}$ Maximum of equipment safety	0 - 4
	$I_{ST, \max}$ Maximum of safe process structure	0 - 5

When scoring  $I_{EQ}$ , the process is divided into the on-site area and off-site area, respectively characterized by the high volume of equipment and piping work within a concentrated area, and large quantities of fluid inventories and hazardous intermediates within a scattered area. Upon obtaining the sub-index values of  $I_{SBL}$  (safety value for the on-site equipment, 0 - 4) and  $O_{SBL}$  (safety value for the off-site equipment, 0 - 3), the maximum of them will be used as the  $I_{EQ}$  value.

### 3.1.2 Health indicators

Safety deals with acute or major catastrophic accidents such as fire, explosion, and leakage. However, health is more associated with chronic or continuous events like fugitive emission. Based on the philosophy of inherent safety, IOH was first formalized by Hassim and Edwards (2006), striving to reduce or eliminate occupational health hazards at the source instead of adding engineered or procedural measures to control the

hazard escalation. For the current health metric, the IOHI (Hassim & Hurme, 2010c) was adopted and modified due to its simple, straightforward, and time-saving procedures. IOHI indexing procedure is two-fold, i.e., Indexing for Physical and Process Hazards ( $I_{PPH}$ ) and Indexing for Health Hazards ( $I_{HH}$ ). The  $I_{PPH}$  describes the possibility for workers being exposed to chemicals, and  $I_{HH}$  expresses the adverse health impacts that arose from the exposure.  $I_{PPH}$  and  $I_{HH}$  are comprised of various secondary metrics, and the values can be respectively computed using Equation 3.3 and Equation 3.4.

$$I_{PPH} = I_{PM} + I_P + I_T + \max(I_{MS}) + \max(I_V) + \max(I_C) \quad (3.3)$$

$$I_{HH} = \max(I_{IEL}) + \max(I_{IR}) \quad (3.4)$$

Where the symbol and indexing procedures are listed in Table 3.2.

**Table 3.2: The indexing procedures of the health indicators**

Symbols	Meanings	Score formation	Penalty
$I_{PPH}$	$I_{PM}$ Mode of process	Continuous	1
		Semi-continuous/semi-batch	2
		Batch	3
	$I_P$ Pressure (bar)	0.5 – 5	0
		5 – 50	1
		20 – 200	2
		> 200	3
		< 70	0
	$I_T$ Temperature (°C)	70 – 150	1
		150 – 200	2
		> 200	3
	$\max(I_{MS})$ Maximum of material phase	Gas	1
		Liquid	2
		Solid	3

Table 3.2, continued

Symbols	Meanings	Score formation	Penalty			
max(I <sub>V</sub> )	Maximum of volatility	Liquid and gas	BP > 150 °C 150 °C ≥ BP > 50 °C 50 °C ≥ BP > 0 °C BP ≤ 0 °C	0 1 2 3		
		Solid	Non-dusty solids	0		
			Pellet-like, non-friable solids	1		
			Crystalline, granular solids	2		
			Fine, light powders	3		
		Corrosiveness of construction material	Stainless steel	0		
			Carbon steel	1		
			Better material needed	2		
		max(I <sub>EL</sub> )	Maximum of exposure limit	Solid (mg/m <sup>3</sup> )	OEL > 10 OEL ≤ 10 OEL ≤ 1 OEL ≤ 0.1 OEL ≤ 0.01 OEL > 1000 OEL ≤ 1000 OEL ≤ 100 OEL ≤ 10 OEL ≤ 1	0 1 2 3 4 0 1 2 3 4
				Vapor (ppm)	No acute toxicity effect	0
R36, R37, R38, R67	1					
R20, R21, R22, R65	2					
R23, R24, R25, R29, R31, R41, R42, R43	3					
max(I <sub>R</sub> )	Maximum of R-pharse			R26, R27, R28, R32, R34, R35	4	
				No chronic toxicity effect	0	
				Chronic	R66	1
				R33, R68/20/21/22	2	

**Table 3.2, continued**

Symbols	Meanings	Score formation	Penalty
		R62, R63, R39/23/24/25, R48/20/21/22 R40, R60, R61, R64,	3
		R39/26/27/28, R48/23/24/25	4
		R45, R46, R49	5

\* BP: Boiling Point, R: R-phrase.

### 3.1.3 Environmental indicators

Inherent safety aims to unearth fundamental choices by eliminating or reducing risks at the source instead of resorting to add-on safeguards. Likewise, inherently environmental processes strive to remove environmental hazards at the earliest possible design stage rather than controlling them by additional protections. This work adopted the environmental hazard metric termed IETH earlier developed by Gunasekera and Edwards (2006), the pioneers in the field of inherent environmental hazard assessment. The IETH is derived from Environmental Hazard Index (EHI) (Cave & Edwards, 1997) and AHI-1 (Gunasekera & Edwards, 2003), and it offers a reconciled methodology for evaluating inherent environmental hazards from aquatic, terrestrial, and atmospheric environments. For a certain process route, the value of IETH can be achieved using Equation 3.5.

$$\text{IETH} = \sum_{i=1}^m (\text{YAi} + \text{YWi} + \text{YTi}) \quad (3.5)$$

Where,  $Y_{Ai}$ ,  $Y_{Wi}$ , and  $Y_{Ti}$  represent the severity scale value of chemical  $i$  in the atmospheric environment, aquatic environment, and terrestrial environment, respectively. Their value estimation can be respectively done through Equations 3.6 to 3.8.

$$Y_{Ai} = \begin{cases} 0 & H_{Ai} < 0.1 \\ 3\log(H_{Ai}) + 4 & 0.1 \leq H_{Ai} \leq 100 \end{cases} \quad (3.6)$$

$$Y_{Wi} = \begin{cases} 0 & H_{Wi} < 80 \\ 2.5\log(H_{Wi}) - 3.75 & 80 \leq H_{Wi} \leq 320000 \\ 10 & H_{Wi} > 320000 \end{cases} \quad (3.7)$$

$$Y_{Ti} = \begin{cases} 0 & H_{Ti} < 80 \\ 2.5\log(H_{Ti}) - 3.75 & 80 \leq H_{Ti} \leq 320000 \\ 10 & H_{Ti} > 320000 \end{cases} \quad (3.8)$$

Where  $H_{Ai}$ ,  $H_{Wi}$ , and  $H_{Ti}$  respectively represent atmospheric, aquatic, and terrestrial, hazard impact value for chemical  $i$ .

#### 3.1.4 Incremental cost indicators

This work adopted and modified the pioneering cost metric – Inherent Safety Implementation Cost ( $C_{\text{Inherent}}$ ) (Khan & Amyotte, 2005) – to indicate the financial aspects of design modifications.  $C_{\text{Inherent}}$  presents a stepwise cost indexing method guided by inherent safety principles, which is straightforward and practical for adapting to the BN-based modeling processes.  $C_{\text{Inherent}}$  is calculated for the application of each principle with the extent of their corresponding applicability, as shown in Equation 3.9, where the indexing procedure of each segment can be found in Table 3.3.

$$C_{\text{inherent}} = \frac{CM}{EM} + \frac{CS}{ES} + \frac{CA}{EA} + \frac{CSi}{ESi} + \frac{CL}{EL} \quad (3.9)$$

Where  $C_M$ ,  $C_S$ ,  $C_A$ ,  $C_{Si}$ , and  $C_L$  represent the costs of implementing inherent safety principles of minimization, substitution, attenuation, simplification, and limitation of effects;  $E_M$ ,  $E_S$ ,  $E_A$ ,  $E_{Si}$ , and  $E_L$  represent the extent of applicability of the respective inherent safety principles.

**Table 3.3: Guidelines to decide the applicability and implementation cost of inherent safety principles**

Descriptions	Applicability and cost indicator
May be applicable and cost may be medium	10
May be applicable and cost may be little	9
Applicable and cost may be medium	8
Applicable and cost may be little	7
Significantly applied with medium cost	6
Significantly applied with little cost	5
Completely applied with major cost	4
Completely applied with medium cost	3
Completely applied with minor cost	2
Completely applied with little cost	1

### 3.2 Determining the indicator weights using Analytic Hierarchy Process (AHP)

The AHP is proposed by Saaty (1977), and it was used to estimate the weights considering its salient functions to deal with the competing criteria with only empirical evidences (Marsh et al., 2017). The AHP is a particularly prevalent solution to weight elicitation and its nature lies in sorting out the relative importance via pairwise comparison. In this work, the hierarchies of the SHEC with their sub-metrics are furnished in Table 3.4. It is worth noting that all the sub-metrics operated the worst case-type (Hassim & Hurme, 2010c) in scoring processes to keep consistency with ISI and the deterministic BN based modeling.

**Table 3.4: The hierarchy of friendly chemical process indicators**

Primary Indicators (PIs)	Codes	Secondary Indicators (SIs)	Codes	Ternary Indicators (TIs)	Codes
Safety indicators	U1	I <sub>CI</sub>	U1_1	I <sub>RM, max</sub>	U1_1_1
				I <sub>RS, max</sub>	U1_1_2
				I <sub>INT, max</sub>	U1_1_3
				I <sub>FL</sub>	U1_1_4
				I <sub>EX</sub>	U1_1_5
				I <sub>TOX</sub>	U1_1_6
				I <sub>COR, max</sub>	U1_1_7
		I <sub>PI</sub>	U1_2	I <sub>I</sub>	U1_2_1
				I <sub>T, max</sub>	U1_2_2
				I <sub>P, max</sub>	U1_2_3
				I <sub>EQ, max</sub>	U1_2_4
				I <sub>ST, max</sub>	U1_2_5
				I <sub>PM</sub>	U2_1_1
				I <sub>P</sub>	U2_1_2
Health indicators	U2	I <sub>PPH</sub>	U2_1	I <sub>T</sub>	U2_1_3
				max(I <sub>MS</sub> )	U2_1_4
				max(I <sub>V</sub> )	U2_1_5
				max(I <sub>C</sub> )	U2_1_6
		I <sub>HH</sub>	U2_2	max(I <sub>EL</sub> )	U2_2_1
				max(I <sub>R</sub> )	U2_2_2
Environmental indicators	U3	Y <sub>A<sub>i</sub>, max</sub>	U3_1		/
		Y <sub>W<sub>i</sub>, max</sub>	U3_2		/
		Y <sub>T<sub>i</sub>, max</sub>	U3_3		/
Incremental cost indicators	U4	C <sub>M</sub> /E <sub>M</sub>	U4_1		/
		C <sub>S</sub> /E <sub>S</sub>	U4_2		/
		C <sub>A</sub> /E <sub>A</sub>	U4_3		/
		C <sub>Si</sub> /E <sub>Si</sub>	U4_4		/
		C <sub>L</sub> /E <sub>L</sub>	U4_5		/

According to the three-step AHP solutions, the first step was done as shown in Table 3.4.

For the second step, the factors in the primary indicators and their sub-metrics are mutually compared using the 1 - 9 numerical scale (see Table 3.5) method based pairwise comparison. The last step is to calculate the maximum eigenvalue ( $\lambda_{\max}$ ) and its

corresponding eigenvector to conduct a consistency test. The Consistency Ratio (CR) - the ratio of Consistency Index (CI) to Random Index (RI) - can be obtained using Equation 3.10 and Equation 3.11. The value of RI can be determined by the factor number (n) in pairwise comparison (see Table 3.6). If  $CR \leq 0.1$ , the normalized eigenvector will be eligible to act as a weight vector. To mitigate the data-intensive procedure, this work developed a set of MATLAB based functions to facilitate the data solution (the running codes can be found in Appendixes A).

**Table 3.5: The 1 - 9 numerical scale for pairwise comparison**

Importance intensity	Definition	Explanation
1	Equal importance	Two activities contribute equally to the objective
3	Moderate importance of one over another	Experience and judgment strongly favor one activity over another
5	Essential or strong importance	Experience and judgement strongly favor one activity over another
7	Very strong importance	An activity is strongly favored and its dominance demonstrated in practice
9	Extreme importance	The evidence favoring one activity over another is of the highest possible order of affirmation
2, 4, 6, 8	Intermediate values between the two adjacent judgments	When compromise is needed
Reciprocals	If activity i has one of the above numbers assigned to it when compared with activity j, then j has the reciprocal value when compared with i.	



**Table 3.5, continued**

Importance intensity	Definition	Explanation
Rationals	Ratios arising from the scale	If consistency were to be forced by obtaining n numerical values to span the matrix.
<hr/>		
	$CI = \frac{\lambda_{\max} - n}{n - 1}$	(3.10)
	$CR = \frac{CI}{RI}$	(3.11)

**Table 3.6: Method for quantifying the Random Index (RI)**

n	1	2	3	4	5	6	7	8	9
RI	0.00	0.00	0.58	0.90	1.12	1.24	1.32	1.41	1.45

### 3.3 Normalizing the indicator scores using fuzzy logics

The adopted inherent SHEC indices are somewhat criticized due to the superposition operations for the hazard scores with different units (Gupta & Edwards, 2003; Hassim et al., 2013). In this context, fuzzy logics were used considering its prominent capabilities of representing the ambiguous factors with unclear boundaries, which can normalize the risk representations to thus develop dimensionless RFPP. When using the fuzzy logics, determining the degree of membership is the basis to distribute the risk fuzziness. Accordingly, the triangular membership function, expressed by p, q, r, was adopted considering its straightforward and easy-to-use procedures. There are three distribution forms (i.e., down-half ridge, intermediate ridge, and ascending ridge) in the triangular

membership function, as shown in Equation 3.12, Equation 3.13, and Equation 3.14, respectively.

$$A(x) = \begin{cases} \frac{r-x}{r-q}, & q < x \leq r \\ 0, & x > r \end{cases} \quad (3.12)$$

$$A(x) = \begin{cases} 0, & x \leq p \\ \frac{x-p}{q-p}, & p < x \leq q \\ \frac{r-x}{r-q}, & q < x \leq r \\ 0, & x > r \end{cases} \quad (3.13)$$

$$A(x) = \begin{cases} 0, & x \leq p \\ \frac{x-p}{q-p}, & p < x \leq q \end{cases} \quad (3.14)$$

Where  $p$ ,  $q$ , and  $r$  represent dependent parameters that can be decided by the range or penalty of the sub-metrics.

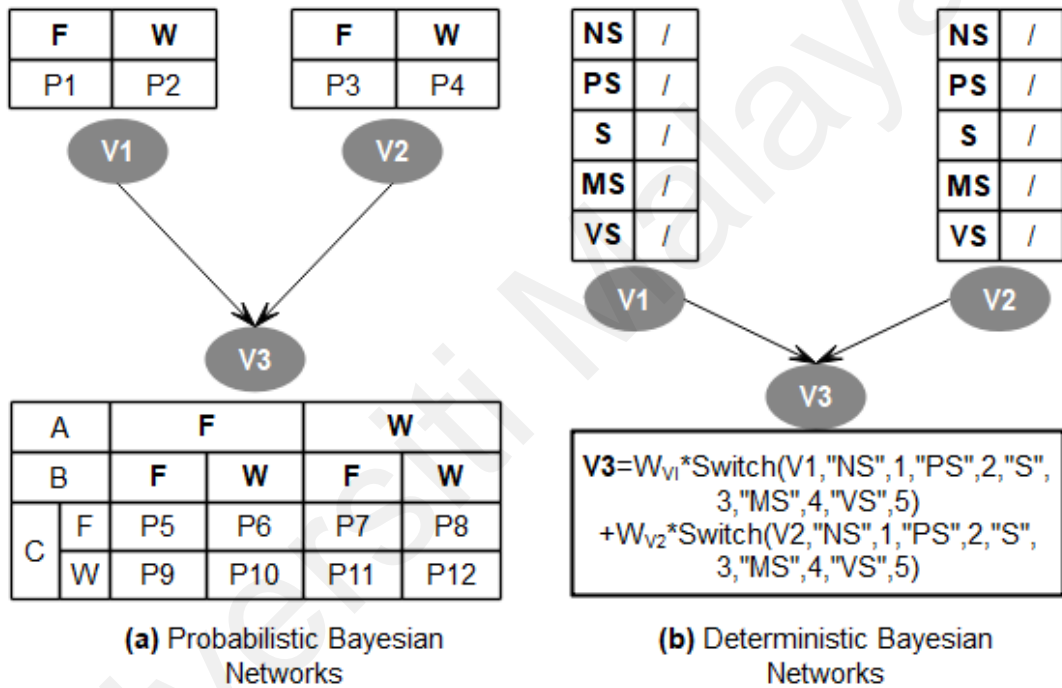
It is pertinent to note that the 'x' values in the Equation 3.12 to Equation 3.14 represent the deterministic values of the separate SHEC metrics. Thus, the determination of the 'x' values follows with the ranges or penalties of the sub-metrics. For example, the 'x' value of  $U1\_1\_1$  ranges from 0 to 4 corresponding to the value range of  $I_{RM, \max}$ . By transferring the deterministic values of the sub-metrics into fuzzy values, the risk representations can be normalized as Very Friendly (VF), Relatively Friendly (RF), Moderate (M), Relatively Hostile (RH), Very Hostile (VH).

### 3.4 Reconciling the indicators using deterministic Bayesian Networks (BN)

Based on the input data, the probabilistic BN inference under the first-order Markov

Chain can be illustrated in Figure 3.2 (a). Where the V1, V2, and V3 are three envisaged variables with binary states, i.e., F (Fail) and W (Work). Where, V1 and V2 are termed Secondary Nodes (SNs) with prior probabilities (i.e., P1 to P4) and V3 is called Primary Node (PN) with joint probabilities (i.e., P5 to P12). With these inputs, the probability of F state of the variable V3 can be obtained using Equation 3.15.

$$P(V3 = F|V1, V2) = P1 * P3 * P5 + P1 * P4 * P6 + P2 * P3 * P7 + P2 * P4 * P8 \quad (3.15)$$



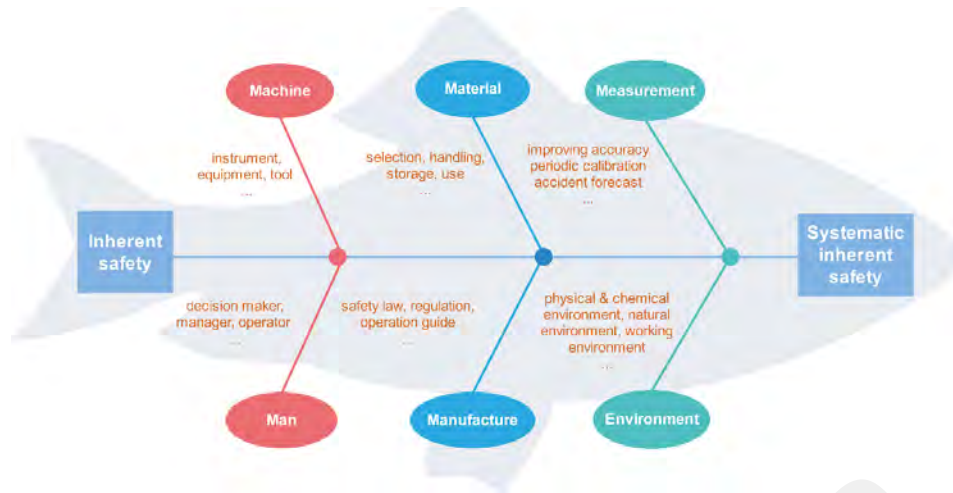
**Figure 3.2: The transition of probabilistic Bayesian Networks (BN) to deterministic Bayesian Networks (BN)**

In this work, the probabilistic BN were symmetrically transited into deterministic BN to adapt to the deterministic input data (i.e., the VF, RF, M, RH, and VH), as shown in Figure 3.2 (b). As such, the data transfer in the deterministic BN follows the dedicated rules that integrate the weights and normalized risk representations. The dedicated rules were used as deterministic CPTs based on the Weighted Average Method (WAM) and

Switch function. This function, as implied by its formula  $\text{Switch}(x, a_1, b_1, a_2, b_2, \dots, [\text{def}])$ , will return a result corresponding to the first matching value. Accordingly, the formula was tailored as  $\text{Switch}(X, VF, 1, RF, 2, M, 3, RH, 4, VH, 5)$  in the context of the normalized risk representations. It is pertinent to note that the BN modeling processes were conducted in the GeNIe 4.0 (<https://www.bayesfusion.com>) environment considering its competent capabilities of constructing the deterministic BN.

### **3.5 Inherently friendlier design modification dimensions**

For the inherent safety principles, there still lacks systematic dimensions to facilitate their implementation. Consequently, the dimensions of Systematic Inherent Safety (SIS) was conceptually proposed based on 5M1E (man, machine, material, method, measurement, and environment). As a heuristic and holistic procedure, the 5M1E approach has been employed as a guide for identifying the possible sources of quality degradation (Han et al., 2008; Kim et al., 2003). Theoretically, the variations from 5M1E during the process design, operation, and maintenance could be transmitted to the process quality and eventually cripple inherent safety and reliability (He et al., 2016). For incorporating proactive safeguards to a relatively full extent, the SIS dimensions were adopted as shown in Figure 3.3 to guide the inherently friendlier design modifications.



**Figure 3.3: The implementation dimensions of the Systematic Inherent Safety (SIS)**

### 3.6 Quality control measures

The quality control measures of this study can be generally described in the following two sections. Firstly, the renowned SHEC metrics were selected to indicate the inherent friendliness. During the literature review, various metrics were collected and compared on the indicator coverage, and eventually the ISI (Heikkilä, 1999), IOHI (Hassim & Hurme, 2010c), IETH (Gunasekera & Edwards, 2006), and  $C_{\text{Inherent}}$  (Khan & Amyotte, 2005) were selected considering their pioneering and trusted solutions to representing the SHEC factors. Also, the four selected metrics use the maximum values for rating the risk severities, which contributed to the consistent data formats and measurement standards. Secondly, the data collection was conducted within the widely used case studies in the "inherent" research community. In this work, for demonstrating the newly developed assessment tool (i.e., the RFPF), the biodiesel production processes were used as a case study. This data of the biodiesel production was collected from the

literatures (Gangadharan et al., 2013; Gómez, 2013; Li et al., 2011; Rathnayaka et al., 2014) where the process parameters are well fitted to this study. Specifically, the process parameters including the maximum of main reaction heat, the maximum of side reaction heat, the maximum of chemical interaction, flammability, explosiveness, toxic exposure, the maximum of corrosiveness, inventory, the maximum of process temperature, the maximum of process pressure, the maximum of equipment safety, the maximum of safe process structure, and other generic information can be matched and reused as the consistent input data.

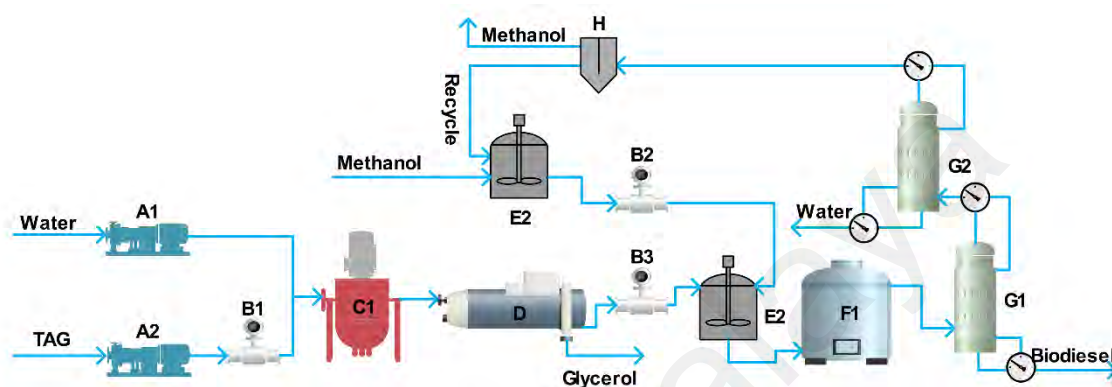
## CHAPTER 4: RESULTS AND DISCUSSION

### 4.1 Baseline design and its friendliness indicators' weighting results

#### 4.1.1 Baseline design descriptions

The biodiesel production process is used as a case study for demonstrating the proposed RFPF. Generally, biodiesel production process can be divided into three main steps (i.e., feedstock pre-treatment, transesterification, and polishing and purification) (Moazeni et al., 2019). Dominated by vegetable oils, diverse feedstocks can be used to generate the synthesis paths for manufacturing biodiesel (Ramos et al., 2019). For the present case study, palm oil (represented by triacylglycerol, TAG) and methanol are utilized as the main feedstocks. This production process and associated data were extracted from the manufacturing process flow used by Gangadharan et al. (2013) and Rathnayaka et al. (2014) who gleaned the biodiesel production information from Li et al. (2011) and Gómez (2013), respectively. In the BDPO as shown in Figure 4.1, TAG, along with water, is transmitted into C1 (hydrolysis tank) by A (charge pump) via B1 (fluid meter). In C1, TAG is hydrolyzed to produce fatty acid, subsequently carried to D (phase separator) for excluding byproduct. Then the separated fatty acid is fed into F1 (transesterification reactor) after being mixed with methanol in E2 (mixer). The crude biodiesel produced in F is lastly sent into G1 (separation distillation column) for purification, and the excess methanol in the overhead product is recovered by G2

(purification distillation column) for recycling via H (fluid divider). If the RFPF result is not satisfactory for the BDPO, design modifications will be conducted using inherent safety principles. The most general and widely applicable principles reported by Khan and Amyotte (2002) are encapsulated in Table 4.1.



**Figure 4.1: The baseline design of biodiesel production process**

**Table 4.1: Key inherent safety principles**

N	Principles	Description
1	Minimization	Reducing hazardous material inventories, operation numbers, plant size, etc.
2	Substitution	Replacing hazardous materials, process routes, non-robust equipment, etc.
3	Attenuation	Moderating hazardous reactions, storage, transportation, etc.
4	Limitation of effects	Limiting accident escalation by changing design and operations.
5	Simplification	Reducing the volume of process facilities and operations.
6	Error tolerance	Making process can bear and withstand unwanted operations and reactions.

#### 4.1.2 Weighting processes and results for the baseline design

For the BDPO, the weights of the metrics were obtained through pairwise comparison using the 1 - 9 scale method (Saaty, 1990, 2008) based on their importance. As an



explanatory example, the pairwise comparison with its weighting results for the primary indicators (U1 to U4) is shown in Table 4.2.

**Table 4.2: Weighting processes for the primary indicators (U1 to U4)**

PIs	U1	U2	U3	U4
U1	1	5	2	2
U2	1/4	1	1/2	1/2
U3	1/2	3	1	1
U4	1/2	2	1	1
CR=0.07<0.1, A=[0.45, 0.11, 0.23, 0.21]				

The weight vector A and CR for the U set were resolved using the developed MATLAB function with judgment matrix N as inputs (an illustrative example for using the developed function was documented in Appendix B). Based on the relative importance of the 1 - 9 scale (Saaty, 1990, 2008) in the AHP method, the values of weight vector A and CR were obtained by repeating the same procedures for the sub-metrics. The results of the pairwise comparison, CR, and eigenvectors are encapsulated in Table 4.3 to Table 4.7. It is worth noting that the weights of RFPF indicators were analytically determined using the AHP method with the authors' expertise and preferences. In practice, the expertise can rely on the designers. And the preferences can refer to the investors based on the fact that the investors often engage external designers, known as Engineering, Procurement, and Construction (EPC) contractors, to conduct the process design (Towler & Sinnott, 2013).

**Table 4.3: Weighting processes for the secondary metrics (U3\_1 to U3\_3)**

Secondary metrics	U3_1	U3_2	U3_3
U3_1	1	1/3	1
U3_2	3	1	2
U3_3	1	1/2	1
CR=0.02<0.1, A=[0.21, 0.55, 0.24]			

**Table 4.4: Weighting processes for the secondary metrics (U4\_1 to U4\_5)**

Secondary metrics	U4_1	U4_2	U4_3	U4_4	U4_5
U4_1	1	1/2	1	1	1/2
U4_2	3	1	2	1	1
U4_3	1	1/2	1	1	1/2
U4_4	2	1	1	1	1/2
U4_5	2	1	2	2	1
CR=0.06, A=[0.13 0.27 0.16 0.16 0.28]					

**Table 4.5: Weighting processes for the ternary metrics (U1\_1\_1 to U1\_1\_7)**

Ternary metrics	U1_1_1	U1_1_2	U1_1_3	U1_1_4	U1_1_5	U1_1_6	U1_1_7
U1_1_1	1	1	1/2	2	1/3	1/2	2
U1_1_2	1	1	1/2	3	1/3	1/2	2
U1_1_3	3	2	1	5	1	1	4
U1_1_4	1/2	1/3	1/3	1	1/6	1/4	1
U1_1_5	3	3	1	5	1	1	5
U1_1_6	2	2	1	4	1	1	4
U1_1_7	1/2	1/3	1/4	1	1/3	1/2	1
CR=0.04, A=[0.10 0.11 0.23 0.05 0.24 0.21 0.06]							

**Table 4.6: Weighting processes for the ternary metrics (U1\_2\_1 to U1\_2\_5)**

Ternary metrics	U1_2_1	U1_2_2	U1_2_3	U1_2_4	U1_2_5
U1_2_1	1	3	3	1	1/2
U1_2_2	1	1	2	1/2	1/3
U1_2_3	1/4	1/2	1	1/4	1/5
U1_2_4	1	2	4	1	1
U1_2_5	2	3	5	1	1
CR=0.07, A=[0.23 0.13 0.06 0.25 0.33]					

**Table 4.7: Weighting processes for the ternary metrics (U2\_1\_1 to U2\_1\_6)**

Ternary metrics	U2_1_1	U2_1_2	U2_1_3	U2_1_4	U2_1_5	U2_1_6
U2_1_1	1	2	1	4	2	2
U2_1_2	1	1	1/2	3	1	1
U2_1_3	1	2	1	5	3	3
U2_1_4	1/4	1/3	1/4	1	1/2	1/2
U2_1_5	1/2	1	1/3	2	1	1
U2_1_6	1/2	1	1/3	2	1	1
CR=0.04, A=[0.25 0.15 0.30 0.06 0.12 0.12]						

Table 4.2 presents a pairwise comparison for the primary indicators (i.e., the Safety, Health, Environment, and Cost metrics) for sorting out their weights. For example, the value of 5 in Table 4.2 demonstrates that U2 has essential or strong importance over U1. Accordingly, all the values in Table 4.2 can be positioned and understood with their relative importance in the 1 - 9 numerical scales. Table 4.2 presents the weight vectors and CR for the secondary metrics (i.e., the S, H, E, and C sub-metrics). The weight vector of U1\_1 and U1\_2 is [0.5, 0.5], which represents equal importance regarding I<sub>CI</sub> and I<sub>PI</sub>. This situation goes the same with Indexing for I<sub>PPH</sub> and I<sub>HH</sub>, and thus the weight vector of U2\_1 and U2\_2 is set as [0.5, 0.5]. In addition, the metrics of U1\_1 versus U1\_2, U2\_1 versus U2\_2, and U2\_2\_1 versus U2\_2\_2 are naturally consistent, which allows the absence of consistency test. By compiling all weight data, the overview of the weighting results of the inherent friendliness metrics was obtained as shown in Table 4.8.

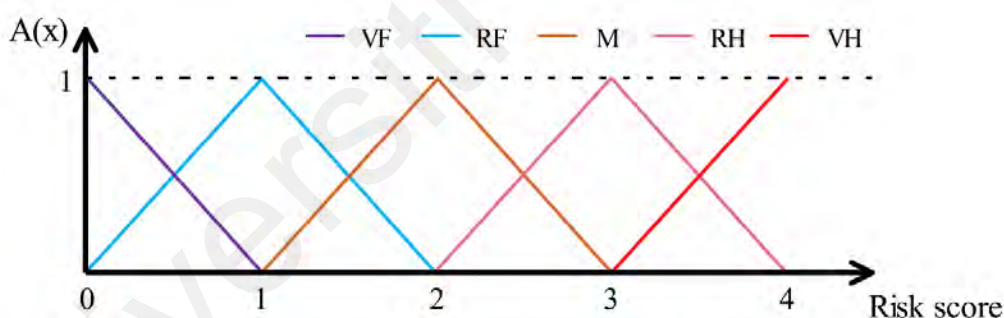
**Table 4.8: Weighting results of the inherent friendliness indicators**

PIs	Weights	SIs	Weights	TIs	Weights
U1	0.45	U1_1	0.50	U1_1_1	0.10
				U1_1_2	0.11
				U1_1_3	0.23
				U1_1_4	0.05
				U1_1_5	0.24
				U1_1_6	0.21
				U1_1_7	0.06
		U1_2	0.50	U1_2_1	0.23
				U1_2_2	0.13
				U1_2_3	0.06
				U1_2_4	0.25
				U1_2_5	0.33
				U2_1_1	0.25
				U2_1_2	0.15
U2	0.11	U2_1	0.50	U2_1_3	0.3
				U2_1_4	0.06
				U2_1_5	0.12
				U2_1_6	0.12
		U2_2	0.50	U2_2_1	0.34
				U2_2_2	0.66
U3	0.23	U3_1	0.21	/	/
		U3_2	0.55	/	/
		U3_3	0.24	/	/
U4	0.21	U4_1	0.13	/	/
		U4_2	0.27	/	/
		U4_3	0.16	/	/
		U4_4	0.16	/	/
		U4_5	0.28	/	/

## 4.2 Normalizing processes and results for the risk scores

This section is to present and discuss the risk scores and normalizing processes based on the results for the case study (see Appendix C and Appendix D). The normalization of the risk scores in the case study followed four steps: 1) grading the value of each

terminal metric, 2) selecting the type of fuzzy membership function, 3) determining the membership function parameters (p, q, and r), and 4) computing the fuzzy memberships. The results for the four steps are integrated into Figure 4.2 and Table 4.9 where U1\_1\_3 is exemplified for computing memberships. It is necessary to note that the risk values for measuring U1\_1\_3 range from 0 to 4, and thus the transverse coordinate was equalized into five nodes (i.e., 0, 1, 2, 3, 4) for determining the membership function parameters. As per the maximum of U1\_1\_3, the maximum of abscissa in the triangular membership function was determined as 4, as shown in Figure 4.2. The parameters in Equation 3.12 to Equation 3.14 were determined as Table 4.9. In the BDPO, as the risk score of U1\_1\_3 was estimated as 2, the membership for VF, RF, M, RH, and VH were obtained as VF=0, RF=0, M=1, RH=0, and VH=0.

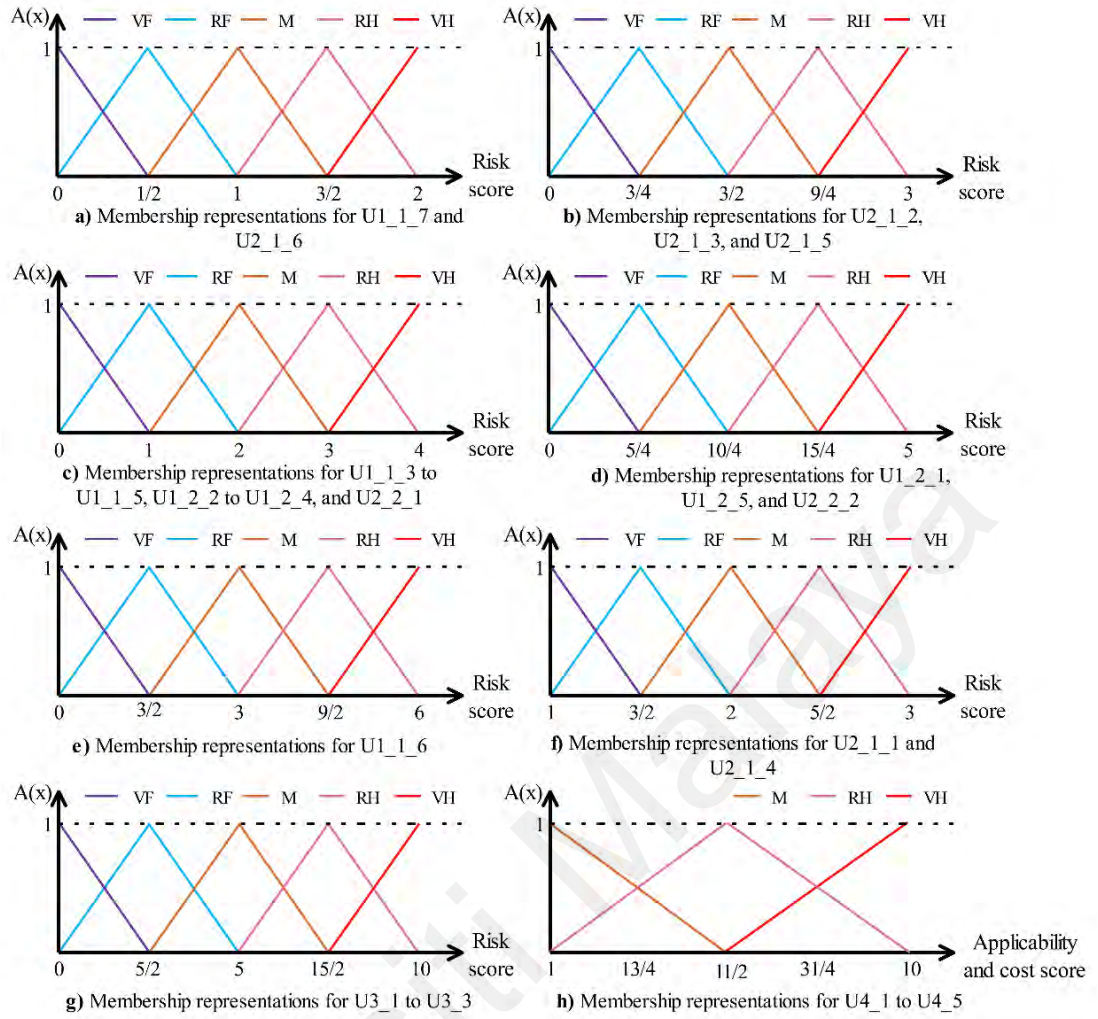


**Figure 4.2: Membership representations for the maximum of chemical interaction (U1\_1\_3)**

**Table 4.9: Determination of membership function parameters for the maximum of chemical interaction (U1\_1\_3) of the baseline design**

Terminal metric	Risk score	Comment set V	Membership functions	Membership function parameters		
				p	q	r
U1_1_3	2	VF	Equation 3.12	/	0	1
		RF	Equation 3.13	0	1	2
		M	Equation 3.13	1	2	3
		RH	Equation 3.13	2	3	4
		VH	Equation 3.14	3	4	/

Table 4.9 demonstrates an illustrative example to calculate the memberships of the terminal metric U1\_1\_3. By repeating the calculating processes for the remaining terminal metrics (i.e., U1\_1\_4 to U1\_1\_7, U1\_2\_1 to U1\_2\_5, U2\_1\_1 to U2\_1\_6, U2\_2\_1 to U2\_2\_2, U3\_1 to U3\_3, and U4\_1 to U4\_5), the full membership representations can be obtained as shown in Figure 4.3. Where, the Figure 4.3 a) to Figure 4.3 h) respectively represent the membership representations with risk scores ranging from 0 - 2, 0 - 3, 0 - 4, 0 -5, 0 - 6, 1 - 3, 0 -10, and 1 - 10. By compiling all the memberships, the results of normalizing the risk scores were obtained as shown in Table 4.10.



**Figure 4.3: The full membership representations for the terminal risk metrics**

**Table 4.10: Results of normalizing the risk scores of terminal metrics**

Terminal metrics	Ranges	Risk Scores	Risk score normalizations				
			VF	RF	M	RH	VH
U1_1_1	0 - 4	N/A	1/5	1/5	1/5	1/5	1/5
U1_1_2	0 - 4	N/A	1/5	1/5	1/5	1/5	1/5
U1_1_3	0 - 4	2	0	0	1	0	0
U1_1_4	0 - 4	3	0	0	0	1	0
U1_1_5	0 - 4	2	0	0	1	0	0
U1_1_6	0 - 6	2	0	2/3	1/3	0	0
U1_1_7	0 - 2	1	0	0	1	0	0
U1_2_1	0 - 5	1	1/5	4/5	0	0	0
U1_2_2	0 - 4	3	0	0	0	1	0
U1_2_3	0 - 4	0	1	0	0	0	0
U1_2_4	0 - 4	3	0	0	0	1	0
U1_2_5	0 - 5	3	0	0	3/5	2/5	0
U2_1_1	1 - 3	3	0	0	0	0	1
U2_1_2	0 - 3	0	1	0	0	0	0
U2_1_3	0 - 3	3	0	0	0	0	1
U2_1_4	1 - 3	2	0	0	1	0	0
U2_1_5	0 - 3	1	0	2/3	1/3	0	0
U2_1_6	0 - 2	1	0	0	1	0	0
U2_2_1	0 - 4	1	0	1	0	0	0
U2_2_2	0 - 5	4	0	0	0	4/5	1/5
U3_1	0 - 10	15/4	0	5/10	5/10	0	0
U3_2	0 - 10	45/8	0	0	3/4	1/4	0
U3_3	0 - 10	23/4	0	0	7/10	3/10	0
U4_1	1 - 10	N/A	1/5	1/5	1/5	1/5	1/5
U4_2	1 - 10	N/A	1/5	1/5	1/5	1/5	1/5
U4_3	1 - 10	N/A	1/5	1/5	1/5	1/5	1/5
U4_4	1 - 10	N/A	1/5	1/5	1/5	1/5	1/5
U4_5	1 - 10	N/A	1/5	1/5	1/5	1/5	1/5

It is necessary to note that the modifications have yet to be conducted for the BDPO.

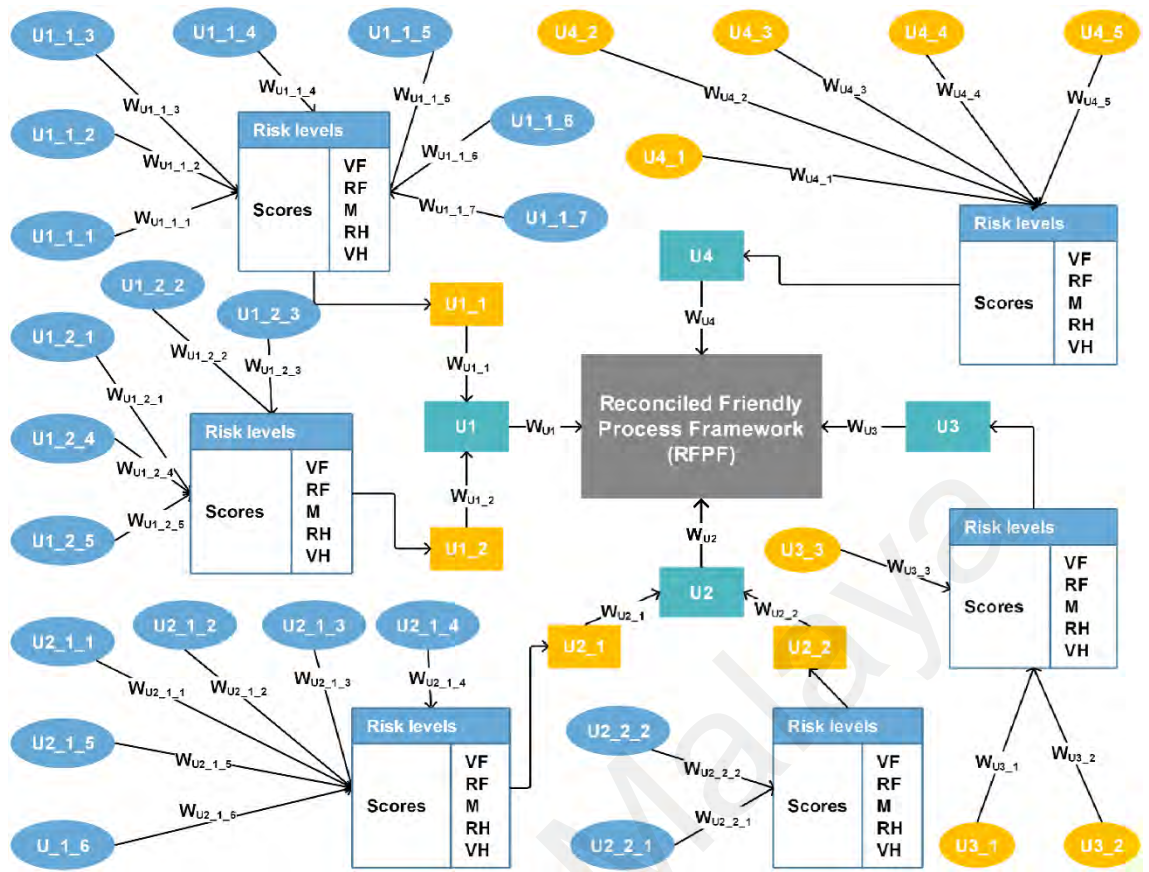
Therefore, the memberships regarding cost metrics (U4\_1 to U4\_5) were evenly assigned as 1/5. As such, the eventual assessment results can be unbiased free from the cost metric. Besides, the main and side reactions for biodiesel production processes are



endothermal, which made U1\_1\_1 and U1\_1\_2 be rated as N/A as they are metrics for measuring the hazards resulting from exothermal reactions. Methanol is deemed as the main chemical to incur environmental hazards since it was involved in most of the reported accidents in the biodiesel production process (Salzano et al., 2010), and it is thus taken as the crucial chemical in attaining the memberships for the environmental hazards.

### 4.3 Demonstration of the Reconciled Friendly Process Framework (RFPPF)

Having the SHEC indicators and their weights and scores in different hierarchies, the RFPPF is figured out, as shown in Figure 4.4. The RFPPF presents a cohesive set of dimensions for integrating the SHE components and their optimized schemes into chemical process design, whilst ensuring that the increased inherent SHE friendliness will not be twisted by the incremental costs. In the RFPPF, the symbols correspond to the hierarchy of the friendly chemical process indicators, and the terminal indicators (e.g., U1\_1\_1 and U3\_1) are designed with risk scores and indicator weights (e.g.,  $W_{U1\_1\_1}$  and  $W_{U3\_1}$ ) as their main attributes. Besides, the intermediate indicators (e.g., U1 and U1\_1) are also designed with indicator weights (e.g.,  $W_{U1}$  and  $W_{U1\_1}$ ) to deliver weighted data for indicating and generating a more realistic chemical process route regarding the inherent friendliness. With these input data, the usability of the proposed RFPPF was first demonstrated for the BDPO.



**Figure 4.4: The overview of the Reconciled Friendly Process Framework (RFPF) with the inherent friendliness indicators**

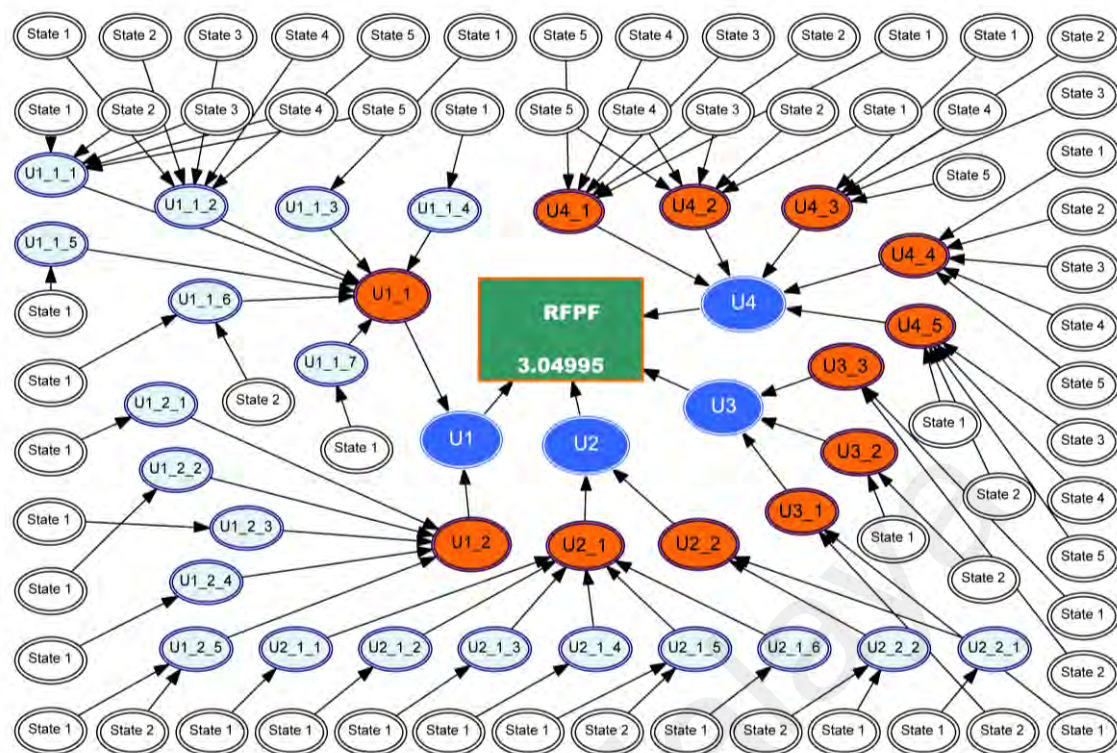
The proposed RFPF was validated in a deterministic BN. In the case study, the weight vector  $A=[0.45 \ 0.11 \ 0.23 \ 0.21]$  indicates the weights of the primary indicators.  $A1=[0.5 \ 0.5]$  and  $RI$  (see Equation 4.1) represent the weights and membership matrix of the secondary indicators, respectively. Comprehensively, the hierarchical weights, along with the membership results, are encapsulated in Table 4.11, which was used as input parameters for validating the RFPF. With the hierarchical weights and normalized risk scores as the inputs, the RFPF validation results for the baseline design were obtained, as shown in Figure 4.5. The results demonstrated that the inherent friendliness of the baseline design is estimated as M level (inherent friendliness  $\approx 3.05$ ), which implies that there necessitates inherently friendlier modifications to move the process design

towards the RF or VF level.

$$RI = \begin{bmatrix} 0 & 4/7 & 3/7 & 0 & 0 \\ 0 & 2/11 & 9/11 & 0 & 0 \end{bmatrix} \quad (4.1)$$

**Table 4.11: Input parameters of validating the Reconciled Friendly Process Framework (RFPF) for the baseline design**

PIs	Weight	SIs	Weight	TIs	Weight	Risk score normalization						
						VF	RF	M	RH	VH		
U1	0.45	U1_1	0.50	U1_1_1	0.10	1/5	1/5	1/5	1/5	1/5		
				U1_1_2	0.11	1/5	1/5	1/5	1/5	1/5		
				U1_1_3	0.23	0	0	1	0	0		
				U1_1_4	0.05	0	0	0	1	0		
				U1_1_5	0.24	0	0	1	0	0		
				U1_1_6	0.21	0	2/3	1/3	0	0		
				U1_1_7	0.06	0	0	1	0	0		
		U1_2	0.50	U1_2_1	0.23	1/5	4/5	0	0	0		
				U1_2_2	0.13	0	0	0	1	0		
				U1_2_3	0.06	1	0	0	0	0		
				U1_2_4	0.25	0	0	0	1	0		
				U1_2_5	0.33	0	0	3/5	2/5	0		
				U2	0.11	U2_1_1	0.25	0	0	0	0	1
						U2_1_2	0.15	1	0	0	0	0
U2_1_3	0.30	0	0			0	0	1				
U2_1_4	0.06	0	0			1	0	0				
U2_1_5	0.12	0	2/3			1/3	0	0				
U2_1_6	0.12	0	0			1	0	0				
U2_2_1	0.34	0	1			0	0	0				
U2_2_2	0.66	0	0	0	4/5	1/5						
U3	0.23	U3_1	0.21	/	/	0	5/10	5/10	0	0		
		U3_2	0.55	/	/	0	0	3/4	1/4	0		
		U3_3	0.24	/	/	0	0	7/10	3/10	0		
U4	0.21	U4_1	0.13	/	/	1/5	1/5	1/5	1/5	1/5		
		U4_2	0.27	/	/	1/5	1/5	1/5	1/5	1/5		
		U4_3	0.16	/	/	1/5	1/5	1/5	1/5	1/5		
		U4_4	0.16	/	/	1/5	1/5	1/5	1/5	1/5		
		U4_5	0.28	/	/	1/5	1/5	1/5	1/5	1/5		



**Figure 4.5: The validation results of the Reconciled Friendly Process Framework (RFPF) for the baseline design**

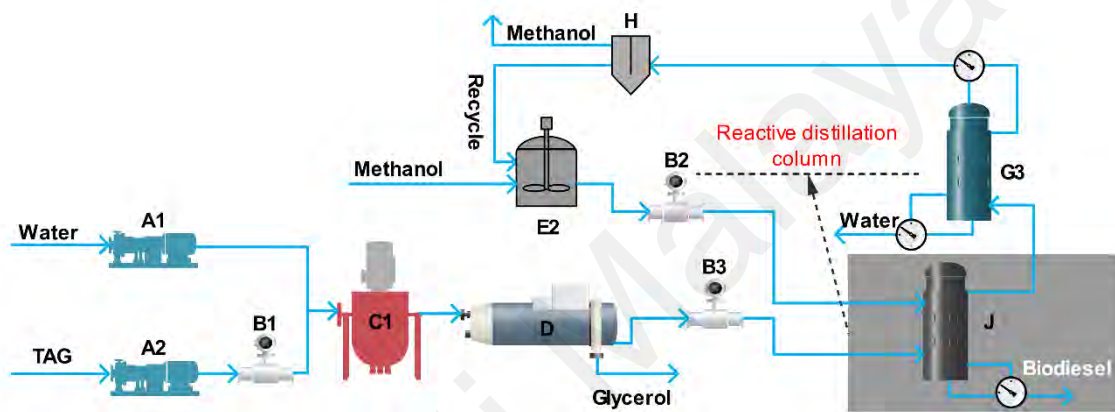
#### 4.4 Inherent friendliness oriented design modifications

The essence of the SIS interventions lies in its inclusive strategies for conducting risk reduction from the perspective of 5M1E, thus creating relatively comprehensive inherent safety interventions that are expected to maximize SHE and cost benefits. Accordingly, the SIS interventions based on the 5M1E have been done for the BDPO to shape the friendlier biodiesel production process. Specifically, the SIS interventions are encapsulated in Table 4.12. The modified flowsheet design is presented in Figure 4.6.

**Table 4.12: Systematic inherent safety (SIS) interventions for the baseline design**

5M1E	Envisaged intervention descriptions	Safety benefits/advantages
Man	1) Substitution: Employment with certificates. 2) Attenuation: Reduction of continuous working hours.	Human error reduction.
Machine	1) Substitution: F and G1 are replaced by a reactive distillation column (J). 2) Simplification: J requires fewer transfer operations and less pipework. 3) Substitution: Existing control instrumentation is replaced by instrumentation with a higher safety integrity level. 4) Simplification: Existing alarm system is simplified to avoid operator overloading with alarms.	1) Inventory reduction for methanol and biodiesel. 2) Risk reduction for human error. 3) Risk reduction in equipment failure. 4) Safety burnout reduction regarding alarm system.
Material	1) Minimization: The inventory of methanol flow is reduced by approximately half of the initial value. 2) Substitution: Alkali based catalyst (NaOH) is replaced by Na <sub>2</sub> O.	1) Risks reduction regarding the accidental release and fugitive emission of methanol. 2) Continuous processes with heterogeneous catalyst process. Fewer vapors will be produced during an unexpected release of methanol; methanol inventory is significantly reduced.
Method	1) Substitution: G2 is replaced by a vacuum distillation column (G3).	
Measurement	N/A	-
Environment	1) Limitation of effects: G3 is equipped with a containment system (H). 2) Attenuation: Equipment noise checking and minimization. 3) Attenuation: Enhancing ventilation system.	1) Limiting the escalation for methanol leakage accident. 2) Enhancing occupational health. 3) Mitigating methanol fugitive emission.

The modified flowsheet, with different reactor systems and same reaction synthesis, was generated by the SIS interventions for the BDPO. The interventions were done with particular focus on the F1, G1, and G2, which were identified as hazardous processing nodes with credible accident scenarios in fire and explosion. As such, the processing nodes were minimized to the reactive distillation column (J) and distillation column (G3).



**Figure 4.6: The modified design of biodiesel production process**

SIS interventions were incorporated into the BDPO, which is expected to create friendlier biodiesel production process. Thus, the friendliness increment needs to be demonstrated, which necessitates re-implementing RFPF for the MDPO. By repeating the computational process for the secondary metrics in the modified process, the input parameters of conducting the RFPF for the MDPO were obtained, as shown in Table 4.13.

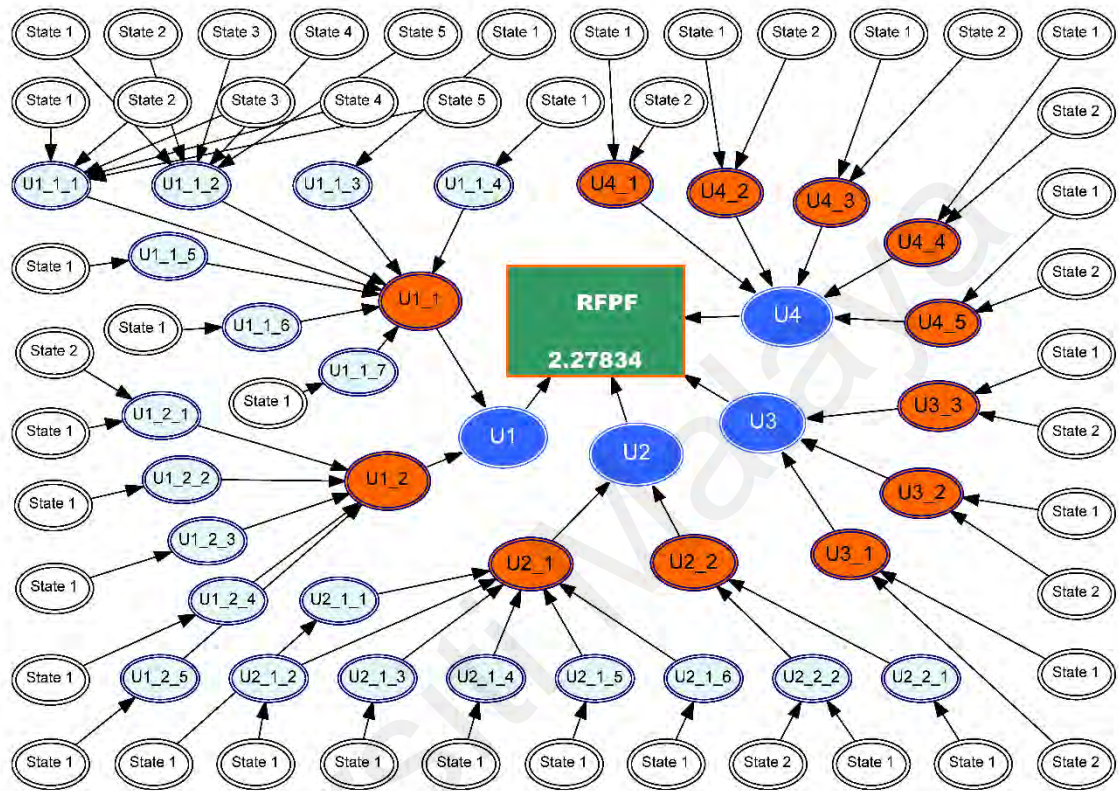
**Table 4.13: Input parameters of validating the Reconciled Friendly Process Framework (RFPPF) for the modified design**

Primary metric	Weight	Secondary metric	Weight	Ternary metric	Weight	Risk score normalization								
						VF	RF	M	RH	VH				
U1	0.45	U1_1	0.50	U1_1_1	0.10	1/5	1/5	1/5	1/5	1/5				
				U1_1_2	0.11	1/5	1/5	1/5	1/5	1/5				
				U1_1_3	0.23	0	1	0	0	0				
				U1_1_4	0.05	0	0	0	1	0				
				U1_1_5	0.24	0	0	1	0	0				
				U1_1_6	0.21	1	0	0	0	0				
				U1_1_7	0.06	1	0	0	0	0				
		U1_2	0.50	U1_2_1	0.23	1/5	4/5	0	0	0				
				U1_2_2	0.13	0	0	0	1	0				
				U1_2_3	0.06	1	0	0	0	0				
				U1_2_4	0.25	0	1	0	0	0				
				U1_2_5	0.33	1	0	0	0	0				
				U2	0.11	U2_1	0.50	U2_1_1	0.25	1	0	0	0	0
								U2_1_2	0.15	1	0	0	0	0
U2_1_3	0.30	1	0					0	0	0				
U2_1_4	0.06	0	0					1	0	0				
U2_1_5	0.12	1	0					0	0	0				
U2_1_6	0.12	1	0					0	0	0				
U2_2_1	0.34	0	1					0	0	0				
U2_2_2	0.66	0	2/5			3/5	0	0						
U3	0.23	U3_1	0.21			/	/	3/10	7/10	0	0	0		
		U3_2	0.55			/	/	0	3/4	1/4	0	0		
		U3_3	0.24			/	/	0	5/10	5/10	0	0		
U4	0.21	U4_1	0.13			/	/	0	0	0	8/9	1/9		
		U4_2	0.27			/	/	0	0	0	2/9	7/9		
		U4_3	0.16			/	/	0	0	0	8/9	1/9		
		U4_4	0.16	/	/	0	0	0	8/9	1/9				
		U4_5	0.28	/	/	0	0	0	8/9	1/9				

With the inherent friendliness oriented design modifications, the SHE performance increased as demonstrated by the parameters in Table 4.13. To indicate the inherent friendliness of the modified design, the parameters in Table 4.13 were imputed to the RFPPF based on the coding of CPTs (see Appendix E). The result ( $\text{RFPPF} \approx 2.28$ )



demonstrated that the inherent friendliness of the modified design is under RF level, as shown in Figure 4.7, implying that the modified design is inherently friendlier than the baseline design.



**Figure 4.7: The validation results of the Reconciled Friendly Process Framework (RFPF) for the modified design**

Compared with other assessment tools for inherent SHE, RFPF highlights its advantages in hierarchically reconciling inherent SHE and incremental cost concerns. In this regard, INSET (2001) acts as the pioneering advocate for integrating inherent SHE into the process development and design activities, and accordingly developed ISHE-PI for measuring and comparing process options. Despite the groundbreaking endeavors, ISHE-PI are often practically constrained due to the subjective scaling and weighting of factors. To this end, Rajagopalan and Nhan (2008) used Principal Components Analysis



(PCA) to objectively scale SHE parameters. However, the intensive procedures in using these mathematical tools may discourage the potential users in practice. In this work, AHP was further programmed in the MATLAB development environment, which contributes to resolving data with fewer time and labor costs.

In addition, by combining the renowned inherent S, H, and E metrics, Warnasooriya and Gunasekera (2017) and Anuradha et al. (2020) presented holistic solutions to comparing chemical routes concerning integrated SHE hazards. Their studies, however, give few thoughts to the cost implications. For bridging this gap, Liew et al. (2014), Liew et al. (2015), and Liew et al. (2016) incorporated economic performance when developing sustainable assessment tools during research and development stage, preliminary engineering stage, and basic engineering stage, respectively. Their solutions are to select inherently better synthesis routes; however, in many cases, there is only one BDPO awaiting ISD modifications, which could pale the utilities of selecting the inherently better design. For improvement, this work addressed this problem through generating inherently friendlier processing scenarios using inherent safety principles on the baseline processing scenario. On the other hand, the cost metrics used by Liew et al. (2014), Liew et al. (2015), and Liew et al. (2016) are mainly to select synthesis routes with inherently cheaper investment and inherently higher revenue. By contrast, this work demonstrated that the expenditures of implementing inherent safety will not override or twist the overall inherent friendliness. In this context, the results work in concert with the conjecture: the systems may turn out to be costlier than those based on

the principles of inherent safety (Khan & Amyotte, 2005).

#### **4.5 Graphical inherent friendliness metrics**

Based on BN topology, the RFPF presented a graphical assessment process with the risk nodes. The first graphical inherent safety metric was proposed by Gupta and Edwards (2003) to address the limitations of the dimensionless addition and arbitrary assignment of the disparate hazard scores in selecting inherently safer process routes. Similarly, the virtues of the graphical methods were introduced to differentiating inherently healthier chemical processes (Hassim et al., 2013) among competing synthesis routes. The main advantages of the two graphical methods lie in visualizing the hazards and comparing them in the same process steps to phase out relatively hazardous process routes. In this study, the advantages were also integrated into the RFPF development, where the normalized metrics were used to generate numerical values. Thus, the nodes with a different number of sub-nodes in the BN can return comparative values from 1 to 5. Besides, the ISM-RL also figured out an overall score for comparing the inherent safety levels before and after implementing design modifications, which is consistent with the Graphical Descriptive Technique for Inherent Safety Assessment (GRAND) (Ahmad et al., 2015) and 2-Dimensional Graphical Rating (2DGR) (Ahmad et al., 2016) with concluded total scores to assist the comparison of different process design alternatives. Notably, the RFPF is positioned at the general design stage, thus enabling relatively stationary graphical parameters as compared with the 2DGR (Ahmad et al., 2016) and

the Graphical Inherent Safety Assessment Technique (GISAT) (Ahmad et al., 2019) with metabolic parameters dedicated to the different phases of the process design stage.

#### **4.6 Costs and timing of inherent friendliness oriented design**

Cost implications of implementing inherent safety concept have been vigorously studied during the past two decades. During the design stage, selecting the relatively economic materials and process equipment can fundamentally reduce the capital and operating costs (Khan & Amyotte, 2005), thus contributing to the inherently cheaper chemical processes. For example, the conventional homogeneous biodiesel processes are modified as a heterogeneous process by changing NaOH based catalyst with the Na<sub>2</sub>O/MgO based catalyst (Gangadharan et al., 2013), leading to the inherently cheaper biodiesel production processes as the latter heterogeneous catalyst can be reused and regenerated and the costs of purifying the products can be reduced. Specifically, developing the inherently cheaper chemical processes is successively dedicated for R&D phase considering the operating cost and revenues (Liew et al., 2014), PE phase considering the operating profits (Liew et al., 2015), and BE phase considering the total annualized costs (Liew et al., 2016). Compared to the current study, the cost assessment was focused on the incremental costs as the cost fluctuation was mainly from the design modifications for the fixed baseline design processing option.

Generally, two kinds of control measures (i.e., preventative and reactive approaches) can be used to improve the inherent friendliness of the chemical processes in the design

and operation stages. The former, as a cost-effective strategy, strives to unearth fundamental measures at the planning stage to prevent or significantly minimize the hazard contributors. The latter, often much costlier, is to cure the SBS symptoms by corrective actions and recovery efforts when observing hazard problems. In this study, the former solution was explored to proactively address the possibly built-in SHE hazards at the source, which could, in turn, reduce the cost of curing the problems such as accidents, harms, and failures in future use. This is consistent with the fact that the inherent safety based process route is well-recognized as the cost-optimal option considering the life-cycle costs (Khan & Amyotte, 2002). Specifically, the conventional chemical process may be cheaper in terms of capital expenditures; however, the later add-on costs from maintenance and modification measures could be prohibitive (Khan & Amyotte, 2005) and greatly reduce the overall economic performance.

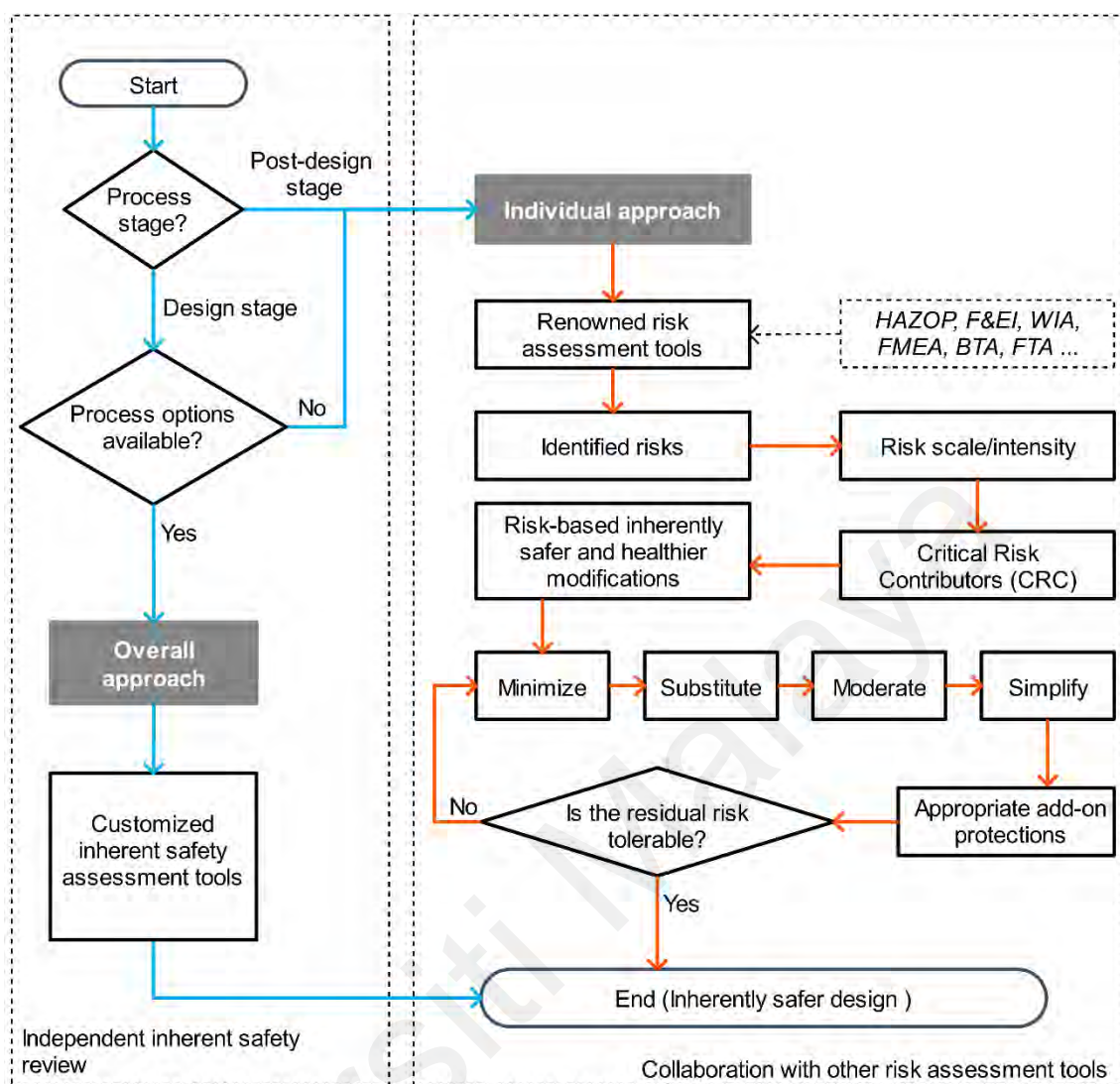
#### **4.7 Inherently friendlier modifications and their intervention manners**

This work first selected the inherent SHE and cost metrics and then developed RFPF using AHP and BN for measuring the inherent friendliness of BDPO and MDPO of biodiesel production processes. The modifications have been done by a newly proposed and validated concept (i.e., SIS) from the perspective of 5M1E. The results showed that the friendliness of the BDPO is under M condition while the MDPO evolved to be RF condition, thus demonstrating that the MDPO is inherently friendlier than the BDPO. Generally, the enhanced performance of the MDPO can be tracked and adumbrated as

follows: 1) The U1\_1 and U2\_2 performance increments are from the explosiveness and toxic exposure risk reduction through methanol inventory minimization, containment and ventilation system; 2) The U1\_2, U3\_2, and U3\_3 performance increments are mainly because of the methanol inventory minimization; 3) The U2\_1 performance increment comes from the reactive distillation column which creates continuous process; 4) The U4\_1 to U4\_5 performance changes are resulting from the financial issues after implementing inherent safety. Overall, according to the features of FCP, lesser safety control systems, waste treatment efforts, occupational hygiene facilities, and even lesser capital and operating costs are going to require, owing to the lesser investments in land, maintenance, piping work, inventory, etc. In this context, the FCP are economically promising and impose lesser risks to the people who design, build, operate, and demolish it, as well as the surroundings around it.

It is pertinent to note that the incorporation of the "inherent" concept can be generally done via two ways, i.e., independent inherent safety review and collaboration with other safety risk assessment strategies (National Research Council, 2012). The former has been vibrantly studied and practiced in developing and applying numerous Inherent Safety Indices (ISIs) (Athar, Shariff, & Buang, 2019; Park et al., 2020). By contrast with the proliferated ISATs, the latter has not yet been fully explored and exploited to integrate "inherent" concept with other renowned risk assessment tools, such as Hazard and Operability Analysis (HAZOP), Dow Fire and Explosion Index (F&EI), What-If Analysis (WIA), Failure Mode Effects Analysis (FMEA), Bow-Tie Analysis (BTA), and

Fault Tree Analysis (FTA). On the other hand, the inherent safety concept can be implemented by overall approach and individual approach (Kidam et al., 2016). The overall approach is to use the customized ISATs to distinguish Inherently Safer Process Routes (ISPRs) that are going to use less hazardous materials, more benign reaction conditions, and simpler processing schemes. This approach could be limited to first comparing and then concluding the safest process routes within available options. However, it is usually prohibitively expensive to generate several alternative process routes to find out the one with the best safety performance (Towler & Sinnott, 2013). On the other hand, the process could have been fixed as a deterministic route with the R&D analysis, which may pale the utilities of some ISIs for identifying ISPRs. In these cases, the interventions can resort to the individual approach using inherent safety principles to modify the fixed process route or scenario. In this context, the general procedures for implementing risk-based ISD could be recommended as Figure 4.8.



**Figure 4.8: The generic risk-based inherent safety intervention routes**

#### 4.8 Hybrid inherent safety concept and solutions

Inherent safety, with primary focus on the chemical industry, is conventionally and preferably used to address material-induced hazards to distinguish the inherently safer synthesis path that involves less hazardous materials and less extreme conditions (Rigas & Amyotte, 2012), implying that inherent safety concept and solutions focus on process safety challenges (e.g., fires, explosions, and toxic releases) and give few attentions on

occupational safety issues (e.g., trips, slips, and falls). To date, however, inherent safety has evolved as a more inclusive concept beyond addressing the material-induced hazards using its fundamental and proactive philosophy (CCPS, 2019). The prominent applications using inherent safety concept are the derived inherent health (Hassim & Hurme, 2010a, 2010b, 2010c), inherent environmental hazard (Gunasekera & Edwards, 2003, 2006), and inherent SHE (Safety, Health, and Environment) (Anuradha et al., 2020; Rajagopalan & Nhan, 2008; Warnasooriya & Gunasekera, 2017). In essence, these prominent applications are in light of the proactive ideologies and fundamental solutions of inherent safety to thus manage the SHE-associated risks. Likewise, guided by the exhortation of "What You Don't Have, Can't Leak" (Kletz, 1978) and ISD principles, this work addressed the CRC in and around the synthesizing scenario, attempting to develop holistic and inclusive Inherently Safer System (ISS) instead of narrow Inherently Safer Synthesis Routes (ISSR). For example, the principle of substitution is originally intended to replace hazardous materials with safer materials to thus obtain ISSR (Amyotte et al., 2012; Kletz, 1985). In this study, however, the principle of substitution is broadly used to replace any hazardous components, including the location of J and H, the flexible slings of L, the synthetic web slings of L, and the small windows of the workshop. In this context, beyond chemical processes, inherent safety concept could be or might have been extended to various other risk-prone processes for managing the hazardous entities (e.g., procedures, human factors, engineering equipment, and working environments), even though there could be no



hazardous materials to minimize, substitute, and moderate. Interestingly, the adoption, adaption, and documentation of using inherent safety outside the chemical processes where it was proposed tend to be fairly loose. Thus, "What You Don't Have, Can't Leak, Harm, Lose, Injure, Fail, and Waste" could be heuristic to inclusively incorporate the inherent safety concept into kinds of risk reduction research and practice.

#### **4.9 Comparison with the existing inherent SHE studies**

Over the past two decades, many inherent SHE-based studies have been presented inspired by the fundamental solutions and tremendous achievements of inherent safety. Like the inherent safety concept, inherent SHE attempts to proactively eliminate or reduce the SHE hazards at the source without relying on extensive end-of-pipe protections or remedial measures. Such promise promoted the development of inherent SHE-based metrics for measuring the corresponding inherent features and selecting inherently safer, healthier, and more environmentally benign process routes. The inherent SHE metrics, together with the newly developed metric of this work, were gleaned and presented in Table 4.14. The methodologies, typical implementation framework, strengths and weaknesses of the existing inherent SHE metrics are compared as follows.

**Table 4.14: SHE-based metrics for assessing inherent SHE**

Terms	Metric indicators												PS	References
	I	T1	P	Y	T2	F	E1	EC	H	E	SC			
Inherent SHE performance index, ISHE-PI	√	√	√		√	√	√	√	√	√		ED	INSET (2001)	
Intelligent benign design tool, iBDT	√	√	√	√	√	√				√		ED	Palaniappan, Rajagopalan and Halim (2002)	
Atmospheric hazard index, AHI-1	√				√					√		ED	Gunasekera and Edwards (2003)	
Inherent environmental toxicity hazard, IETH					√					√		ED	Gunasekera and Edwards (2006)	
Process route healthiness index, PRHI	√	√							√			LC	Hassim and Edwards (2006)	
Inherent benign-ness indicator, IBI		√	√		√	√	√		√	√	√	R&D	Rajagopalan and Nhan (2008)	
Inherent occupational health index, IOHI		√	√		√				√		√	R&D	Hassim and Hurme (2010c)	
Health quotient index, HQI					√				√		√	PE	Hassim and Hurme (2010b)	
Occupational health index, OHI					√				√		√	BE	Hassim and Hurme (2010a)	
Occupational chemical exposure and risk estimation, OCERE	√								√		√	ED	Hassim and Hurme (2010d)	
Fugitive emission assessment tool, FEAT	√				√						√	ED	Hassim et al. (2012)	
Inherent SHE assessment tool (1), ISHEAT-1	√	√	√	√	√	√	√	√	√	√		R&D	Liew et al. (2014)	
Heuristic framework of inherent health assessment tool, HFIHAT		√	√		√				√		√	ED	Ng and Hassim (2015)	
Inherent SHE assessment tool (2), ISHEAT-2	√	√	√	√				√	√	√		PE	Liew et al. (2015)	
Inherent SHE assessment tool (3), ISHEAT-3		√	√		√			√	√	√		BE	Liew et al. (2016)	
Inherent chemical process route index, ICPRI	√	√	√		√	√	√		√	√		PE	Warnasooriya and Gunasekera (2017)	
EHS-fuzzy index, EHSI	√	√	√		√	√	√		√	√	√	PE	Anuradha et al. (2020)	
Product safety and health index, PSHI		√			√	√	√			√	√	ED	Raslan et al. (2020a)	
Product ingredient safety and exposure index, PISEI					√						√	ED	Raslan et al. (2020b)	
Enhanced inherent occupational health index, EIOHI		√	√		√						√	R&D	Ying So et al. (2021)	
Reconciled Friendly Process Framework (RFPF)	√	√	√	√	√	√	√	√	√	√	√	ED	The current study	

#### **4.9.1 The methodologies for the inherent SHE studies**

The most pioneering inherent SHE study is the three-year European Union co-funded research project, aiming to promote the systematic application of inherently better ideology during the process invention stages. The ISHE-PI (INSET, 2001) is the major output in this project, and it consists of eleven tailored indices for various hazards that may be involved during the process or plant design stage. However, the eleven indices were developed to be relatively independent and stand-alone, by which it could be uneasy to indicate the overall inherent SHE level for a certain processing scenario. In this respect, Liew et al. (2014), based on the information available during the R&D stage, developed an integrated assessment tool (i.e., the ISHEAT-1), where the separated three indices, together with cost metric, were reconciled via fuzzy optimization for measuring the overall inherent SHE level. After that, another two inherent SHE metrics tailored for the BE stage (Liew et al., 2016) and PE stage (Liew et al., 2015) were developed as the ISHEAT-2 and the ISHEAT-3 according to the data availability. As it implies literally, besides the inherent safety index, the inherent SHE-based metrics also include the inherent health index and inherent environment index. In this domain, the PRHI (Hassim & Edwards, 2006) and the IETH (Gunasekera & Edwards, 2006) were developed in the light of inherent safety concept as the respective pioneering tools for inherent health and environmental assessment,. In general, the methodologies of the IETH and the PRHI can be illustrated by Equation 4.2 (Gunasekera & Edwards, 2006) and Equation 4.3 (Hassim & Edwards, 2006).

$$IETH = \sum_{i=1}^m (YA_i + YW_i + YT_i) \quad (4.2)$$

$$PRHI = ICPHI \times MHI \times HHI \times \frac{WEC_{\max}}{OEL_{\min}} \quad (4.3)$$

$$IOHI = IPPH + IHH \quad (4.4)$$

Where  $YA_i$ ,  $YT_i$ , and  $YW_i$  stand for the toxicity impact severity scale value of chemical  $i$  in the atmospheric environment, terrestrial environment, and aquatic environment, respectively. The ICPHI, MHI, HHI, WEC, and OEL denote the Inherent Chemical and Process Hazard Index, Material Harm Index, Health Hazard Index, Worker Exposure Concentration, and Occupational Exposure Limit, respectively.

As the initial exemplar of assessing inherent environmental factors, the IETH is evolved from the IEH (Cave & Edwards, 1997) and the AHI-1 (Gunasekera & Edwards, 2003). It is composed of three aggregated sections (see the factors in Equation 4.2) to indicate the inherent environmental toxicity hazard taking MMA (methyl methacrylate) production process as a case study. Similarly, this case study was also employed to validate the PRHI (Hassim & Edwards, 2006), a prototype of the inherent healthiness metric. Although the PRHI procedure cannot be and is not intended to be precise due to the still missing data during the initial process design stage, its methodology offers a heuristic guide for selecting inherently healthier process routes. Thereafter, for the R&D stage, this methodology was further tailored as the IOHI (Hassim & Hurme, 2010c) which comprises the Index for Physical and Process Hazards ( $I_{PPH}$ ) and the Index for Health Hazards ( $I_{HH}$ ). The two sub-indices respectively represent the likelihood of exposure to chemicals for workers and the health impacts and dangers caused accordingly, and eventually, the sum (i.e., the IOHI) of sub-indices is used to characterize inherent health level, as shown in Equation 4.4

(Hassim & Hurme, 2010c). Based on the methodologies of the IOHI, a more holistic metric with Layers of Protection (LOP) control strategies was presented (Ying So et al., 2021). As process proceeds, the HQI (Hassim & Hurme, 2010b) for the BE process stage and the OHI (Hassim & Hurme, 2010a) for the PE process stage were developed according to the available process parameters. Furthermore, the IOHI, OHI, and HQI were respectively reconciled with safety, environmental, and economic concerns for assessing alternative biodiesel production pathways during the R&D stage (Liew et al., 2014), BE stage (Liew et al., 2016), and PE stage (Liew et al., 2015). More inclusively, the IOHI, HQI, and OHI were compiled as the HFIHAT (Ng & Hassim, 2015) for selecting the inherently healthier process route based on chemical exposure and operating conditions. Considering the chemical exposure is one of the two vital contributors to occupational health, Hassim and Hurme (2010d) further elucidated the Occupational Chemical Exposure Risk Metric (OCERE) for measuring and comparing the concentration-based and intake-based exposure risks of process routes. Besides, as most of the chronic chemical exposure results from fugitive emission, Hassim et al. (2012) further identified its incentives from the numbers of piping components and equipment fittings together with the type of process units.

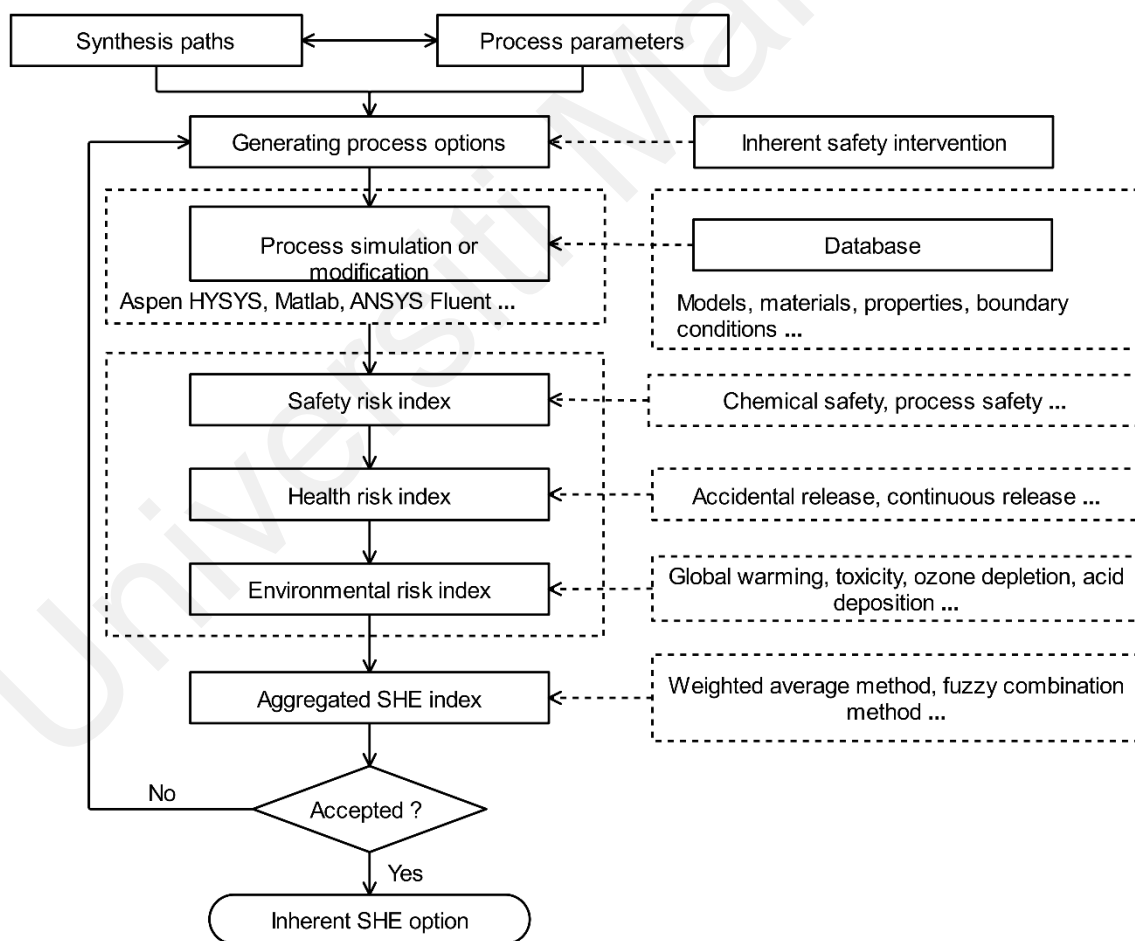
Similar to the methodologies of the reconciled SHE assessment tools, the ICPRI (Warnasooriya & Gunasekera, 2017) integrated the SHE concerns through three separate indices (i.e., chemical route safety index, occupational health hazard index, and environmental toxicity hazard index), and their values were aggregated with relative importance from expert elicitation. Similarly, the EHSI (Anuradha et al., 2020),

based on a fuzzy hierarchical model, also incorporated the three similar indices for assessing the inherent SHE hazards with special concerns on accidental and daily operational chemical release. With special concern on explicitly scaling the disparate the SHE hazards, the IBI (Rajagopalan & Nhan, 2008) adopted an objective scaling mechanism by specifying relative and absolute parameter values. In practice, the SHE hazards could vary depending on the chemical inventories, which necessitates selecting corresponding hazard forms either from safety, health, or environmental consideration. For instance, based on the safety and health hazards of formulated products, the PSHI (Raslan et al., 2020a) and the PIEI (Raslan et al., 2020b) were customized for identifying and eliminating the involved hazardous ingredients during product design.

#### **4.9.2 Typical implementation framework of the inherent SHE studies**

Like the previous three kinds of ISMs, the inherent SHE-based metrics also attempt to compare and select the optimal process alternative. In the comparison and selection, inherent safety no longer works as an independent indicator but is integrated into the inherent health and inherent environmental assessment. Concerning the individual metric selection, the inherent safety metric is always adapted from the previously analyzed pioneering ISMs, and the inherent health and environmental metrics generally prefer the IOHI (Hassim & Hurme, 2010c) and the IETH (Gunasekera & Edwards, 2006), respectively. Then, the three fundamental metrics would be aggregated using, for example, the weighted average method (Warnasooriya & Gunasekera, 2017) and the fuzzy combination method (Anuradha et al., 2020).

Moreover, the SHE metrics could also include cost considerations to select the process alternative with better SHE and cost performance. It is worth noting that inherent safety can also be aggregated with varied implications such as sustainability and profitability. In this regard, Guillen-Cuevas et al. (2018) developed the SASWROIM during the conceptual design stage to investigate the economic viability and the impact on environment and process safety between base and modified processing scenarios. Overall, the typical implementation framework for the SHE-based metric could be presented in Figure 4.9.



**Figure 4.9: The typical implementation framework of the SHE-based metrics**

#### 4.9.3 Strengths and weaknesses of the inherent SHE metrics

The developments of inherent health and environmental concept were inspired by inherent safety. In practice, the index-based inherent safety metrics have been preferable, thus facilitating the developments of index-based inherent health and environmental metrics. In this context, the inherent SHE-based metrics share the common strengths with the index-based inherent safety metrics, like the ease of indicator selection and the ease of indexing procedures with limited information during process design stages. On the other hand, there also exposed some weaknesses in the following aspects: 1) the inherent environmental metrics were not developed for specific phases of process design, which reduced the consistency when developing the SHE metrics with safety and health considerations; 2) when determining the presence of airborne contaminants, the inherent health metrics gave little thought on the Breathing Zone, a hemisphere forward of the shoulders with a radius of 6 to 9 inches and therefore the major area from which the employee draws airborne hazardous particulates; 3) the SHE-based metric may neglect the identification and reconciliation of the possible intersecting indicators in the separate S, H, and E metrics. Compared with the existing inherent SHE metrics, the newly developed metric (i.e, the RFPF) in this work highlights its capacities of weighting the competing SHEC indicators and aggregating the dimensionless SHEC indices, so that the accuracy of the assessment results can be improved to develop more realistic inherently FCP. Also, the RFPF integrated incremental cost considerations, which is useful to reveal whether the design modifications can twist the overall inherent friendliness of the modified process routes.

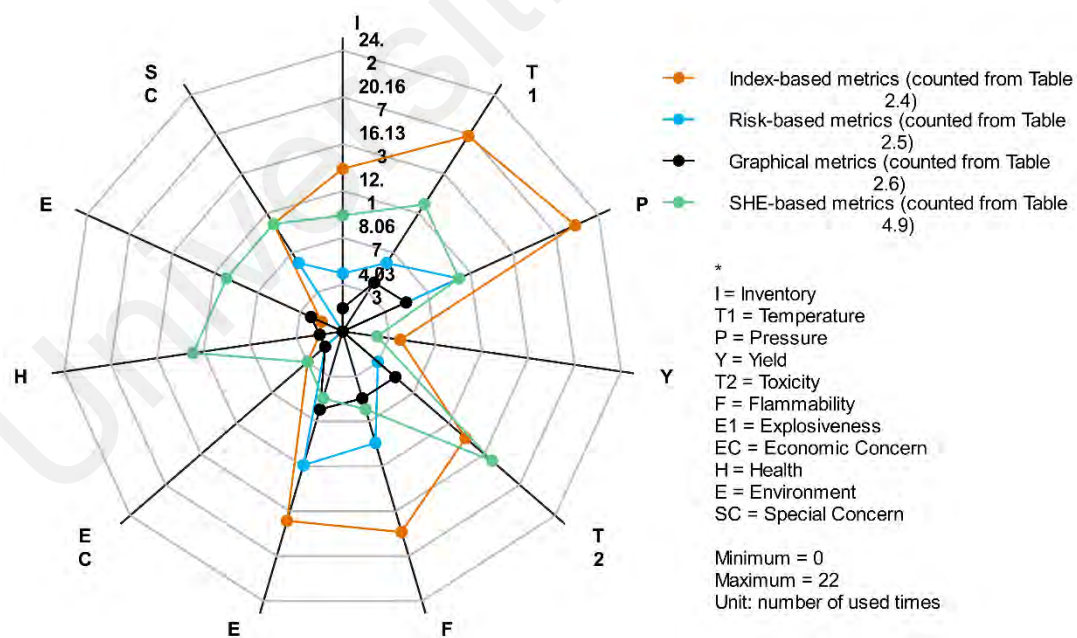


Another advantage of the RFPF is that the assessment processes and results present graphical solutions, which can absorb the virtues of the graphical inherent safety metrics to facilitate the comparison and modifications of the process routes. With these strengths and weaknesses of the SHE-based "inherent" metrics, some general challenges in practical use also arose. Firstly, the phase classifications and data availability at the process design stage are yet to be established, making the indexing procedures inevitably use empirical SHEC grades. Secondly, the design modifications are often based on the EPC contractors' interests to fulfill the prescribed inherent friendliness, which may make a less desirable process design for the investors. Thirdly, the inherently FCP modifications are static at the design stage, thus the dynamic risks from the chemistry development to the process development and construction can be neglected. To overcome these challenges, the corresponding endeavors can be made. Firstly, sharp boundaries that are consistent in SHEC data availability can be defined to divide the process design stage into clear boundaries. Secondly, risk-based inherently FCP modifications can be explored to reduce the identified risks with minimal incremental costs. Thirdly, multi-stage decision strategies can be introduced to generate the optimized process routes and sustain the inherent friendliness from the earliest design stage to the successive stages.

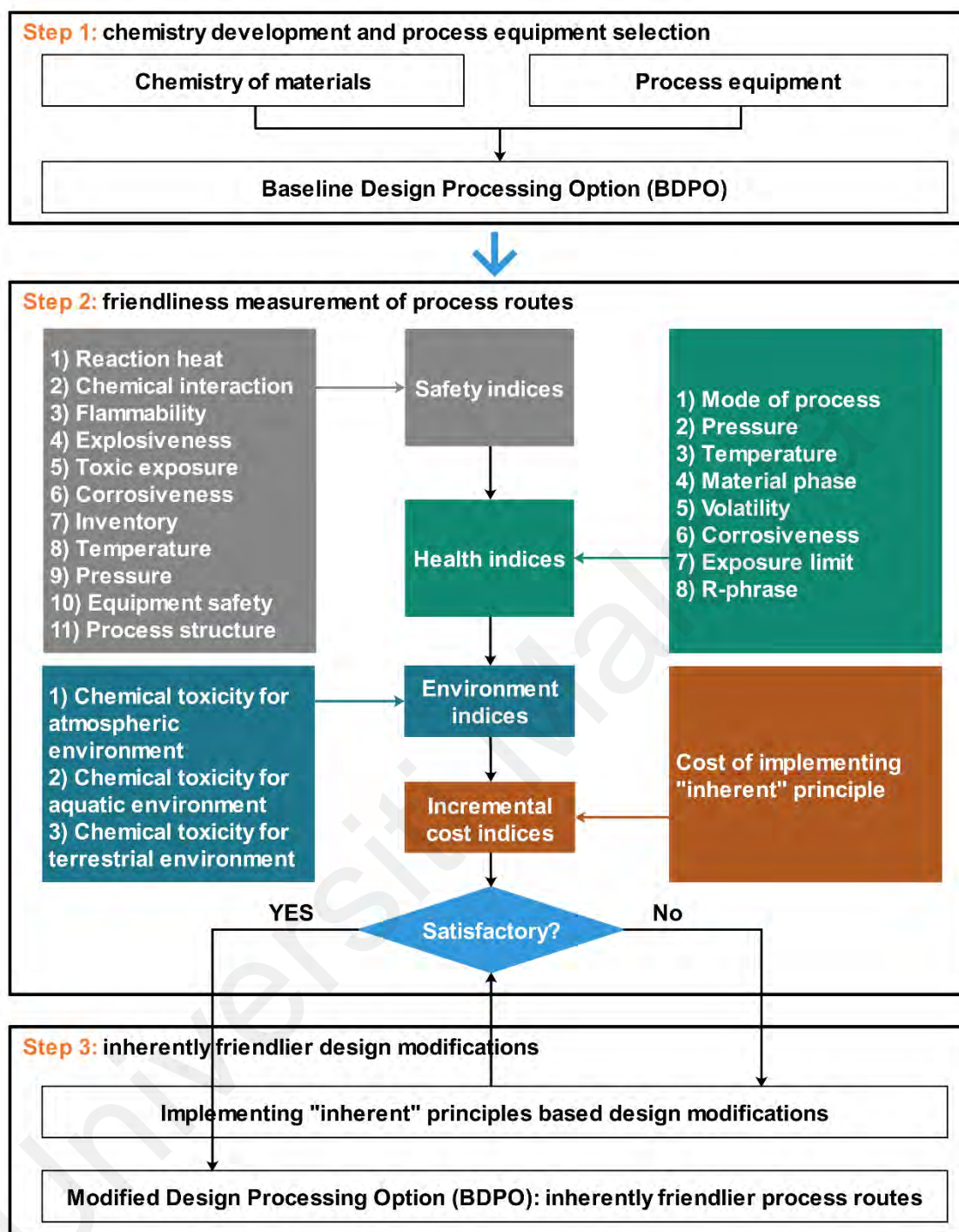
#### **4.10 The selection and application of appropriate "inherent" metric**

When selecting appropriate ISMs, users often suffer from the metric indicators, implementation stages, and benchmarking resources. Accordingly, the commonly used

indicators were extracted and compared (see Figure 4.10) for first determining the preferable metric type from the four kinds. Then, the implementation stages and concerns of case studies can be considered for guiding the further metric selection. If the users are interested in the SHE indicators and want to ensure that the cost increments of the "inherent" concept based design modifications will not cover or twist the overall inherent SHE performance, it will come to the newly developed RFPF. The RFPF is a comprehensive assessment tool for generating inherently FCP by modifying a baseline design using "inherent" principles. Generally, the RFPF can be used as the three-step standard implementation procedures, including 1) chemistry development and process equipment selection, 2) friendliness measurement of process routes, and 3) inherently friendlier design modifications, as shown in Figure 4.11.



**Figure 4.10: The spectrum of commonly used indicators in the Inherent Safety Metrics (ISMs)**



**Figure 4.11: Standard implementation procedures of using the Reconciled Friendly Process Framework (RFPF)**

## CHAPTER 5: CONCLUSION AND RECOMMENDATION

### 5.1 Conclusions

Inspired by the inherent safety concept, this study developed the Reconciled Friendly Process Framework (RFPF) as a dedicated tool for indicating and generating inherently Friendlier Chemical Processes (FCP) during design stage. With the development and validation of the proposed RFPF, the following research objectives were defined, explored, and realized.

Firstly, the "inherent" concept and its applications to developing inherently safer, healthier, and more environmentally benign processes were gleaned and compared, thus identifying the appropriate indicators to develop inherently FCP with Safety, Health, Environment (SHE) elements.

Secondly, with the identified "inherent" indicators, a dedicated tool termed Reconciled Friendly Process Framework (RFPF) was developed for indicating the inherent friendliness of chemical process routes before and after the "inherent" principles based design modifications.

Thirdly, the incremental cost indicators resulting from the "inherent" principles based design modifications were incorporated into the measurement of the inherent friendliness of the modified process routes for ensuring that the modifications are economically worthwhile in contrast to the increased SHE performance.

Fourthly, the proposed RFPF was successfully demonstrated and validated by

indicating and generating inherently friendlier biodiesel production processes.

Fifthly, a cohesive set of standard implementation procedures were presented to facilitate the application of the proposed RFPF in general chemical processes.

With the achieved research objectives, it can conclude that the aim of developing a dedicated framework (i.e., the RFPF) for indicating and generating inherently FCP through the "inherent" principles based modifications for the SHE and cost problems has been realized. The newly developed RFPF highlights its holistic solutions to incorporating the risk weights and uncertainties and graphically aggregating the separate SHE and incremental cost indicators compared with the existing studies. Using the RFPF, the generated inherently FCP can be characterized to be inherently cheaper, safer, healthier, and more environmentally benign. As such, this study can be useful to promulgate the "inherent" concept by proactively enhancing process safety, occupational health, and environmental protection while operating economically. Besides, this study addressed the cost conflicts when doing SHE modifications, which can be used as a trade-off tool for the chemical process developers and investors. With these advantages, it can be envisaged that, like cleaner production and sustainable development, the RFPF can be used as a broad concept more than a narrow technique for proactively and economically minimizing the SHE risks of chemical processes. These attempts are also expected to gradually break the boundaries of green chemistry and inherently friendlier processes by developing fundamental and proactive solutions to reducing the wastes, hazards, losses, injuries, and other process problems at their sources.

## **5.2 Knowledge contribution**

The knowledge contribution of this study can be concluded as the following three dimensions: 1) the proactive concept of inherent safety is expanded to a more inclusive way for preventing the SHE and cost problems by design approaches; 2) the RFPF is developed as a dedicated tool to indicate and generate inherently friendlier chemical process routes; 3) a set of standard procedures for using the RFPF is presented to obtain inherently friendlier process options.

## **5.3 Future research recommendations**

### **5.3.1 Inherent resilience for the infrastructure system**

Engineering resilience is an emergent safety concept to cope with the intractable hazards induced by the Volatility, Uncertainty, Complexity, and Ambiguity (VUCA) in the present ever-changing production systems. Particularly, the engineering resilience concept has been extensively employed to strengthen the infrastructure system with the capabilities of resisting the disruption events such as natural disasters, power loss, migration, and terrorist attacks. However, the current resilience management for the infrastructure system is dominated by the vulnerability reduction and disruption recovery strategies in the commission stage. How to proactively eliminate the vulnerable factors or disruption contributors in the planning and design stage to generate inherently resilient infrastructure system remains to be further elucidated. In addition, the conventional safety management, known as the Safety-I, has been advancing as the Safety-II by many renowned safety researchers and practitioners. The

Safety-II is not just to do reactive safety risk reduction but also to sustain the system in case of going wrong, which shares significant commonalities with the engineering resilience concept regarding the resistance to the disruption events. As such, using the inherent safety concept, it can be possible to incorporate proactive resilience during the infrastructure system planning and design stage. This can create a new gateway, which can be termed as inherent resilience, to develop fundamentally, permanently, and naturally resilient infrastructure system that needs little maintenance and few recovery efforts.

### **5.3.2 Metric development for lifetime economic benefits**

There is a widely recognized belief that inherent safety based friendlier process is a cost-optimal option. By contrast, there are limited reported cases to explicitly verify this cost benefit. In practice, the cost consideration is occasionally integrated with SHE considerations to select cheaper and more SHE compelling synthesis paths during the process design stage. However, the endeavors generally answer whether we can afford it and may be unable to tell us a whole cost story since the affordable synthesis path can be unequal to a cheaper entire footprint. In this context, together with the cost Life Cycle Assessment (LCA), it would be interesting to incorporate SHE, socio-political, and socio-technical factors into the development of LCA based Inherent Safety Metrics (ISMs), thus better answering the question of how the materials or processes affect the inherent friendliness from cradle to grave.

### **5.3.3 Collaborating with Preliminary Safety Analysis (PSA) tools**

Inherent safety is often conducted independently based on various tailored ISMs but seldom collaborates with other simple and well-practiced PSA tools, such as Preliminary Hazard Analysis (PHA), Concept Safety Review (CSR), Critical Examination (CE), Concept Hazard Analysis (CHA), and Preliminary Consequence Analysis (PCA2). PSA shares the safety vision with inherent safety in striving to eliminate hazards at source, which makes their collaboration feasible and synergistic in the process design stage. In this context, the PSA based implementation procedures can be encouraged to treat inherent safety as a more inclusive way of thinking (guided by the inherent safety principles) instead of a narrow safety technique, expecting to further promote the recognition, application, and documentation of inherent safety in failure and accident prone industries.

### **5.3.4 Risk-based inherently friendlier design using HAZOP**

For decades, the development of ISMs tailored for various process stages (especially for the multiple phases of the process design stage) and hazards (e.g., fire, explosion, and toxic release) has been the principal research interest of inherent safety. In the practical application, however, few of the developed metrics are available to work as a consensus with generic capacity, constrained by their complexities and accessibilities. This problem makes us questioned whether we still need more ISMs. Regarding this question, maybe, there is still no unanimous answer at present. However, a new inherent safety assessment procedure, without elaborating new metrics, can be



recommended as Figure 5.1. This procedure presents a risk-based inherently friendlier design in the light of HAZOP. With the HAZOP or its derived tools, if the modified processing scenario met the risk acceptance/tolerance criteria, the intended inherently friendlier design processing option would be generated.

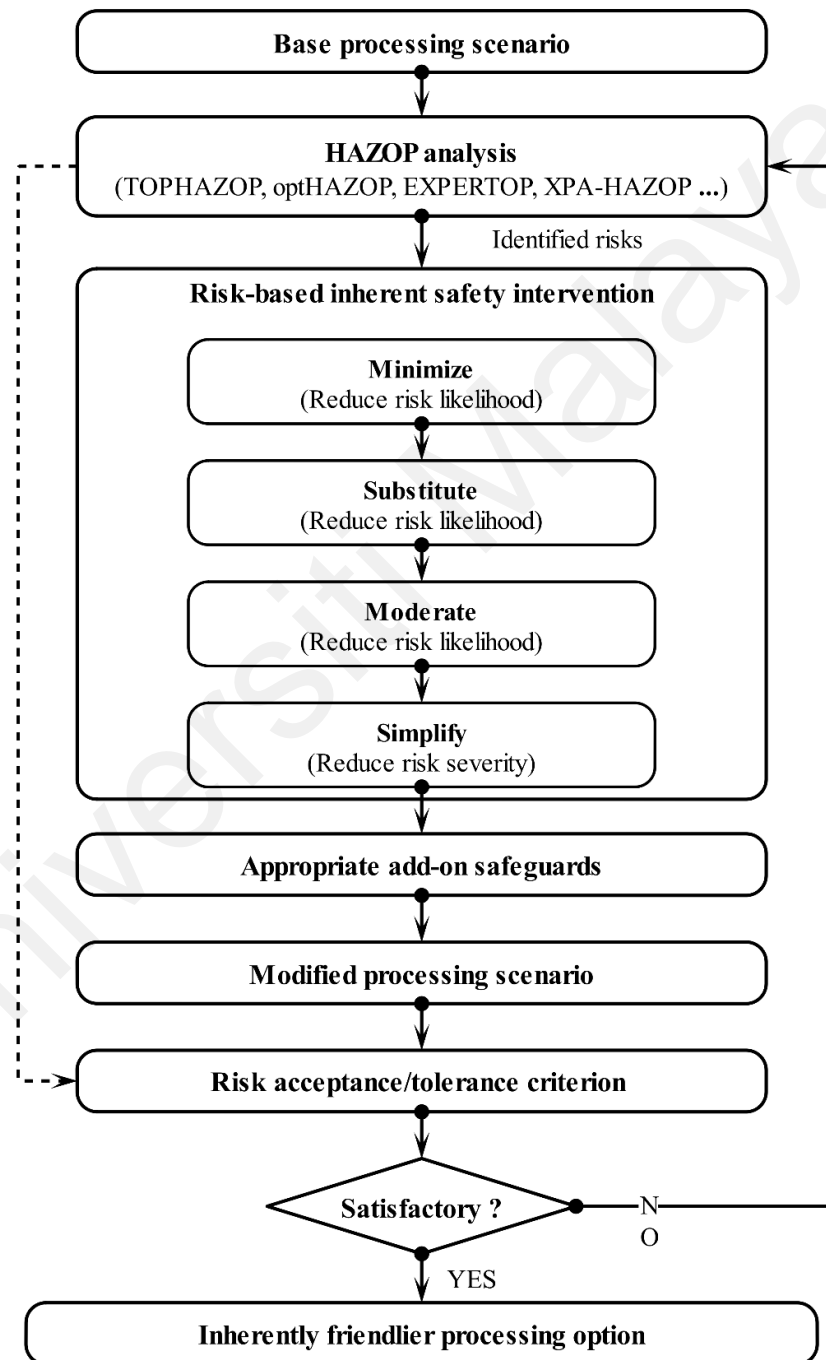


Figure 5.1: Procedures for implementing risk-based ISD using HAZOP

### **5.3.5 Intelligent inherent friendliness consolidation**

In chemical processes, the inherent friendliness is conventionally achieved by optimizing the process route design scheme towards using less hazardous materials and less extreme conditions. However, as the processes evolve to the operation stage, the built-in inherent friendliness can degenerate with the equipment aging and process retrofitting, which necessitates the consolidation of the inherent friendliness for the processes in commission. The solutions to the inherent friendliness consolidation are closely related to the intelligent chemical process operation and maintenance, where big data technologies are utilized to predicate and isolate the potential failures or accidents. Especially, with the development of the big data technologies, advanced safety instrument systems, and big data collection approaches, extensive research and practice of using data mining technologies (e.g., machining leaning, deep learning, transfer learning) have been presented to do fault diagnosis and prognosis for the existing chemical processes. This can be a heuristic for creating and sustaining the inherent friendliness of chemical processes from the lifecycle perspective. With the data mining technologies, the possibly degenerated process units regarding the inherent friendliness can be predicated and timely reduced. As such, the built-in inherent friendliness in the design stage can be monitored and intelligently consolidated in the operation stage.

### **5.3.6 Development of inherently friendlier materials**

The "inherent" concept is generally used to develop inherently better (cheaper, safer,

healthier, and more environmentally benign) process routes. By contrast, the researcher and practitioners give limited attention to developing inherently better materials, or the associated studies have not yet been seen or documented as the "inherent" solutions. However, with certainty, the possible inherently better materials are conducive to developing the inherently better processes. For example, the intrinsic (inherent) flame-retardant materials have been extensively studied with numerous published findings. Developing and introducing such new safer materials into the process design scheme can result in inherently safer process routes with lesser fire and explosion potentials. Another good example is the development and use of non-toxic sticky rice-based glue as wallpaper adhesive, which is inherently healthier than using the Polyvinyl Acetate (PVA) based glue that always needs air purification equipment (add-on protection) for cleaning the underlying emitted pollutants. Understandably, it is the inherently safer and healthier materials that make the processes inherently safer and healthier. In this context, the "inherent" concept is worth being extended to the material science fields to achieve the cohesive development of inherently friendlier materials and inherently friendlier processes. Also, this initiative may be heuristic for the chemists to find inherently friendlier materials together with the chemical engineers to build inherently friendlier processes.

#### **5.4 Research outputs**

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- 2) Gao, X., Abdul Raman, A.A., Hizaddin, H.F., Archina, B., Bello, M.M., 2020. Systematic inherent safety and its implementation in chlorine liquefaction process. *Journal of Loss Prevention in the Process Industries* 65, 104133. ISI-indexed, Q2, IF= 3.916.
- 3) Gao, X., Abdul Raman, A.A., Hizaddin, H.F., Buthiyappan, A., Bello, M.M., 2021. Dynamic Inherently Safer Modifications: Metric development and its validation for fire and explosion prevention. *J. Loss Prev. Process Ind.* 71, 104483. ISI-indexed, Q2, IF= 3.916.
- 4) Gao, X., Abdul Raman, A.A., Hizaddin, H.F., Bello, M.M., Buthiyappan, A., 2021. Review on the Inherently Safer Design for chemical processes: Past, present and future. *J. Clean. Prod.* 305, 127154. ISI-indexed, Q1, IF= 11.072.
- 5) Gao, X., Abdul Raman, A.A., Hizaddin, H.F., Buthiyappan, A., Bello, M.M., 2021. Developing friendlier biodiesel production process via systematic inherent safety interventions. *J. Clean. Prod.* 308, 127291. ISI-indexed, Q1, IF= 11.072.
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