Journal of Loss Prevention in the Process Industries 51 (2018) 112–124

Contents lists available at ScienceDirect

Journal of Loss Prevention in the Process Industries

journal homepage: www.elsevier.com/locate/jlp

Inherently safer design of a reactor network system: A case study

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ABSTRACT

The strategies of Inherently Safer Design (ISD) provide a conceptual approach in order to design equipment and processes with substantially improved safety level. However, this may lead to a less economically attractive design. This study aimed to obtain optimal decision parameters of a reactor network system to produce allyl chloride. The objective functions were the risk level, including the severity and the frequency of the accidents, which were associated with the hazards in the network and the economic profit of the process. Based on this optimization approach, an array of optimal solutions (called Pareto front) was obtained as a trade-off between the objectives under investigation. A final design point was ultimately selected using Shannon's entropy and Bellman-Zadeh's techniques of decision making in a fuzzy environment. Results showed that the optimum reactor network leads to a highly complex system and more process control difficulties. This result was inconsistent with the simplification strategy of Inherently Safer design. In order to deal with this problem, a sensitivity analysis was performed that yielded a decision guide to decide about the desirable level of the risk as well as the optimum design.

1. Introduction

Reactor systems usually represent a large portion of the total risk in a chemical process. Innovative reactor designs that improve mixing of the reactive fluids may result in much smaller reactors. Such designs are usually cheaper to build and operate, as well as being safer due to their smaller inventory. Consequently, safer design of rectors system, as the main part of the processes, is crucial in order to make the overall process safer. This can be done using any category of the risk reduction strategies, including Inherent, Passive, Active, and Procedural (CCPS, 2009).

The two most important tools to make a plant safer are inherently safer design philosophy in the preliminary stages of the design and the operational acts to control hazards. A process that is inherently safer will require fewer and less robust layers of protection. This is due the fact that an inherently safer design can either reduce the magnitude of a potential incident or make the occurrence of the accident highly unlikely (Mannan, 2012).

There are four basic principles of inherently safer design. These principles are shown in Table 1 (Shariff and Zaini, 2010).

Development of a chemical process consists of many sequential stages, namely research and development (R&D), conceptual design, detailed design, construction, start-up and commissioning, and plant operations (Thiruvenkataswamy et al., 2016). Although it is applicable to implement inherently safer design concepts and to improve the inherent safety characteristics of a plant during any stage of its lifecycle, the greatest opportunities for making major improvements in inherent safety are provided in the first stage (R&D), when the designer may have many choices of basic technology and chemistry available, and may be free to choose less hazardous alternatives (Mannan, 2012).

Generally, the evaluation and comparison of the inherent safety level with respect to different design options can be categorized in two groups (Eini et al., 2015) as follows:

- Evaluation by scoring the process features and the development of indices,
- Quantitative assessment using consequence modeling and the calculation of accidents' consequences,

The majority of the attempts have been made in order to obtain indices to evaluate the inherent safety level (Eini et al., 2015). Several studies reviewed available tools and techniques for evaluating inherent safety using indices (Khan and Amyotte, 2005; Kletz and Amyotte, 2010; Khan et al., 2015). Despite the simplicity of using inherent safety indices, they only provided a relative evaluation of the level of risk between different design options and did not consider vulnerable

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https://doi.org/10.1016/j.jlp.2017.12.004
Received 22 June 2017; Received in revised form 8 December 2017; Accepted 8 December 2017
Available online 09 December 2017

Table 1
Pareto frontier of a multi-objective optimization.

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

elements in the surrounding environment as the possible hazard receptors. However, more important point is that these indices did not demonstrate the possible, and often important, economic benefits of implementing inherent safety. But, evaluating inherent safety using consequence modeling approach considers hazard receptors and provides a clearer understanding of the risk (Eini et al., 2015). Table 2 shows the studies that have considered consequence modeling in order to evaluate inherent safety level.

It should be noted that, it is almost impossible to simultaneously maximize all desired characteristics of a process. The central problem of all engineering designs is to find the optimum combination of characteristics that best meets the overall objectives (Mannan, 2012). Inherent safety is one of the many characteristics of a process, which should be evaluated as an optimization problem. In many cases, making a process inherently safer may conflict with the economics of the plant. On the other side, reducing a hazard may result in increasing another hazard. Consequently, for decision making and designing an "economically optimum and inherently Safer" process, it is important to consider a multi-objective optimization algorithm in which different objective functions are addressed to reach their optimum values; one objective function with respect to risk level and another one with respect to economics. Multi-Objective Optimization (MOO) method is an efficient approach for optimizing the problems dealing with conflicting objectives. Table 3 represents the research studies that have considered multi-objective formulation for inherently safer design.

Although, Medina-Herrera et al. (2014) proposed a multi-objective formulation and performed a sensitivity analysis in their study, they didn't solve the problem using MOO.

In order to assess a realistic measure of risk, it is crucial to consider the frequency of the accidents as well as the consequences. Eini et al. (2015) did not employ the probabilistic approach in risk assessment. They considered economic damages arising from the accidents as the measure of inherent safety and combined the objective functions in order to convert the multi objective problem into a single objective. Moreover, Eini et al. (2016a) conducted the same case study as the previous research. However, they combined detailed quantitative risk assessments considering the frequencies and consequences of the incidents. Indeed, they utilized NSGA-II in order to solve the MOO formulation. In order to develop MOO framework for inherently safer design, Eini et al. (2016b) considered exergy efficiency as a third objective besides the economic and safety objectives for a cascade refrigeration unit.

To the best of the authors' knowledge, there is no comprehensive study on the synthesis of inherently safer reactor networks in the open literature. In this paper, in order to design an inherently safer reactor network for allyl chloride production, a multi-objective optimization (MOO) of the system was performed in order to minimize the risk posed by the hazards in the network and maximize the process of the economic profit as objective functions. In the allyl chloride process, both toxic and flammable hazards are expected. This suggests an opportunity for the implementation of ISD's strategies in order to make the process inherently safer. In the analysis, both Intensification and Moderation strategies were considered. In this paper, the capital and maintenance costs of system components, the operational cost, and the profit due to selling of the product were included in the process of the economic profit of the plant. In order to calculate the frequency of the probable accidents, a multivariable model based on event tree was used, which yielded more accurate risk calculation. In this study, an evolutionary algorithm (EA) method based on the elitist NSGA-II was employed to obtain the Pareto optimal set and Pareto frontier in objective space. In the next step, Euclidian and fuzzy non-dimensionalization was employed for non-dimensionalization of the Pareto front results, and the final optimal solutions from available solutions located at the Pareto frontier were selected by the decision makers, including Shannon Entropy and Fuzzy methods proposed by Bellman-Zadeh.

2. Economically optimum-inherently safer design of a reactor network system

Economic profitability is the main goal of the design of a reactor system. However, several additional considerations such as safety aspects, environmental regulations, etc. should be respected in the design work. These considerations may have either direct or indirect effects on overall plant profits. However, safety aspects, has the most important effects on the overall profits. On the one hand, this issue arises from the fact that controlling hazards in a plant requires safety functions that need a considerable efforts and costs in chemical processes. On the other hand, occurrence of an accident produces all types of direct and indirect costs (Reniers and Audenaert, 2009). Therefore, if a hazard leads to an accident, large monetary losses would be imposed to the plant. Accordingly, one of the aspects that should be considered in plant design is process safety to reduce the overall risk level of the plant. This can be done using any category of the risk reduction strategies, including Inherent, Passive, Active, and Procedural (CCPS, 2009). Inherent safety principles not only can reduce or maybe eliminate the high risk nature of the plant (both accidents magnitude and probability of occurrence), but also reduce the required expenses in safety functions.

It should be noted that different process options and alternatives differ in level of potential of accident occurrence and severity. It is possible that a design, which has lower processing costs, has more associated hazards and consequently more accident costs (Eini et al., 2015). To perform a realistic optimization, all costs associated with a process, including accident costs, which are influenced by decision parameters of a design procedure, should be taken into account. Consequently, it is essential to find an "Economically Optimum-Inherently Safer design" using an optimization framework.

In order to deal with risk level as a measure of inherent safety, probabilistic risk assessment can be performed in which the consequence and the frequency of the probable accidents are combined. Therefore, any effort to lower the calculated risk leads to higher level of inherent safety. This risk reduction should be done simultaneously in connection with enhancing the profits of the plant using a Multi-Objective Optimization (MOO) procedure. This procedure is briefly described below and is presented in more details in Section 3.

2.1. Objective functions: the overall risk level and profit of the plant

There are many alternatives, options, and operational conditions that should be determined to finalize a process design. For reactor network systems, the following options may be considered:

- ✓ Different reaction routes to obtain a specific product,
- ✓ Contacting pattern and technology (plug flow reactor, mixed flow reactor, etc.),
- ✓ Number of reactors in series or parallel,
- ✓ Operation condition (temperature distribution along the reactor,