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Progress in Inherently Safer Design for Chemical Processes

Sunhwa Park[a,b], Hans J. Pasman[a]*, Mahmoud M. El-Halwagi[a,b,c]

[a] TEES Mary Kay O'Connor Process Safety Center, Texas A&M University System, College Station, Texas 77843-3122
[b] Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas 77843-3122
[c] TEES Gas and Fuels Research Center, Texas A&M University System, College Station, TX, USA
hjpasman@gmail.com

Traditionally, process design has been primarily driven by techno-economic criteria while safety is often considered after preliminary design decisions have already been made. Such an approach implies that most of the design's degrees of freedom, including technology and configuration issues, have already been determined when considering safety. Modifying a process at later stages is costly and may be afflicted with complexity. To resolve this issue, there have been numerous attempts by safety engineers and researchers to consider process safety during the early design stages. Special attention to adopting inherently safer design (ISD) has been made because ISD is deemed the most cost-effective risk reduction strategy. However, it is still challenging for process engineers to adopt ISD at the early design stages. This study summarizes those challenges. Progress in ISD applications over the last three decades is analyzed. The question is raised as to how to quantify and reconcile inherent safety of the process while considering economics, plant resilience, environmental protection, sustainability, and life cycle requirements. So, the question is raised how to quantify the inherent safety level of a process concept. Lately, besides our own, several other extensive review papers have been published on different aspects and approaches to solve this question. Based on these findings, this paper provides insights, data, and detailed guidance for making further progress of ISD, particularly at the early process design stages.

1. Introduction

There is much literature on inherently safer design (ISD) but only scarce application. Without the fundamental removal or reduction of chemical hazards, merely installing safety devices proves much less reliable to avoid possible incidents (Kletz, 1985). To resolve this issue, safety engineers and researchers have attempted to effectively consider ISD during the early design stages. This is because ISD principles (e.g., intensification, substitution, attenuation, and simplification) are proactive strategies for reducing the incidents' likelihood or the impact and endeavouring to achieve cost-optimal safety solutions (Kletz & Amyotte, 2010). Despite greater efforts over the last three decades, it is still challenging for designers and decision-makers in the chemical process industry to adopt ISD, even during the early design stage. A likely explanation for the challenges how ISD principles can be adopted is the lack of detailed process information during the early design stages as this is mostly limited to a simple flowsheet, nature of chemicals, and process conditions, and further the lack of data on chemical properties, and practical guidance. A team at Texas A&M University attempted to break the deadlock, which resulted in three papers (Park et al., 2020, Park, Mendez et al., 2021, and Park, Bailey et al., 2021). These studies begin by summarizing previous works on ISD index measures, searching whether ISD features can be found or not in detailed accident descriptions for design practice convenience. In addition, results of three meanwhile published papers of other authors will be briefly described.

2. Research to apply ISD principles during the early design stages

Over the last three decades, there have been numerous efforts to apply ISD principles during the early design stages. Of these efforts, the Park et al. studies focus on three research approaches: (1) metrics of inherently safer design (Index-based types), (2) research on safety indicators, and (3) metrics for various process design factors along with safety.

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2.1 Metrics of Inherently safer design (ISD) levels (Index-based types)

Prior to applying ISD principles, the measurement capability of process designs' ISD levels (or safety levels) is fundamental. Therefore, a host of researchers have actively engaged in proposing Inherent Safety Assessment Tools (ISATs). Of various ISAT types, it is necessary to concentrate on the indexing methods that usually measure an inherent hazard level, because these methods are straightforward for practitioners to use. Since Edwards and Lawrence (1993) proposed the first index-based ISAT, Prototype Index for Inherent Safety (PIIS), many different indices have been proposed to prudently use the limited process information at the early design stage. Given the amount of information available, one distinguishes 22 *hazard-based* inherent safety assessment tools (H-ISATs) according to a certain procedure, 33 *risk-based* inherent safety assessment tools (R-ISATs), and 18 *cost-optimal* inherent safety assessment tools (CO-ISATs) (Park et al., 2020). The R-ISATs embrace a group that is solely based on potential *consequences* of a release and another group in case also occurrence probability values can be estimated yielding *risk.* The CO-ISATs determination is completed by a decision procedure, applying a multi-criterion or multi-objective method.

Based on a proposed index metric, the feasible design alternatives (of process routes, units, pieces of equipment, or streams) can be ranked according to their inherent safety. Fundamentally, the indices are based on safety indicators, which can be classified into two categories: chemical indicators and process indicators. Chemical indicators consider the hazards presented by the properties of chemicals (e.g., flammability, explosiveness, or toxicity), while process indicators represent the hazards of the process operating conditions (e.g., process pressure or temperature) (Park et al., 2020). Hence, these safety indicators would enable practitioners to easily calculate the relative safety levels of alternatives using the value of a given formula, because chemical indicators and process indicators can be readily available during the early design stages.

2.2 Research on safety indicators

For a more reliable ISD index value, many efforts were made to use trustworthy safety indicators. As observed by Leong & Shariff, 2009, the hazard of chemical substances included in the process design was initially considered based on the properties of each pure substance with subsequent consideration of mixtures. Also, researchers proposed safety indicators assuming a highly plausible process incident scenario. Based on the assumed scenarios, relevant theoretical equations were taken into account. For instance, process route index (PRI) was proposed by assuming an explosion incident (Leong & Shariff, 2009) and toxic release route index (TRRI) (Zaini et al., 2014). Nonetheless, given the limited availability of empirical data, there are uncertainties in the validity of estimated values of selected variables and their combinations without the availability of empirical data. Therefore, the problem-solving approach of the previous safety indicator selection methods was tried to improve via the following two recent studies.

2.2.1 Accident analysis for identifying key safety indicators

Park, Mendez, et al. (2021) analyzed at a granular level of detail 94 chemical process incidents investigated by the US Chemical Safety and Hazard Investigation Board (CSB) reports. Since many CSB reports contain detailed process incident information for high-profile US process incidents, these reports were utilized to find out whether ISD features by key safety indicators, identified in accident analysis, can be better defined. This research was the first to study the potential of low-level information extracted from the CSB reports to use in ISD strategy. To systematically analyze the incident information, this study established a guideline to collect data of incidents causal factors, scenario factors, and consequence factors. In particular, causal factors were composed of 12 chemical and 5 process indicators, while 7 scenario factors represent incident sequences, equipment types, operating modes, process units, domino effects, detonation likelihood for explosion incidents, and population densities. Consequence factors include types of chemical incidents, casualties, population densities, and economic losses. Despite the fact that the CSB reports offered detailed incident information, the findings of this study indicated that data available from the CSB reports and existing chemical databases did not allow drawing firm conclusions on identifying key safety indicators and their weights due to numerous missing data. To resolve this limitation, standardized formats in process incident reports and hands-on predictive models of chemical properties were recommended.

2.2.2 Easy method to determine important hazardous properties

Based on a recommendation of the previous CSB study, Park, Bailey, et al. (2021) proposed hands-on predictive models of the four representative safety indicators for the relatively frequent combustion incidents: flash point, heat of combustion, lower flammability limit (LFL), and upper flammability limit (UFL). Compared to previous predictive models (e.g., physical property model, group contribution model, and quantitative structure-property relationship (QSPR) model), the newly proposed models were not only easy-to-use, but also provided highly competitive performance. This study only used readily available variables — the numbers of atomic elements, molecular weights, and normal boiling points — or their proper combinations as predictors to propose easy-to-use models. Multiple linear regression (MLR) models were built based on the selected predictors by adopting machine learning algorithms to set proper predictors among numerous default variables and to build MLR models such as:

- The constructed predictive model of the flash point, T_f, for pure organic compounds:

$$T_f\ [K] \approx f(the\ numbers\ of\ C, O, N, F, Cl, Si, S\ and\ T_b)$$
$$= 2.7735 - 1.8443\, nC + 2.7454 nO\ + 2.3241 nN + 2.9889 nF + 6.2254 nCl - 3.2484 nSi - 7.9198 nS + 0.7665\, T_b \quad (1)$$

- The constructed predictive model of the heat of combustion, ΔH_C^o, for pure organic compounds:

$$\Delta H_C^o \left[\frac{kJ}{mol}\right] \approx (the\ numbers\ of\ C, H, O, N, F, Cl, Si, S, P, Pb\ )$$
$$= -30.514 - 425.831 nC - 90.766 nH + 169.7306 nO - 106.9996 nN + 224.3168 nF + 62.7552 nCl - 683.1319 nSi - 295.9456 nS - 419.4349 nP - 647.0202 nPb \quad (2)$$

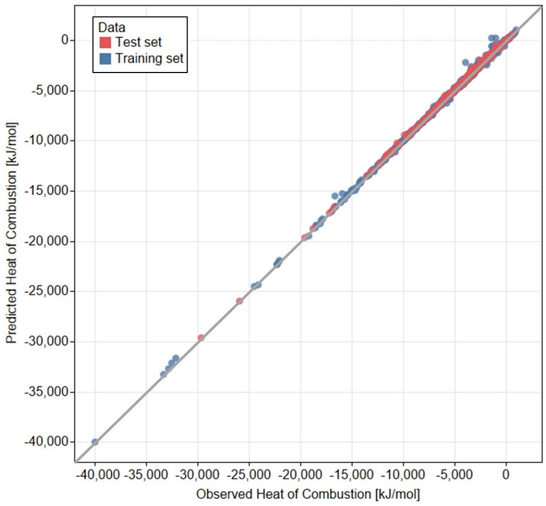

Figure 1: Predicted (Eq. 2) vs. observed heats of combustion after to Park, Bailey et al. (2021)

- The constructed predictive model of the LFL for pure organic compounds:

$$LFL\ [vol.\%] \approx f(Interactions\ of\ C, H, O, F, Cl, Si, S)$$
$$= -0.1014 + nCl(0.3103 nO - 0.0613 nH) + \frac{1}{nC}(10.3579 + 1.6783 nF + 2.0032 nCl) + \frac{1}{(nC)^2}(-1.1007 nH + 0.496(nO)^2 - 4.3578 nS - 6.896 nSi) \quad (3)$$

- The constructed predictive model of the UFL for pure organic compounds:

$$UFL\ [vol.\%] \approx f(nC, nH, nO, nN, nF, nCl, nBr, nSi, nS, MW, interaction\ terms)$$
$$= 3.636 - 0.0686 nH + 0.00001(MW)^2 + 0.2266(nO)^2 + 0.1740\,(nN)^2 + 0.8261(nS)^2 - 0.0118(MW \times nO) + 0.1799(nC \times nF) + 0.0746(nH \times nO) + \frac{1}{nC}(46.62 + 5.476 nO + 38.47 nSi) + \frac{1}{(nC)^2}(-5.749 nH - 2.051(nCl)^2 - 7.024 nBr - 0.0009(MW)^2) \quad (4)$$

where MW and T_b refer to the molecular weight [g/mol] and boiling point [K] of an organic compound of interest, respectively. UFL is considered as the most difficult parameter of the four considered. In Figure 2 the result is presented of the UFL prediction compared with observed values excluding 15 exotic compound outliers, e.g., hexadecamethylcyclooctasiloxane.

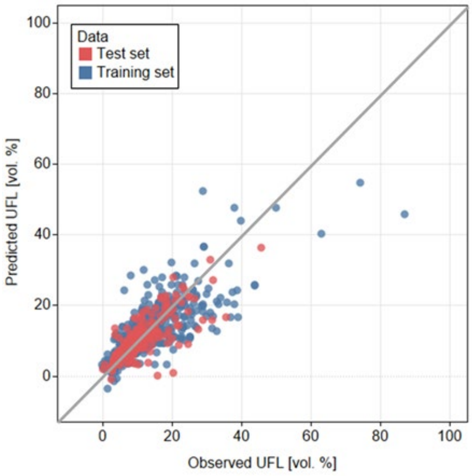

Figure 2: Predicted (Eq. 4) vs. observed UFLs without 15 outliers after to Park, Bailey et al. (2021)

2.3 Results of other recent studies

In 2021 three other ISD papers with some interesting aspects have been published, which shall be briefly summarized here.

Gao et al. (2021a) extended the scenario idea to a dynamic one for conducting Inherently Safer Modifications (ISMs) after an incident occurred. This was accomplished by applying IFAM (Information-Flow-based Accident-causing Model) accident causation model, which among other takes care of human error factors, and is further modeled by means of a rather extensive DBN (Dynamic Bayesian Network). The many required prior probability values were determined via weighted aggregation of estimates of experts, of whom the importance weights were determined by the comparative pairwise judgment of their background and expertise level. The DBN consisted of ca. 135 mostly parent nodes and 4 dynamic nodes, the latter to model the changes during the run-up of the event. Given parent probabilities, the DBN can be used to infer a final event probability and the other way around given the accident the causation probabilities. The effect of inherently safer measures can be examined using the model. Considering the method described in the paper, one comes to the conclusion that the effort to create the causal structure and estimate the probabilities is not at all negligible and requires specialist knowledge, and therefore, it is not to be expected that designers will easily apply it.

Gao et al. (2021b) reviewed the existing literature on inherent safety from a different, more broadly oriented point of view, not focused only on detailed practical guidance of early process design. It presents an overview of various metric methodologies (index-, risk-, graphical-, SHE-based, and others). It also treats cost metrics. Further, implementation literature is summarized at off-shore and nuclear industry, and finally, future research directions are discussed. There are good examples of ISD, but in has generally been treated too much as a topic on its own. It should be implemented at least with cost consideration but even better with other aspects such as health and environment. Cost should be considered over the entire plant life cycle. More attention should be given to how to reduce effects of human failure (“inherently safer human”), Because practical ISD application is still rather limited, it is recommended to include ISD thinking in Preliminary Safety Analysis, while also a HAZOP-based Inherently Safer Design and Modifications (ISD&M) procedure development is proposed.

The third paper, Sultana and Haugen (2022), describes a proposed Inherent System Safety Index (ISSI) to evaluate inherently safer solutions at the detailed engineering stage or later. ISSI is the sum of 4 sub-indices: inflow of materials and energy, production safety characteristics, a complexity index, and an equipment vulnerability. Methods for the calculation of these sub-indices are described. Production safety distinguishes 4 so-called deviation contributions: material properties and inventory, heat of reaction, emissions of vapors, and waste material effluents. Complexity is composed of 14 parameters, while for equipment vulnerability, a classification ranking order is developed. On the vulnerability index are also penalties to implement: Special risky processes, unwanted reactions, parameter interactions that increase risk, e.g., pressure increase due to temperature going up, and an extreme value of a parameter, e.g., an extremely toxic material increasing risk level exceptionally. To demonstrate the method, a case study on the production of methyl methacrylate has been carried out. The application becomes only possible when sufficient data are available; hence, this will be the case in the detailed design and later life cycle stages. The method still does not cover all risk aspects.

These papers appear to add little to the earlier described ones of the Park-team on early process design.

3. Proposed further research paths for a reliable ISAT in early design

Regarding safety considerations during the early design stage, in the studies of the Park-team two main limitations are found with current multi-objective metrics (i.e., CO-ISATs): (1) using older, simplistic safety index tools rather than enhanced ISATs for early design, and (2) lack of research related to the financial benefits from ISD (Park et al., 2020). Therefore, efforts should be made to more actively share proposed ISATs, which are suitable for use at early design with process designers and/or researchers. For designers this should be incorporated in software to be queried following a certain protocol. Also, further research on the strategic estimation of ISD benefits into a monetary value should be conducted. Several further efforts are proposed to identify optimal safety indicators, types of their combination, and ISATs.

3.1 Additional non-safety metrics for an optimal process design

The consideration of only safety aspects via an ISD metric, excluding other process aspects, would fail to incorporate different process design factors effectively. In a practical approach based on market prices of products, process engineers should optimize a design under multiple constraints. Therefore, many researchers have developed metrics that measure multiple constraints including safety, by differentiating multi-objectives, safety indices, and decision-making tools. Examples include the work of Moreno Sader et al. (2019) and Guillen-Cuevas et al. (2018) who made an optimized weighted trade-off of safety, sustainability, reliability, and resilience in terms of a return-on-investment metric. This metric provides a convenient approach to the incorporation of inherent safety, resilience, and sustainability early enough in design.

3.2 Hands-on predictive models for chemical mixture properties

As the extension of Park, Bailey, et al. (2021)'s work, a study is suggested that proposes easy-to-apply machine learning predictive models of flammability properties for chemical mixtures. Since most chemicals used in the chemical industry are mixtures, rather than pure substances, establishing hands-on predictive models of chemical mixtures would help to use accurate chemical indicators that reflect more realistic incident scenarios. However, generally in mixtures properties do not fully follow the proportional change of the properties of the mixture constituents. Also, it will be more difficult to validate results against observed data, because there is less data published of mixtures, both regarding their physical properties as well as their hazardous ones.

3.3 Identifying key safety indicators via data-driven analysis and machine learning techniques

Once enough possible indicators (i.e., chemical indicators and process indicators) are secured as key indicators, such data can be profitably used with the latest data science techniques. For example, key safety indicators might be empirically identified from previous incident information, and theoretical incident equations applying a data-driven analysis via a machine-learning technique, as illustrated in Figure 3. The findings of this approach can contribute to a better understanding of key safety indicators to apply ISD effectively. Subsequently, such selected key indicators (or their appropriate combinations) from this finding can be used to propose a more reliable ISAT.

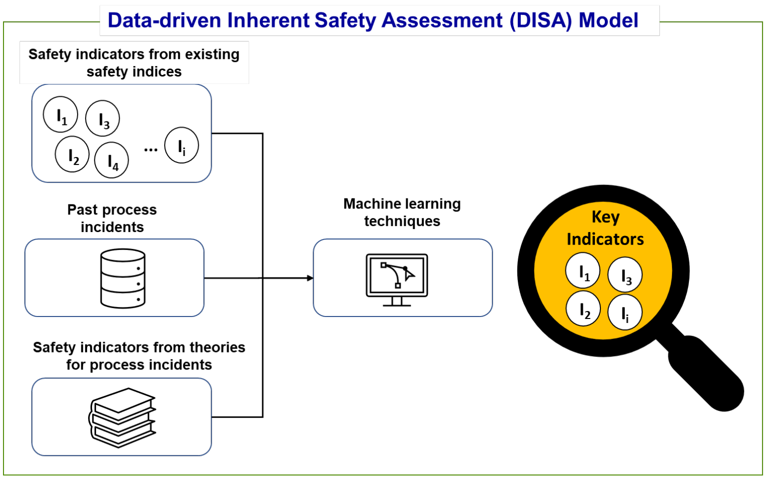

Figure 3: Proposed research approach to identify key safety indicators for ISD (Park, 2022)

4. Conclusions

This study presented the previous works for the ISD application attempts in early design and addressed possible future research based on current research progress. However, the reliability of the selected safety indicators or the proposed equations of these indicators is uncertain without verification based on actual incident data. Therefore, some further not quite successful efforts were described on how to obtain information/data that can be used as possible safety indicators before determining key indicators. Furthermore, as the importance of data application in the chemical engineering field is emphasized, the rapid development of data science applications, such as machine learning algorithms, will enable future ISD applications to be adopted more effectively.

Nomenclature

CSB – the US Chemical Safety and Hazard Investigation Board
DBN – Dynamic Bayesian Network
H-ISAT – Hazard-based ISAT
IFAM – Information-Flow-based Accident-causing Model
ISAT – Inherent safety assessment tool
ISD – Inherently safer design
ISD&M – Inherently Safer Design and Modifications
ISM – Inherently Safer Modification
ISSI – Inherent System Safety Index
LFL – Lower flammability limit
MLR – Multiple linear regression
PIIS – Prototype index for inherent safety
PRI – Process route index
QSPR – Quantitative structure-property relationship
R-ISAT – Risk-based ISAT
TRRI – Toxic release route
UFL – Upper flammability limit

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