

Saeed Eini, Hamid Reza Shahhosseini, Majid Javidi, Mahdi Sharifzadeh, Davood Rashtchian. Inherently safe and economically optimal design using multi-objective optimization: The case of a refrigeration cycle. *Process Safety and Environmental Protection*, 2016, 104 (Part A), 254–267.

Inherently safe and economically optimal design using multi-objective optimization: the case of a refrigeration cycle

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1 **Abstract**

2 The Economic viability of industrial processes strongly depends on their safe and reliable
3 operation. The method of inherent safe process design enables systematic consideration of safety
4 measures in order to ensure process safe operation at the early stages of process design. The
5 challenge is that the economic measures that are often considered for the design of industrial
6 processes are often incommensurable with the safety measures. In the present research, a novel
7 framework is proposed in which the safety criteria are quantified based on consequence
8 modeling and aggregated with the economic performance using multi-objective optimization
9 programming. The developed methodology was applied to the design of a simple refrigeration
10 cycle. The optimization algorithm was NSGA-II. The results suggested a strong trade-off
11 between the competing economic and safety objectives in terms of Pareto frontiers that clearly
12 quantified the required compromise. It was observed that only with a minor increase in the
13 capital investment, it is possible to significantly improve the safety. While the case of the LNG
14 refrigeration cycle was selected as a demonstrating case, the research methodology is to large
15 extend general and deemed to be acceptable to design and operation of other industrial processes.

16

17 **Keywords**

18 Inherent safety, Consequence Modeling, Multi-objective Optimization, Layout Optimization,
19 Simple refrigeration cycle

20

21 **1. Introduction**

22 The modern approach to chemical process safety is to apply risk management systems theory.
23 This includes identification of the hazards, and assess the associated risks, in order to reduce

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24 them to an “as low as reasonably practicable” (ALARP) level, while balancing other business
25 objectives (CCPS, 2009). In general, the risk reduction policy, whether directed toward reducing
26 the occurrence or the severity of potential accidents, falls into one of the inherent, passive,
27 active, and procedural categories. The ideal way of dealing with a hazard is to remove it
28 completely if possible. This principle has been incorporated in the systematic application of
29 inherent safety (Mannan, 2013). The provision of the means to control the risk associated with a
30 hazard is very much the second best solution.

31 There are four basic principles to design an inherently safer process (Kletz, 1991): (1) Minimize:
32 use smaller quantities of hazardous substances (also called intensification); (2) Substitute:
33 replace a material with a less hazardous substance; (3) Moderate: use less hazardous conditions,
34 a less hazardous form of a material, or facilities that minimize the impact of a release of
35 hazardous material or energy (also called attenuation or limitation); (4) Simplify: design facilities
36 which eliminate unnecessary complexity and make operating errors less likely.

37 An inherently safer design (ISD) can either reduce the magnitude of a potential incident, or make
38 the occurrence of the accident highly unlikely, or perhaps impossible. Consequently, a process
39 that is inherently safer will require fewer and less robust, layers of protection (Mannan, 2013).

40 Although this strategic ideally should be implemented at an early stage in the process design
41 phase (CCPS, 2009), it may become necessary to implement the concepts of inherent safe design
42 and required major enhancements for existing plants at various phases of the process life cycle
43 (Khan and Amyotte, 2002, 2003; Mannan, 2013). As the process moves through its life cycle and
44 enters the operational phases, it becomes more difficult to change the basic process (CCPS,
45 2009). At the conceptual design stage, the process configuration and equipment design are
46 developed, their implications are explored, and potential problems are identified. In most cases,

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47 the conceptual design stage may be quite short and associated with many uncertainties in the
48 involved physical and chemical phenomena and the process model parameters. However, if the
49 safety measures are neglected during the process design phase, it may have costly implications
50 during operational phases in terms of hazardous accidents and production interruptions.
51 Therefore, at the earliest phases of process design, the designers are encouraged to incorporate
52 ISD concepts. In order to do so, one can integrate these design concepts into the process design
53 by using optimization-based techniques (Mannan, 2013).

54 The inherent safety level can be evaluated either using (1) consequence modeling (calculation of
55 accidents' consequences) or (2) scoring the process features in terms of safety indices. The
56 majority of the research in the field has focused on developing safety indices in order to evaluate
57 the inherent safety level, for which extensive literature reviews are provided by Khan and
58 Amyotte (2003, 2005), Kletz and Amyotte (2010), and Khan et al. (2015). However, there are
59 little studies on the application of consequence modeling for designing inherently safer
60 processes. In the following, firstly, a brief survey of the methods which apply safety indices is
61 presented. Then the discussion continues with further elaboration of the methods which apply
62 consequence modeling for designing inherently safer processes. The aim is to identify the
63 research gaps and put the present research in the context.

64 The inherent safer design of heat exchanger network (HEN) has been the focus of researchers.
65 Chan et al. (2014) and Hafizan et al. (2016) integrated the STEP (stream temperature vs.
66 enthalpy plot) graphical approach and the inherent safety index (ISI) which had been developed
67 by Heikkilä (1999). In addition to the inherent safety concepts, Hafizan et al. (2016) considers
68 process operability of the HENs as well.

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69 Ng et al. (2014a) proposed a framework in which various index-based methods can be selected
70 based on the availability of process data during process development and design. One of the
71 shortcomings of the index-based methods is scaling in which the physical or chemical properties
72 are divided into various ranges, in which each range has a score. The scaling procedure may
73 result in subjective measures and discontinuities at the sub-range boundaries. Ahmad et al.
74 (2014) proposed a new measure called Logistic function. Logistic function is a continuous
75 function that relates a score (as the dependent variable) to a safety parameter (as the independent
76 variable) in order to prevent discontinuity issues.

77 Ahmad et al. (2015) proposed a methodology in which the inherent safety of a separation process
78 is assessed during the design stage. In this approach, four parameters (volatility, toxicity,
79 flammability, and explosiveness) were used to find the total score in order to rank the alternative
80 designs. A systematic framework was proposed by Ng and Hassim (2015) to assist process
81 designers and engineers in assessing and reducing inherent occupational health hazards or
82 the potential risks based on process information availability. Pandian et al. (2015) proposed a
83 systematic methodology for designing an inherently healthier process during the R&D stage
84 using ISD principles.

85 Groos-Gerardin et al. (2015) presented a framework by combining product engineering and
86 inherent safety to improve the powder impregnation process. They have used minimum ignition
87 energy as a measure of inherent safety. A combined approach for inherent safety and
88 environmental (CAISEN) assessment was presented by Ee et al. (2015). They integrated a life
89 cycle assessment (LCA) and the Inherent Safety Index (ISI) scoring system.

90 Several researchers have focused on developing inherently safer and healthier bioprocesses using
91 index-based approaches. Ng et al. (2013, 2014b) and Liew et al. (2014, 2015) utilized fuzzy

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92 optimization approach in order to analyze inherent safety, health, environment, and economic
93 performance of biorefineries. With respect to the same objectives, Liew et al. (2016) proposed a
94 sustainability assessment framework for a biorefinery including uncertainty in some parameters
95 (feed flow rate and price).

96 Ramadhan et al. (2014) developed a multi-objective fuzzy-based optimization model in order to
97 minimize work-related casualties within a palm-based bioprocess during its life cycle, while
98 simultaneously minimizing the operating costs. Due to the stochastic nature of workplace
99 accidents, realistic statistical data has been used for estimating the best possible pathway for the
100 desired process. Ng et al. (2015) presented a process-graph (P-graph) methodology for the
101 planning of bioenergy supply chains. The methodology was developed in order to take into
102 account both total cost minimization and supply chain risk reduction. The p-graph approach
103 enables embedded algorithms for solution structure generation and optimization to be used for
104 planning the supply chain. Ling et al. (2015) reviewed the sustainability assessment
105 methodologies which were used during the process synthesis of an integrated biorefinery system.

106 Ahmad et al. (2016) discussed the inherent safety assessment of biodiesel production pathways
107 from the flammability parameter. The numerical descriptive inherent safety technique (NuDIST)
108 for flammability score calculation was used in this research. Scarponi et al. (2016) proposed a
109 methodology for the selection of inherently safer biogas technology during early design stages.

110 In this method, Monte Carlo sensitivity analysis was applied for the uncertainty of the input
111 parameters and addressing the robustness of the ranked solutions.

112 The application of inherent safety indices is a simple approach to quantify the level of safety that
113 a process features. However, these methods only provide a relative evaluation of the level of risk
114 between different design options and do not consider vulnerable elements in the surrounding

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115 environment that are the true hazard receptors. More importantly, these indices do not
116 demonstrate the potential economic benefits of implementing inherent safety strategies.
117 Quantification of the opportunities for ISD based on consequence modeling approach provides a
118 clearer understanding of the risk (Eini et al., 2015).

119 Several researchers have focused on developing computing tools based on consequence
120 modeling. Mohd Shariff et al. (2006) developed a tool called integrated risk estimation tool
121 (iRET) that applies the TNT equivalence method and the TNO correlation method to study
122 explosion consequences. Later, Shariff and Zaini (2010) developed toxic release consequence
123 analysis tool (TORCAT) in order to analyze the consequence of a toxic release. A model known
124 as inherent fire consequence estimation tool (IFCET) was developed by Shariff et al. (2016) to
125 assess process plant for the potential boiling liquid expanding vapor explosion (BLEVE).

126 Patel et al. (2010) integrated consequence modeling and regulatory guidance from
127 “environmental protection agency risk management program” (EPA RMP) in order to select
128 inherently safer solvents.

129 Jha et al., 2016 developed a hybrid methodology using both index-based and consequence
130 modeling-based methods in order to select the inherently safer design. In this framework, the
131 best process route and the inherent safety level of all process streams are estimated using
132 different indices. Finally, a risk assessment approach (based on consequence modeling) is
133 applied to the worst stream in order to evaluate the acceptability of the design. Methyl
134 methacrylate (MMA) routes were selected for demonstrating the methodology.

135 Unlike the abovementioned works which have not considered the plant economic during
136 incorporation of ISD concepts, Medina et al. (2009) have proposed an optimization methodology
137 in which both cost and risk were taken into account. They studied the optimum number of

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138 storage tanks in a chemical plant. Bernechea and Arnaldos Viger (2013) have used a
139 probabilistic approach to assess risk and to optimize the design of storage plants and for
140 minimizing the risk. None of these studies has considered inherent safety measures in their
141 optimization procedure.

142 Medina-Herrera et al. (2014) developed a methodology that can be applied in order to design
143 inherently safer distillation systems. They used the principles of quantitative risk analysis
144 combined with economic objectives for the design of two types of distillation arrangements,
145 namely conventional distillation and multi-effect distillation. However, they didn't present an
146 optimization framework for systematic selection of the optimum design.

147 Since making the processes inherently safer seem to be conflicting with the plant economics in
148 some cases (Medina-Herrera et al., 2014), an optimization framework is required to find an
149 economically inherently safer design.

150 Nowadays, inherent safety has gained acceptance, with law initiatives and is included in codes.
151 Although considering the costs of hazardous accidents an ISD is necessarily the cost-optimal
152 option (CCPS, 2000; Edwards and Lawrence, 1993; Hendershot, 2000; Khan and Amyotte,
153 2002), it requires quantification of safety risks and consequences, in addition to bridging
154 between the incommensurable economic and safety objectives (Medina-Herrera et al., 2014; Eini
155 et al., 2015). In addition, a holistic method is needed that systematically generates alternative
156 solutions and screen the candidate decisions in order to find the optimal solution. Such a
157 framework conforms to optimization programming.

158 Eini et al. (2015) proposed an optimization procedure which integrates both plant economics and
159 accident costs based consequence modeling for different design schemes. They applied the sum
160 of accident costs and processing costs all through the plant lifespan, as the objective function.

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161 They applied consequence modeling and “Probit” function for assessing the costs of the
162 accidents. However, they didn’t consider the probability of the accidents. To assess the risk of
163 any accident scenario, it is necessary that the probability of that event and associated
164 consequences be quantified (Javidi et al., 2015).

165 Due to the uncertain nature of accidents, incorporation of accidents costs directly in optimization
166 problems do not necessarily represent the real risk level. The implication is that ISD concepts
167 should be based on a probabilistic approach. Even if the accident risks are fully quantified by a
168 cost function, the probabilistic nature of the frequency and the intensity of the potential accidents
169 makes the economic function highly uncertain. Therefore, in order to underpin a design solution
170 which is inherently safer and economically optimum, the optimization program should minimize
171 risk levels and plant costs simultaneously. In the present research, multi-objective optimization
172 programming is applied in order to quantify the trade-off between the production economy and
173 the costs of accidents. The solution of a multi-objective optimization is not unique but a set of
174 solutions that form a Pareto front. At one extreme, more weight is given to the economic
175 objective. Here, the risks of potential accidents are assumed to be relatively low. On the other
176 extreme, the safety objective is dominant and the risk of accidents is considered to be likely in
177 order to achieve an inherently safer design. Such a Pareto front can quantify the trade-off
178 between the costs of inherently safe design strategies and process profitability and enable
179 decision-maker to underpin a practical compromise.

180 In this paper, a multi-objective optimization (MOO) framework is proposed to optimize
181 simultaneously inherent safety level and plant economic. The applicability of the framework is
182 shown using a case study. To evaluate inherent safety level probabilistic risk analysis is
183 considered which combines accidents costs with the likelihood of accidents occurrence. The

184 inherent safety strategies are incorporated into the optimization algorithm by considering
185 decision parameters associated with each strategy. The novelties of the present study in
186 comparison to the previous research (Eini et al., 2015) are as follows:

- 187 • Multi-objective optimization programming is applied in order to simultaneously optimize
188 economics as well as inherent safety measures
- 189 • Detailed quantitative risk assessment is applied in order to measure inherent safety
190 considering incidents frequencies and consequences
- 191 • The combination nature of accident scenarios is formulated in the optimization program.
- 192 • Layout optimization considering land cost in the economic analysis as well as safe
193 distances in the case study

194 Accidents frequencies have not been considered in the procedure presented by Eini et al. (2015).
195 Their defined objective function comprised of summing plant processing costs and accident
196 costs. Consequently, the optimization procedure concerned finding the optimum design using a
197 single-objective function.

198 Due to the probabilistic nature of the accidents, the consequence modeling results should be
199 corrected by accidents frequencies and accidents occurrence combination to show more realistic
200 risk calculation. Therefore in addition to the plant costs (considering both operating and capital
201 costs) as an objective function, risk can be introduced to the optimization problem as another
202 objective function. According to the different nature of these two objective functions (plant costs
203 and risk), a multi-objective optimization (MOO) problem should be implemented.

204 The outline of the paper is as follows. The present section explored the research background and
205 justified the necessity of the research. Section two discusses the research methodology and
206 presents the formulation of the multi-objective optimization (MOO). In Section three, the case

207 study is described and the details of risk analysis, as well as the economic objective function, are
208 presented. The results are reported and discussed in Section four. Finally, Section five
209 summarizes the research and concludes the paper.

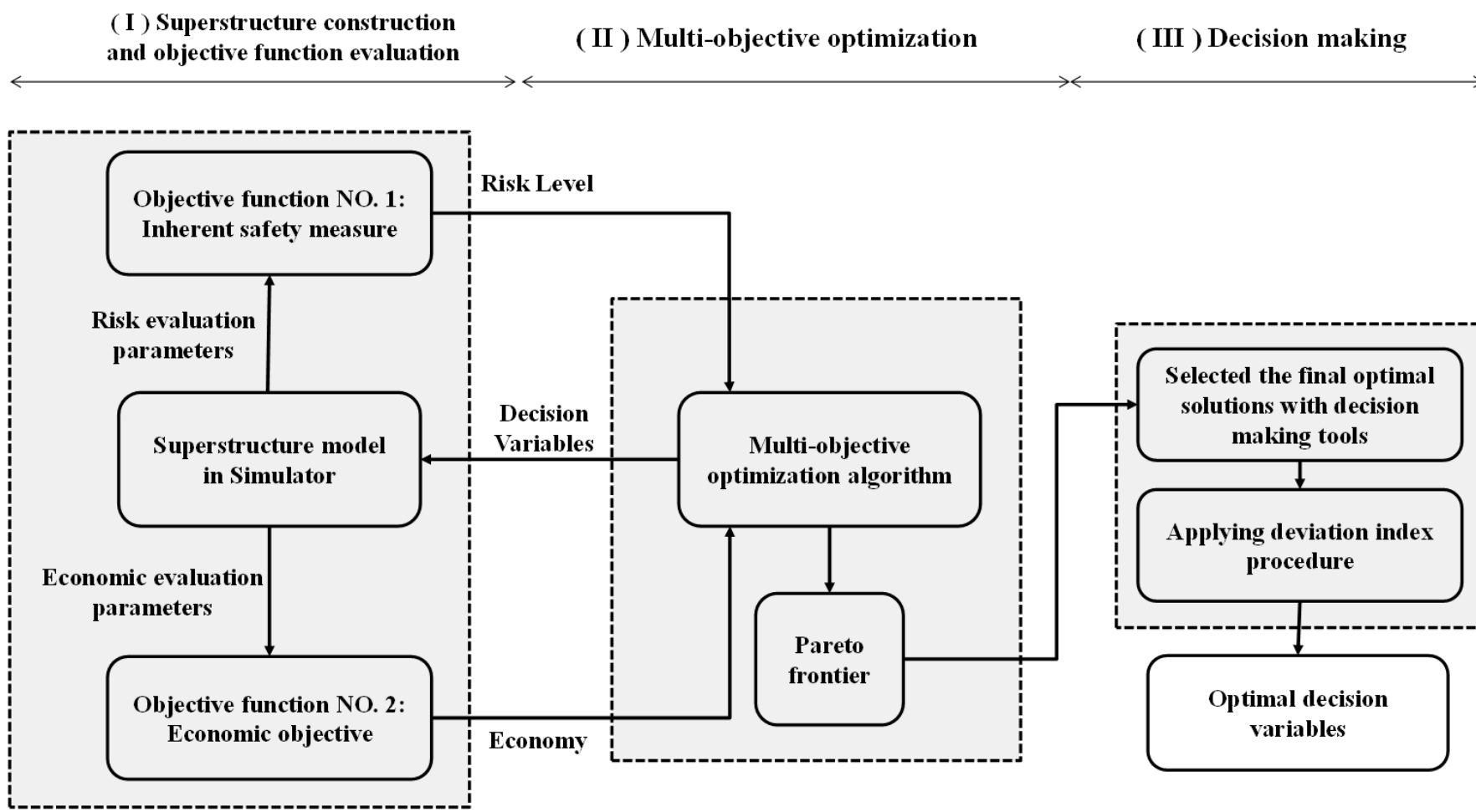
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211 **2. Methodology: Multi-objective optimization for inherently safer design**

212 To Design a process it is required to consider and to compare all feasible alternatives. These
213 alternatives may differ either in their structure, or operation, or both. Different structural and
214 operational decision variables result in different design alternatives. The final selected design
215 scheme should be economically feasible and be consistent with environmental regulations.
216 Nevertheless, the safety level of a design should be of high standards. Considering risk
217 management strategies in the process design provides the opportunity to enhance the process
218 reliability and reduces the losses associated with potential accidents. Therefore, the aim of the
219 present research is to propose a computational algorithm in which inherent safety criteria are
220 systematically considered in the early design stages. The main parts of the proposed algorithm
221 are shown in Figure 1. They are (I) superstructure constriction and objective function
222 evaluations, (II) multi-objective optimization (MOO), and (III) decision-making. Once a
223 superstructure is developed, the MOO algorithm proposes different values for the decision
224 variables. The fitness of the candidate solution is benchmarked against economic and safety
225 criteria. The output of the MOO algorithm is a set of optimal solutions that forms a Pareto front.
226 Finally, using decision-making tools a single solution that established the trade-off between
227 competing objectives is selected as the optimal design. The details of each of these three
228 calculation steps are discussed in the following.

229

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231
232

Figure 1 - The general algorithm to select an inherently safer and economically optimal design using multi-objective approach

233 **2.1. Superstructure construction and objective function evaluation**

234 The ideal treatment for potential hazards in the first place is to completely remove them.
235 However, there is often a very low chance to make a process absolutely “safe” and the goal of
236 safe process design is to find a configuration that is rather inherently “safer” and more reliable
237 compared to other alternatives. Therefore, the provision of means to control the risk associated
238 with a hazard is very much the second best solution (Mannan, 2013). Inherent safety strategies
239 reduce or permanently eliminate the hazards and guarantee lower risk levels by changing the
240 nature of the process. In order to make a process inherently safe, it is necessary to generate
241 alternative solutions systematically. Afterward, the solutions should be screened based on the
242 desired performance criteria. In the following subsection, the required methods for superstructure
243 construction and evaluation of the objective functions are discussed.

244 **2.1.1. Superstructure construction**

245 To take into account all feasible options, a superstructure should be created which embeds all
246 alternative process configurations, processing technologies and their feasible interconnections
247 (Smith, 2005). Such a superstructure should also include various strategies for enhancing the
248 inherent safety of the process, including substitution, simplification, and minimization,
249 moderation. Examples of such strategies are:

- 250 • Selection of safer reaction pathways;
- 251 • Substitution of hazardous energy transfer mediums, solvents, and adsorbents;
- 252 • Selection of alternative safer process equipment (e.g. reactor type, separation
253 technology);
- 254 • Moderating processing conditions such as temperature and pressure, or reducing
255 concentration of hazardous materials using inert;

- 256 • Reducing the inventory of hazardous materials

257 The general algorithm to select an inherently safer and economically optimal design (ISEOD)
258 using multi-objective approach is shown in Figure 1.

259 **2.1.2. Objective functions**

260 The two objective functions that should be considered in order to develop an ISEOD are inherent
261 safety measure as well as an economic objective. The economic objectives can be expressed
262 using one of the common methods: total annualized cost, capitalized cost, net present value, and
263 so on. In addition, layout optimization considering land cost as well as safe distances between
264 plant elements may be required. Besides, in order to measure the inherent safety level of a
265 process plant, risk level calculated using quantitative risk assessment (QRA) can be utilized.
266 Nowadays, QRA has become an efficient tool in decision-making to evaluate the risk level. QRA
267 procedure is carried out in several stages: (i) Hazardous scenario selection, (ii) Frequency
268 estimation, (iii) Consequence modeling, and (iv) Risk level calculation. These stages are
269 discussed in the following.

270 **(i) Hazardous scenario selection:**

271 The first stage of the QRA procedure is hazardous scenario selection. For this purpose, all
272 necessary data such as environmental conditions, physical and chemical specification, and
273 process specifications must be collected. Afterward, the potential sources of the hazards which
274 can lead to an accident in the plant are selected as the accident scenarios.

275 **(ii) Frequency estimation:**

276 When the accident scenarios are selected, the second stage of QRA procedure is scenarios
277 frequency estimation. A method for estimating the accident frequencies is event tree analysis
278 (ETA) (Casal, 2008). Having the frequency of a release (as the initial event in each accident

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279 scenario), Event Tree is applied for calculating the frequency of final possible outcomes. For
280 example, upon a flammable chemical release, the potential outcomes can be a pool fire, a jet fire,
281 vapor cloud explosion (VCE), vapor cloud fire (VCF) and boiling liquid expanding vapor
282 explosion (BLEVE). Two ways can be applied in order to estimate the frequency of an initial
283 event. They are fault tree analysis (FTA) or using failure frequency databanks (Casal, 2008).
284 Failure frequency databanks are constructed based on past accident records. There are several
285 databanks available such as API (2008), OGP (2010), and Handbook of failure frequencies
286 (LNE, 2009).

287 **(iii) Consequence modeling:**

288 Consequence modeling is the third step in the QRA approach. The outputs of this stage are the
289 effects associated with accidents on people, equipment, environment, and so on. Consequence
290 modeling is supposed to be carried out in several steps to model the effects of various scenarios.
291 First, source modeling is performed that provides discharge rate and the total discharged volume
292 over a time horizon. Dispersion modeling is subsequently used in order to describe how the
293 hazardous material is dispersed to certain concentration levels. Then, fire and explosion models
294 convert the dispersion model information into hazard potentials such as thermal radiation and
295 blast overpressure. Consequently, using appropriate effect modeling, the number of individuals
296 affected and the property damage can be calculated. Finally, using of individuals affected and the
297 property damage, and associated costs, the total imposed costs of any accident scenario can be
298 obtained.

299 **(iv) Risk level calculation:**

300 The final stage of the QRA is risk level calculation. The general expression to calculate the risk
301 level associated with an accident scenario (R_i) imposed to a risk receptor can be shown as
302 follows (CCPS, 2000).

$$R_{(x,y)_i} = f_i \times C_{(x,y)_i} \quad (1)$$

303 Where i refers to the accident scenario, f is the scenario frequency, C is the scenario
304 consequence, and (x, y) represents the risk receptor location.

305 Based on Equation (1), the risk level associated with all scenarios in the (x, y) location can be
306 represented as Equation (2).

$$R_{(x,y)} = \sum_i f_i \times C_{(x,y)_i} \quad (2)$$

307 Finally, the risk level imposed to all risk receptors can be calculated using Equation (3).

$$Risk\ level = \sum_{(x,y)} R_{(x,y)} \quad (3)$$

308 **2.2. Multi-objective optimization procedure**

309 Simultaneous consideration of process economy and the level of inherent safety using
310 mathematical programming conforms to multi-objective optimization. A multi-objective
311 optimization program consisted of several competing objectives as follows:

$$\begin{aligned} & \text{Optimize } \{f_1(\vec{x}), \dots, f_k(\vec{x})\} \\ & \text{Subject to } x \in S \end{aligned} \quad (4)$$

312 Here, the instances of the economic objectives are the capital investment required for purchasing
313 process equipment, operating costs, raw material costs. Often capital and operating costs are
314 aggregated based on the plant lifespan for example in terms of total annualized costs. The
315 quantification of the level of inherent process safety was discussed in subsection 2.1.2. In the

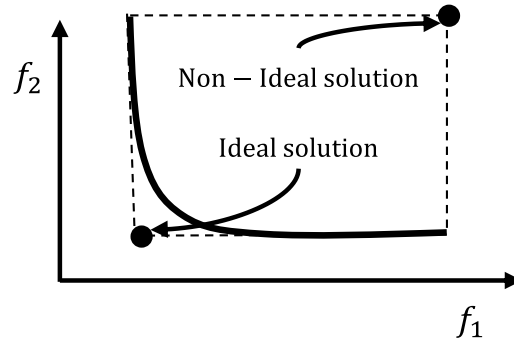
316 Optimization problem (Equation (4)), x is a vector of decision variables. Examples of decision
317 variables include process configuration, equipment design, process inventory, and process
318 operating conditions. The decision variable can be decided within a range of feasible candidates
319 $S \subset \mathbb{R}^n$ which include alternative process configurations, practical size of equipment, and the safe
320 operating conditions.

321 In multi-objective optimization problems, the optimal solution is not unique, but compromises a
322 Pareto front or Pareto set. For a given solution on the Pareto front, it is not possible to improve
323 an objective function without compromising other objective functions. For the case of
324 simultaneous optimization of economic and inherent safety, such a Pareto front represent the best
325 comprise that can be reached among these competing objectives. In other words, if further
326 improvement is desired in the level of process safety, more investment is required. Conversely, if
327 further economic saving is needed, the designer should make sure that the safety will not be
328 compromised. The ideal solution vector F^{ideal} and a non-ideal solution
329 vector $F^{\text{non-ideal}}$ represent the upper and lower bounds for the objective function values of the
330 Pareto optimal solutions, respectively (Gebreslassie et al., 2009; Konak et al., 2006; Madetoja et
331 al., 2008). Figure 2 displays Pareto front, ideal and non-ideal solutions for four possible
332 combinations of the minimization and maximization procedures. The solid curve marks the
333 Pareto optimal solution set. In the algorithm proposed in this paper (Figure 1), there are two
334 objective functions: $f_1(\vec{x})$: Total annualized costs and $f_2(\vec{x})$: Plant risk level which both should be
335 minimized. Therefore it is expected that the Pareto front matches the figure shown in case (a).
336 With respect to this case, the ideal solution is the point in which the risk level, as well as the total
337 annualized costs, have their minimal values. However, this ideal solution cannot be reached in
338 reality.

339 Subsection 2.2.1 describes the multi-objective optimization algorithm used in this paper in order

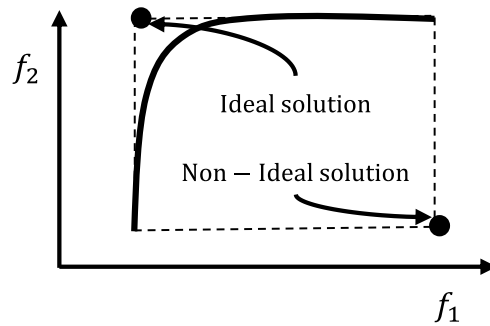
340 to generate the Pareto front.

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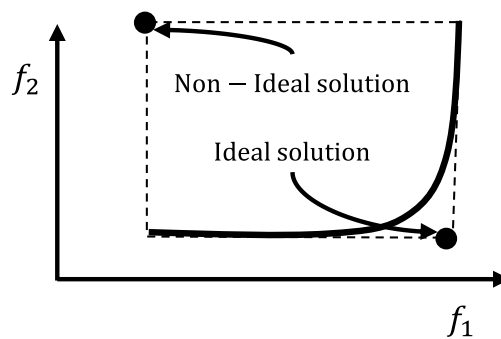
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Case (a): Minimize f_1 , Minimize f_2



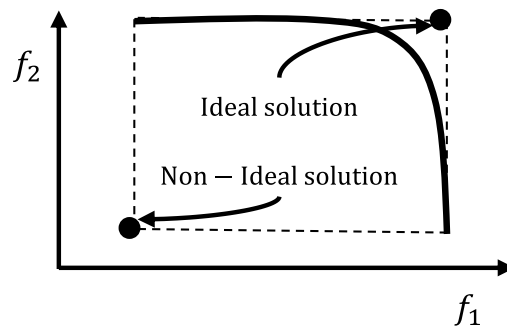
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Case (b): Minimize f_1 , Maximize f_2



344

Case (c): Maximize f_1 , Minimize f_2



Case (d): Maximize f_1 , Maximize f_2

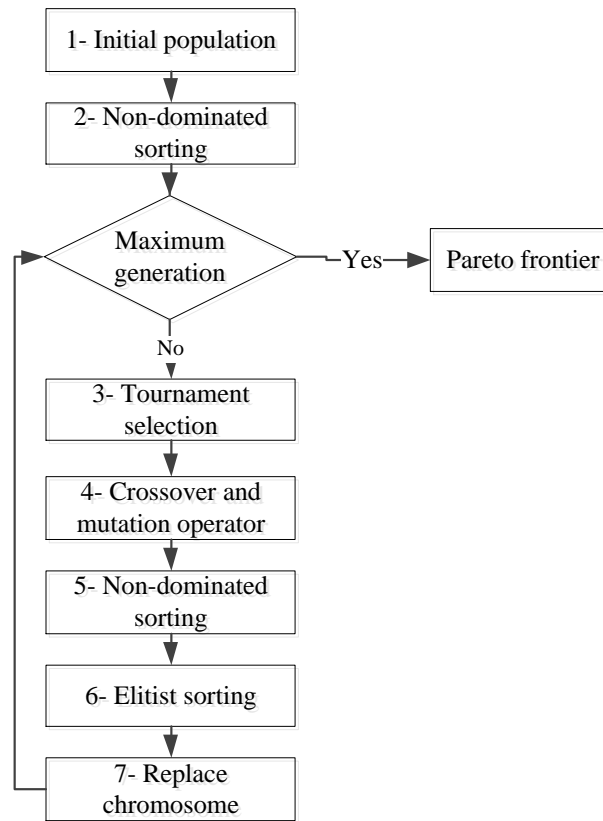
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346

Figure 2 - Pareto set for four combinations of two types of objectives

347 **2.2.1. Visualizing the Pareto furniture, Non-dominated sorting genetic algorithm (NSGA-**
348 **II)**

349 In this study, NSGA-II algorithm which was introduced by Deb (Deb, 2005) is utilized as a multi-
350 objective optimization method in order to find the optimal Pareto set and the corresponding
351 Pareto front. Deb investigated the simulation outcomes from a number of difficult problems and
352 concluded that NSGA-II outperforms two other contemporary multi-objectives evolutionary
353 algorithms (EAs) (Pareto-archived evolution strategy (PAEs) and strength Pareto EA (SPEA))
354 (Knowles and Corne, 1999) in terms of finding a diverse set of solutions and in converging
355 near the appropriate Pareto optimal set. According to Figure 3, NSGA-II as an Elite-preserving
356 technic and an explicit diversity-preserving structure can be depicted through the seven steps (Li
357 et al., 2015).



358

359

Figure 3 - Flow chart of NSGA-II algorithm

360 In an evolutionary cycle of NSGA-II, initially, a random parent population is generated. The

361 population is sorted based on the non-domination procedure (rank and crowding distance).

362 Parent selection for crossover and mutation operation is performed based on the tournament

363 selection. In the next step, crossover and mutation are used to generate the child populations.

364 Then all previous and current population members are integrated together to create a combined

365 population, then the population is sorted according to non-domination. Since all previous and

366 current population members are included in combined population, the elitism is insured. It means

367 that solutions with better fitness are chosen by elitist sorting and these become the parent

368 individuals. These steps are repeated until the maximum generation number is reached and

369 Pareto front developed.

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370 All of the point on the Pareto front can be a candidate for the optimal solution. Therefore, to
371 select a single point on the Pareto front, a decision-making tool is needed. Subsection 2.3
372 presents the basic concepts of two well-known decision-making methodologies.

373

374 **2.3.Decision-making on multi-objective optimization**

375 In multi-objective optimization problems, all the points on the Pareto set are optimal solution
376 with different weights to various objective values. However, in the practical point of view, only
377 one optimal solution should be chosen. In this paper most well-known and the common type of
378 decision-making processes including the LINMAP and TOPSIS methods are applied in parallel
379 in order to specify the final optimal solution. TOPSIS estimates the alternatives adoptability
380 according to their distance with the ideal and the non-ideal points. Meanwhile, LINMAP method
381 follows the nearest alternative to the ideal point. The following sections are presented here in
382 order to describe these decision-making algorithms.

383 **2.3.1. LINMAP decision-making (Linear Programming Technique for Multidimensional** 384 **Analysis of Preference) (Yu, 2013)**

385 The distance of every solution on the Pareto front from the ideal solution marked by d_{i+} is
386 defined as:

$$d_{i+} = \sum_{j=1}^m (F_{ij} - F_j^{ideal})^2 \quad i = 1, \dots, n \quad (5)$$

387 Where F_j^{ideal} is the ideal solution of the j th objective in a single-objective optimization. In the
388 LINMAP decision-making, the solution with minimum distance from the ideal point is selected
389 as a final desired optimal solution.

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390 **2.3.2. TOPSIS decision-making (Technique for Order Preference by Similarity to an Ideal**
391 **Solution) (Yue, 2011)**

392 Besides the ideal solution, the non-ideal solution is considered in TOPSIS decision-making.
393 Therefore, besides the distance of each solution from ideal solution d_{i+} , the distance of each
394 solution from the non-ideal solution denoted d_{i-} is implemented as a criterion for the selection of
395 final optimal solution:

$$d_{i-} = \sum_{j=1}^m (F_{ij} - F_j^{non-ideal})^2 \quad i = 1, \dots, n \quad (6)$$

396 A new assessment parameter is defined as follows:

$$Y_i = \frac{d_{i-}}{d_{i+} + d_{i-}} \quad (7)$$

397 In TOPSIS decision-making, a solution with maximum Y_i is selected as a desired final solution.

398 In order to explore the reasonable status of various solutions obtained using above-mentioned
399 tools, the deviation index of each solution from the ideal solution is calculated as Equation (8).

$$d = \frac{\sqrt{\sum_{j=1}^m (F_j - F_j^{ideal})^2}}{\sqrt{\sum_{j=1}^m (F_j - F_j^{ideal})^2} + \sqrt{\sum_{j=1}^m (F_j - F_j^{non-ideal})^2}} \quad (8)$$

400

401 **3. Case Study**

402 Vapor-compression refrigeration systems are used in the many types of the industrial plants for
403 separation purposes or chemical storage at low temperatures. It is very common to use
404 hydrocarbons as the refrigerant in gas and petroleum processing plants with respect to the
405 availability of hydrocarbons. However, hydrocarbons have a great flammability hazard potential.
406 Nevertheless, due to the usually high power demand of the compressors (Sharifzadeh et al.,

2011), refrigeration cycle shares great costs in a plant. Therefore, the optimal design of this particular unit, in terms of both economic and safety, is very important.

In the present study, the case of a pre-cooling natural gas using single refrigerant propane cycle is considered, (Manning and Thompson, 1991). Figure 4 shows the process flow diagram. The cycle consists of two compressions stages and aims at cooling dry natural gas down to $-13.2\text{ }^{\circ}\text{C}$.

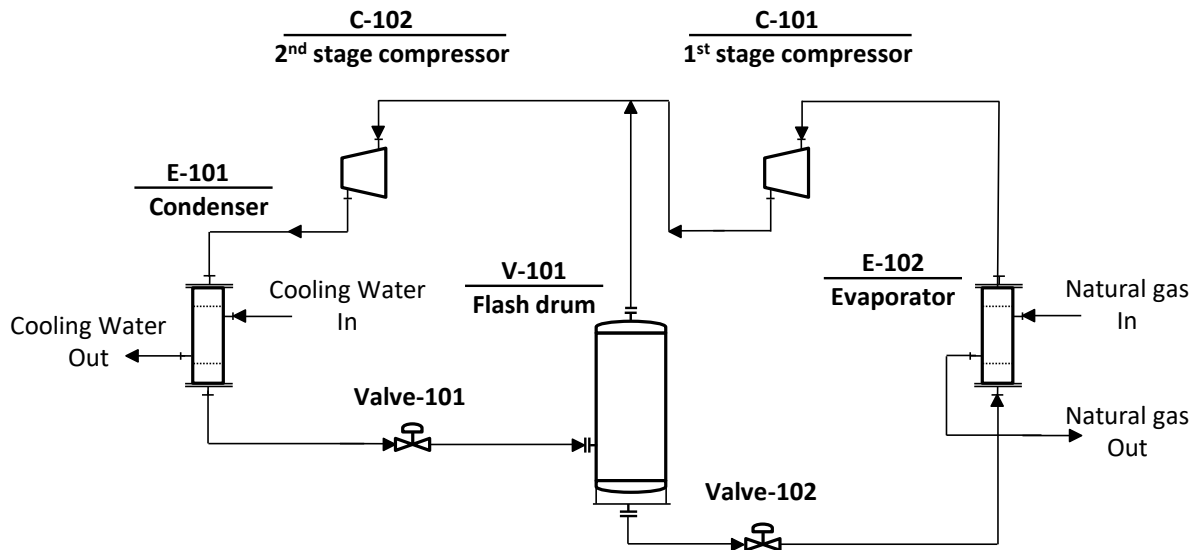


Figure 4 – Simple Refrigeration Cycle

The optimal operating pressure of the flash drum in the propane refrigeration cycle can be estimated as following (Manning and Thompson, 1991):

$$P_{econ} = P_{ch} (P_{cond} / P_{ch})^{0.614} \quad (9)$$

Where: P_{econ} = optimum drum operating pressure, kPa

P_{ch} = chiller (evaporator) pressure, kPa

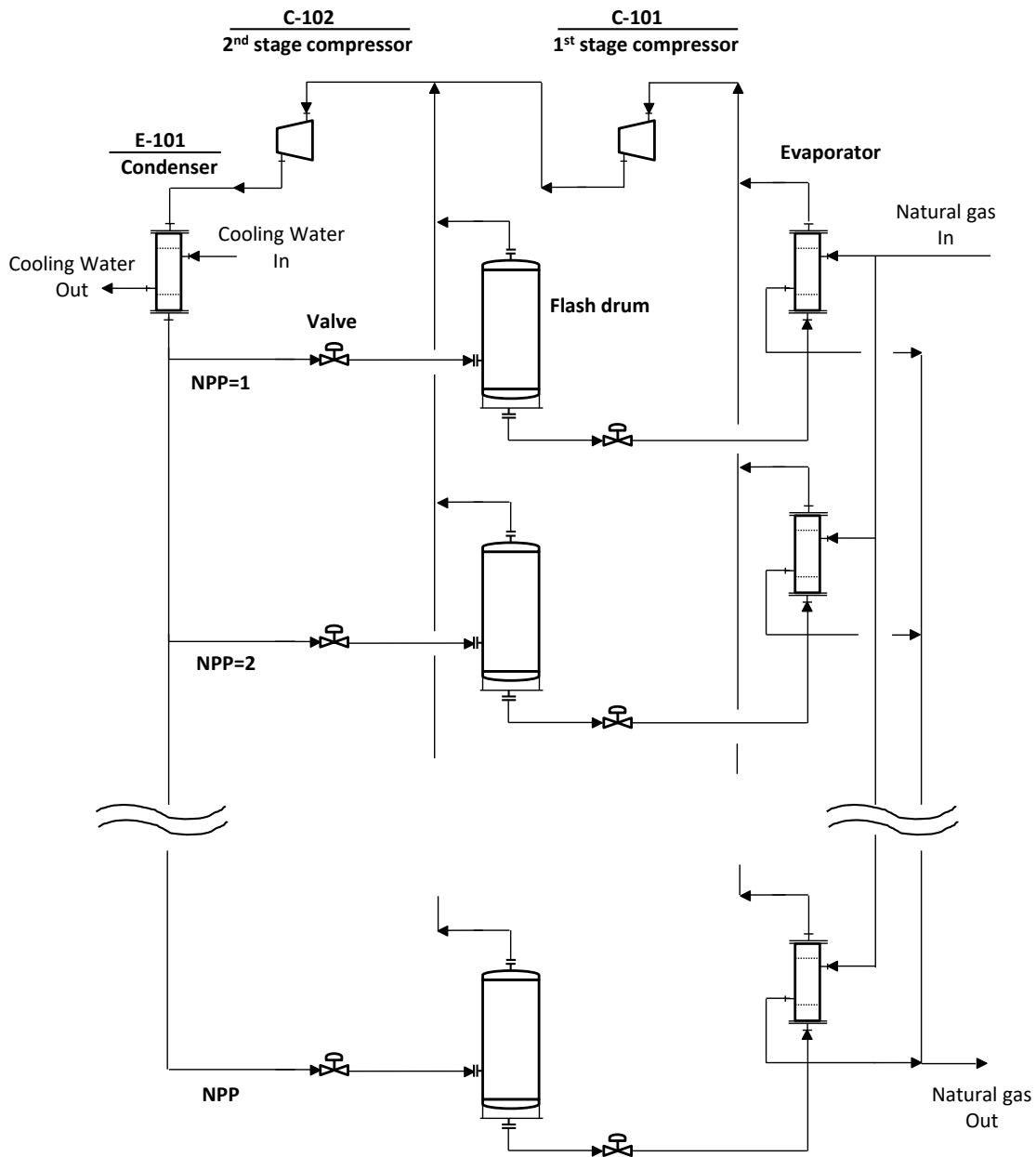
P_{cond} = condenser pressure, kPa

For the cycle under study, cooling water (entering and leaving the condenser at 25°C and 30°C , respectively) is used as the coolant in the condenser. A typical approach temperature of $5\text{ }^{\circ}\text{C}$ is used for both the condenser and the evaporator (Smith, 2005). Consequently, the temperature of

419 the propane in the condenser and evaporator is 35 °C and -18.2 °C, respectively. The saturation
420 pressure of propane in these temperature levels is 1234 kPa for the condenser and 260 kPa for
421 the evaporator. Using Equation (9) the optimal operating pressure of the drum is equal to 676
422 kPa.

423 The cycle with above-mentioned specification is considered as a base-case in this paper. The
424 optimum pressure calculated by Equation (9) may not be the optimal value if one considers both
425 economic and safety aspects. Therefore, drum operating pressure is one of the decision variables.

426 One of the principal ways to make a process inherently safer is to limit the inventory of
427 hazardous material. It is better to have only a small inventory of hazardous material rather than a
428 large one which needs highly engineered safety systems. Thus, according to the minimization
429 strategy of inherent safety, the number of parallel paths (NPPs) of pressure drop, shown in
430 Figure 5, also can be a decision variable. Because increasing the NPP reduces the refrigerant rate
431 in each path and consequently, the size of the drum and the refrigerant inventory of the drum will
432 be smaller. The NPP as a structural variable is determined in the superstructure. The
433 superstructure which is used in the present study is shown schematically in Figure 5 (Eini et al.,
434 2015). The lower and upper bound values of drum operating pressure are considered to be 300
435 kPa and 1200 kPa, respectively. These ranges of operating pressures are selected according to the
436 saturation temperature of the propane refrigerant in the condenser and evaporator. Also, it is
437 assumed that NPP can have the values in the range of 1 to 20.



438

439

Figure 5 - Intended superstructure of refrigeration cycle

440 Making the plant inherently safer and economically more profitable are the two objectives of the
 441 present research. Here, the plant risk level is chosen as the first objective function for the plant
 442 inherent safety. In subsection 3.1 the methodology applied for calculating the risk level is

443 discussed in more detail. Furthermore, subsection 3.2 presents the details of the economic
444 objective function. Afterward, the optimization procedure is presented in subsection 3.3.

445

446 **3.1. Risk analysis**

447 The failures of vessels and columns account for 21% of accidents in refineries, (CCPS 2003).

448 Since in the present case study (Figure 5) the largest material inventory is located in the flash
449 drums, this paper focuses on the drum(s) as hazard source(s).

450 In the present research, it is assumed that the phenomena of boiling liquid expanding vapor
451 explosion (BLEVE) occurs during the accident, in which a sudden loss of containment of a
452 pressure vessel (containing a superheated liquid or liquefied gas) occurs due to the explosion.

453 The release of hazardous material is assumed to be followed by a fireball that consumes all of the
454 released material. Since the propane refrigerant is a flammable material, the consequence of the
455 combustion of the entire contents of hazardous materials in the release point is worse than any
456 dispersion scenario. Therefore, a design based on BLEVE is more conservative than any other
457 scenario and is in fact, the worst-case scenario. Consequences of this type of accidents can be
458 very severe, especially in areas close to the release point (CCPS, 2000). It should be noted that
459 for the case of toxic materials (e.g., ammonia, or chlorine), the dispersion may represent more
460 hazard and need to be fully modeled.

461 In this study, different potential damage receptors were supposed:

- 462 • 80 operators in the surrounding area (in 130m radius).
- 463 • 8 buildings (B4-Type according to API (1995) definition) at a distance of 300 m
464 downwind; each building has four occupants.

465 The meteorological data of the region in the present study comprising temperature, humidity,
466 atmospheric stability class, and wind velocity, are very important to consequence modeling and
467 for QRA procedure (Table 1).

468 **Table 1 - Metrological data of the region**

Ambient temperature	30 °C
Ambient pressure	1 bar
Ambient relative humidity	40%
Class stability	F
Wind speed	1.5 m/s

469

470 3.1.1. Frequency estimation:

471 Table 2 displays some generic frequency data for pressure vessels (LNE, 2009). According to
472 this table, the release frequency for the selected scenario (catastrophic rupture of the drums) is
473 equal to 5E-5.

474 **Table 2 - Frequency data (LNE, 2009)**

475

Loss of equipment event	Frequency(year-1)
Catastrophic rupture	5×10^{-5}
Large breach	2.2×10^{-3}
Medium breach	2.2×10^{-3}

476

477 According to the BEVI guide (2009), for the medium size instantaneous spill, the probability of
478 BLEVE/fireball is 50% among all outcomes. This probability is calculated by the product of the
479 probability of immediate ignition rather than non-immediate ignition and probability of
480 BLEVE/fireball rather than explosion. Therefore, the frequency of a BLEVE/fireball outcome
481 can be calculated using Equation (10):

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$$\begin{aligned} f_{BLEVE/FIREBALL} &= f_{leak/rupture} \times (P_{immediate\ ignition} \times P_{BLEVE/fireball}) \\ &= (5 \times 10^{-5}) \times (0.50) = 2.45 \times 10^{-5} \text{ year}^{-1} \end{aligned} \quad (10)$$

482

483 3.1.2. Consequence analysis:

484 There are several damages such as loss of human life, structural damages and environmental
485 damages related to accidents. In this study loss of human life, human injuries and structural
486 damages are considered as the accidents consequences.

487 To model the consequences of the selected scenarios, it should be noted that a BLEVE has
488 various effects; fireball is the important effect for flammable release materials. The combined
489 action of BLEVE and fireball can be summarized as the following effects:

- 490 • Blast wave
- 491 • Thermal radiation

492 For these outcomes, detailed procedure to model the consequences has been presented by Eini et
493 al. (2015). The applied consequence modeling has two features. The explosion severity is
494 calculated based on the TNT equivalence indicator (Casal, 2008), which is used in order to
495 quantify the severity of overpressure conditions produced under boiling liquid expanding vapor
496 explosion (BLEVE) conditions. The potential for fire damage is quantified in terms of fireball
497 duration and thermal radiation, using the source point method (Casal, 2008). Then, the Probit
498 analysis is applied in order to relate the overpressure and fire effects, to the probability of
499 damages for any of the above mentioned vulnerable elements in specified distances. Therefore,
500 the outdoor fatality and injuries due to overpressure and thermal radiation, as well as the
501 damages to buildings (either collapse or major structural damage) due to overpressure, are

502 calculated using appropriate Probit models. Finally, by using the following items, the total
503 accident costs can be estimated:

- 504 • The percentage of collapsed buildings
- 505 • The percentage of buildings which receive major structural damage
- 506 • The number of fatalities
- 507 • The number of injuries

508 The building cost has been considered to be 100% of the cost of the building in the case of
509 collapse and 70% for major structural damage (Medina et al., 2009).

510 Finally, the total cost of the accident (C_{total}) can be calculated summing the cost imposed to each
511 vulnerable element. In other words, the accident cost is expressed as Equation (11):

$$\begin{aligned}
 C_{total} = & \text{(number of fatalities * cost of a fatality)} & (11) \\
 & + \text{(number of injuries * cost of an injury)} \\
 & + \text{(number of collapsed building * cost of a building)} \\
 & + \text{(number of damaged building * 70 \% of the cost of a building)}
 \end{aligned}$$

512 Table 3 shows the cost data that have been used in the consequence modeling.

513 **Table 3 - Cost data (Eini et al., 2015)**

Cost parameters	Cost (\$)
Cost of a fatality	350,000
Cost of an injury	160, 000
Cost of one building	100,000

514

515 **3.1.3. Risk level calculation:**

516 As it is shown in Figure 5 the superstructure consists of several drums in parallel. Consequently,
517 it is possible that a number of drums prone to the similar accident at the same time. Therefore,

518 the general equation that determines the risk should be expanded to consider all of the scenario
519 combinations to obtain the realistic results.

520 The risk associated with the simultaneous explosion of “ n_f ” drums in terms of its probability and
521 financial consequence can be calculated as:

$$R_{n_f} = n_f \times C_{total} \times P_{n_f} \times f_{BLEVE/FIREBALL} \quad (12)$$

522 In the above equation, C_{total} is the total cost of the accident and P_{n_f} is the probability of
523 occurrence of this accident as an independent event (Equation (13)).

$$P_{n_f} = \left(\frac{1}{n}\right)^{n_f} \quad (13)$$

524 The number of accident combinations that can occur when n_f units suffer an occurrence out of
525 “ n ” (the total number of drums in the cycle) is calculated as the Equation (14):

$$C_n^{n_f} = \frac{n!}{n_f! (n - n_f)!} \quad (14)$$

526 Finally, overall risk ($R_{overall}$, as the second objective function to be optimized) can be expressed
527 as Equation (15):

$$R_{overall} = \sum_{n_f=1}^n C_n^{n_f} \times (n_f \times C_{total}) \times P_{n_f} \times f_{BLEVE/FIREBALL} \quad (15)$$

528

529 **3.2. Economic Objective function**

530 As mentioned earlier, the refrigeration cycle shown in Figure 5 includes four major elements: (i)
531 compressor, (ii) condenser, (iii) evaporator, and (iv) flash drum. Consequently, the costs
532 associated with these elements are as follows:

533 • Purchasing cost and energy cost of the compressors.

534 • Purchasing cost and energy cost of the condenser.

535 • Purchasing cost of the evaporators(s).

536 • Purchasing cost of the flash drum(s).

537 The methods applied for designing and sizing process equipment were adopted from Towler and
538 Sinnott (2008). Also, the cost estimation methods were taken from Seider et al. (2009). Other
539 costs included the instrumentation and piping as well as land-use costs. Instrumentation cost was
540 estimated to be 10 percent of the total plant investment cost (Perry, 1950). The piping cost was
541 considered to be 86.3 \$/m (Han et al., 2013). The land-use cost depends on the plant location and
542 may vary case by case. In this paper, the value of 100 \$/m² was considered.

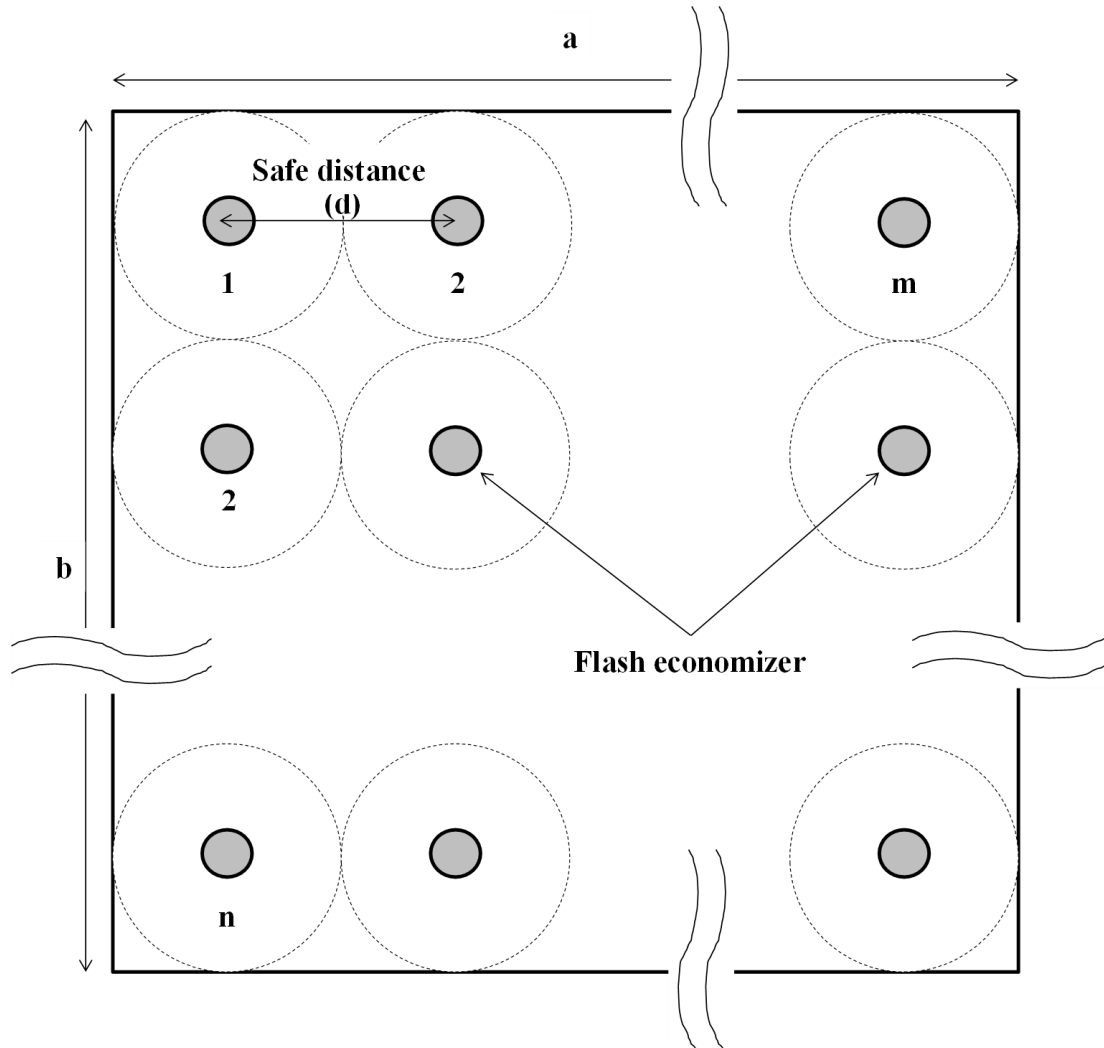
543 The total annualized cost (TAC) was considered as the economic objective function. The TAC
544 includes the capital costs of procurement and the installation of process equipment and costs
545 associated with the operation of the refrigeration cycle.

$$TAC = \text{Annualized cost of the investment} + \text{annual operating costs} \quad (16)$$

546 For this purpose, the investment cost (such as the purchasing cost of the equipment and land
547 cost) should be annualized using capital recovery factor (CRF) (Peters et al., 2003). In this paper,
548 the annual interest rate and the plant life time are considered as 18% and 15 years respectively.

549 In the present study, the number of parallel paths (NPP) was being optimized which affects the
550 required land area. For a plant consisting of $m \times n$ flash drum (NPP = $m \times n$), the layout is shown
551 in Figure 6. Here, “a” and “b” are the length and the width of the plant, respectively. The
552 parameter “d” as shown in this figure is the safe distance between two flash drums. This
553 parameter is determined using consequence modeling and is based on the maximum heat flux
554 that reaches the nearby vessels through radiation upon the evaporation of the total material
555 inventory and fire accident. According to General Specification for safety GS 253 (TOTAL,
556 2012), the radiation level of 9.5 kW/m² can be considered conservatively. Therefore, for the case

557 study in this paper, a fire (flash fire) consequence modeling was performed in order to determine
558 the safe distances of the flash drums (Casal, 2008).



559

560

Figure 6 - Flash drum layout

561 The layout optimization involves two additional decision- variables, “a and “b”. The area of the
562 layout is calculated by multiplying a and b, (Equation (17)). This area needs to be larger than the
563 summation of flash drum safe areas (Equation (18)). The required cost of piping was assumed to
564 be proportional to the total perimeter.

$$Area = a \times b \tag{17}$$

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$$a \times b \geq \pi \left(\frac{d}{2}\right)^2 \times NPP \quad (18)$$

$$\text{Perimeter} = 2 \times (a + b) \quad (19)$$

565 In conclusion, the economic objective function (the annualized cost of the plant) can be
566 presented as follows:

$$\text{Annualized cost} \quad (20)$$

$$= \left[\text{Purchasing costs of the } \begin{cases} \text{compressors} \\ \text{condenser} \\ \text{evaporators} \\ \text{flash economizers} \end{cases} \right. \\ \left. + \text{Instrumentation cost} + \text{Piping cost} + \text{Land cost} \right] \times CRF \\ + [\text{Compressors and condenser energy costs}]$$

567

568 3.3. Implementation of the optimization–simulation program

569 In this paper, the superstructure is developed in the HYSYS process simulator. The formulations
570 of both risk level and plant annualized cost are codified in MATLAB as well as the MOO
571 algorithm. The optimization algorithm proposes the values of the decision variable and sends
572 them to the simulator. By fixing the specifications of the superstructure (i.e., degrees of
573 freedom), it is possible to execute the simulation program. The value of the objective functions
574 in terms of the performance of each candidate solution is evaluated using the extracted data (such
575 as flow, density, etc.) from the simulator. The iterative calculation of objectives functions
576 provides the opportunity to the optimizer to generate all non-dominated solutions (Pareto front)
577 based on the elitist non-dominated sorting genetic algorithm (NSGA-II). In the last step, final
578 optimum points are then chosen using LINMAP and TOPSIS decision-making methods. Also in

579 this part, in order to explore the reasonable status of various solutions, the deviation index of
580 each solution from the ideal and non-ideal solution is evaluated.

581

582 **4. Results and discussion**

583 The proposed multi-objective optimization problem including economic and safety measures was
584 optimized using the NSGA-II procedure. In this regard, flash drum operating pressure (“P”), the
585 number of parallel paths (“NPPs”), the length of the plant layout (“a”), and the width of the plant
586 (“b”) with corresponding constraints expressed in Equations (21) were considered as the decision
587 variables. In order to define the optimum design variables, the multi-objective optimization
588 problem can be formulated as follows:

$$\begin{aligned} & \text{Minimize Risk Level } f_1(\vec{x}) \\ & \text{Minimize Plant annualized costs } f_2(\vec{x}) \\ & x = \{P, NPP, a, b\} \\ & \text{Subject to} \\ & 300 \leq P \leq 1200 \\ & 1 \leq NPPs \leq 20 \\ & 10 \leq a \leq 2000 \\ & 10 \leq b \leq 2000 \end{aligned} \tag{21}$$

589 In the present case study, the plant annualized cost (TAC) and risk level must be minimized
590 simultaneously (Figure 2- case a). The tuning parameters selected for the NSGA-II algorithm
591 procedure are presented in Table 4. In addition, it is possible to visualize Pareto front in a two-
592 dimensional space. Visualization of the Pareto front enables decision-makers to compare
593 different solutions according to their fitness with respect to the competing objectives.

594

595

Table 4 - Specified NSGA-II options for multi-objective optimization

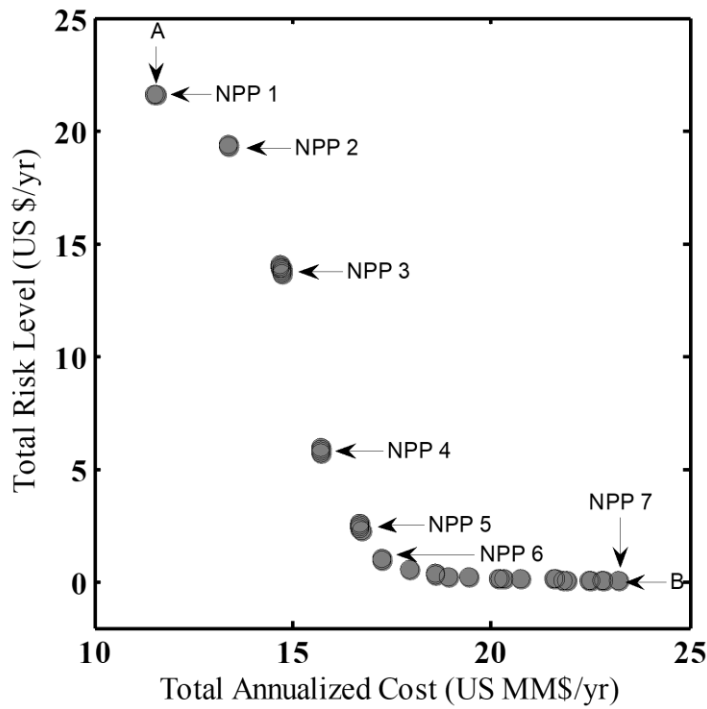
Specified Options	value
Population Size	30
Maximum Generations	300
Tournament Size	2
Crossover Function	Intermediate
Crossover Probability	0.9
Mutation Function	Constraint Dependent
Mutation Probability	0.1
Pareto Fraction	0.6

596

597 Figures (8a) show the Pareto front for multi-objective optimization of designing an inherently
 598 safer refrigeration cycle, in which the competitions and conflicts between the considered
 599 objectives are clearly demonstrated. Since, the range of varying of the objective functions in a
 600 multi-objective optimization problem might be different, in order to facilitate the optimization
 601 procedure, the dimension and scales of the objective functions were normalized. To do so, the
 602 method of Euclidian was applied (Farsi and Shahhosseini, 2015). In this method, the matrix of
 603 objectives at various points of the Pareto front is denoted by F_{ij} where i is the index for each
 604 point on the Pareto front and j is the index for each objective in the objectives space. Therefore a
 605 non-dimensionalized objective F_{ij}^n is defined as:

$$F_{ij}^n = \frac{F_{ij}}{\sqrt{\sum_{i=1}^n F_{ij}^2}} \quad (22)$$

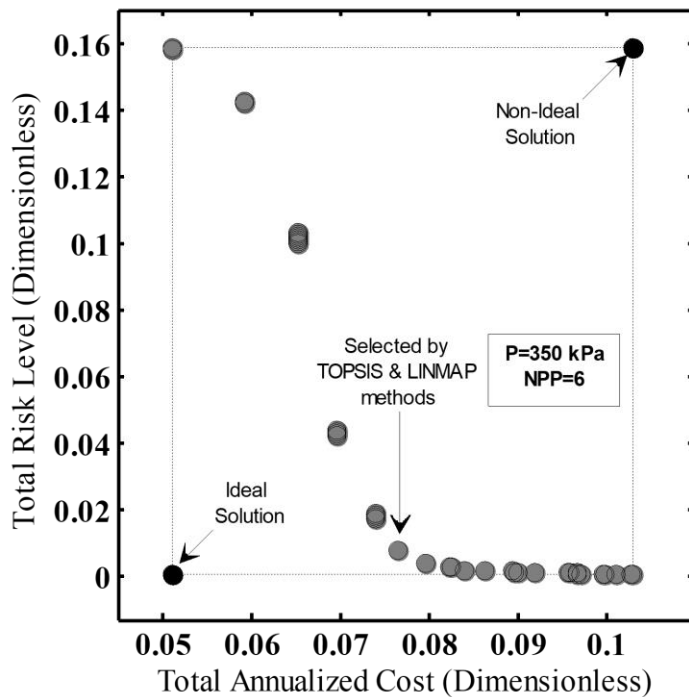
606 Therefore, all non-dominated optimal solutions are plotted in non-dimensional form in Figure 8.



607

608

Figure 7 - Pareto optimal Front in the objectives space



609

610

611

Figure 8 - The set of non-dimensional Pareto optimum solutions using LINMAP and TOPSIS methods to specify the final optimal design point

612 The Pareto front in Figure 7 shows that the lowest risk level is at design point B (0.0727 US
613 \$/yr), while the TAC has its highest value at this point (23.2×10^6 US \$/yr). On the other
614 extreme, the lowest TAC is at design point A (11.5×10^6 US \$/yr) while the risk level has its
615 highest value at this point (21.621 US \$/yr).

616 The values of decision variables are shown in Figure 7 for some of the points on the Pareto front
617 in order to clarify the trend of the Pareto front with respect to the decision variables.

618 If only the TAC was considered as the objective function (single-objective optimization), the
619 design point A (Figure 7), would be chosen as the optimal solution point of the system, while the
620 design point B (Figure 7), indicates the optimum system performance considering the risk level
621 as the objective function. In Figure 8, the ideal point is the point at which each single objective
622 has its optimum value regardless of satisfaction of other objectives (Points A and B, as discussed
623 earlier). In contrast, the non-ideal point is the point at which each objective has its worst value.
624 In Figure 8, the final optimal solution selected by LINMAP and TOPSIS decision-makings is
625 indicated. The results are an ideal solution and also a non-ideal solution.

626 Table 5 lists the final optimal results of multi-objective optimization and single-objective
627 optimization in detail. In order to quantify the fitness of various solutions, the deviation index of
628 each solution from the ideal solution is also calculated and reported. The fifth column of Table 5
629 represents the deviation indexes for the results in each optimization approach. As is clear, the
630 deviation indexes (0.0055 and 0.0055) for the multi-objective optimization are less than those
631 for minimum Cost and maximum Risk which are 0.9820 and 0.018, respectively. Therefore, the
632 final optimal solution selected by both of TOPSIS and LINMAP decision-making methods
633 which show the minimum deviation index from ideal solution in multi-objective optimization is

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634 most preferred. The last row of Table 5 represents the numerical values of optimum design
 635 parameters and objective functions which were corresponded to the coordinate that was
 636 determined by decision-making methods.

637 **Table 5 - Comparison between optimal solutions for multi-objective and single-objective optimizations**

Optimization algorithms	Decision- makings	Objectives		Deviation index d	P (kpa)	NPP
		Non-dimensional TAC	Non-dimensional Risk			
NSGA-II	LINMAP	0.0766	0.0075	0.0055	350	1
	TOPSIS	0.0766	0.0075	0.0055	350	1
Minimum TAC		0.0511	0.1585	0.9820	383	1
Minimum Risk Level		0.1029	0.0053	0.018	351	20
Optimum design variables and objective functions based on TOPSIS and LINMAP decision-making						
P (kpa)		NPP		TAC (US \$/yr)		Risk (US \$/yr)
350		6		17.3×10 ⁶		1.0262

638
 639 The value of optimization variables for the base case design (Figure 4), P=676 kPa, NPP=1), the
 640 solution reported by Eini et al. (2015) (P= 600kPa, NPP= 11), and the optimum solution found in
 641 this study (P= 350 kPa, NPP= 6) are shown in Table 6. Table 6 suggests that, in comparison to
 642 the base-case, for 19 percent increase in the TAC, it is possible to increase the level of process
 643 safety by 1 order of magnitude. With respect to the previous results by Eini et al. (2015), the new
 644 solution is much more realistic as the number of parallel paths is almost halved (i.e., less
 645 complexity) but the associated risk is only increased by 17%, In addition, the new solution
 646 considers the costs of land-use, piping, and instrumentation that were ignored in the previous
 647 study.

648 **Table 6 - Comparison of optimum point characterizations of base-case, single-objective optimization case**
 649 **(Eini et al., 2015), and multi-objective optimization case (present work)**

Optimum point characterizations	Base-case	Eini et al. (2015)	Present study
Drum operating pressure (kPa)	676	600	350
Number of parallel paths (NPP)	1	11	6
Plant annualized costs (US \$/yr)	14.5×10 ⁶	22.1×10 ⁶	17.3×10 ⁶
Risk (US \$/yr)	21.8256	0.4462	1.0262

650

651 **5. Conclusion**

652 In this paper, a general framework to design inherently safer processes is developed. In the
 653 proposed framework, the two competing and conflicting objectives of process economy and
 654 inherent safety are considered simultaneously. The new algorithm is developed in order to
 655 consider the level of process inherent safety based on the frequency and the consequence of
 656 potential accidents. The solution of the multi-objective optimization (MOO) forms a Pareto front
 657 which quantifies the trade-off between competing objectives and enables the decision-makers to
 658 choose the optimal design based on the satisfaction of the objectives.

659 The proposed optimization framework was implemented for the case of a simple refrigeration
 660 cycle. The objective functions used in the case study were the plant risk level as well as the plant
 661 total annualized costs. Furthermore, a layout optimization was implemented in order to consider,
 662 the costs of instrumentation, piping, and land-use. NSGA II was utilized as the MOO algorithm
 663 in order to produce the Pareto front. Two well-known and common types of decision-making
 664 techniques (LINMAP and TOPSIS) were applied in order to specify the final optimal solution.
 665 The results of multi-objective optimization problem suggested that for about 19 percent increase
 666 in the total annualized costs, it is possible to decrease the risk level by one order of magnitude in

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667 comparison with the base-case. While the demonstrating example of the refrigeration cycle
668 provides the proof of concept, the results are deemed to be general and extendable to other
669 industrial processes.

670 The dynamic behavior of a process strongly depends on its design. Therefore, the decision-
671 making domains of process and control engineers overlap (Sharifzadeh and Thornhill, 2012,
672 2013; Sharifzadeh, 2013a, 2013b). Moreover, it should be noted that accidents have a dynamic
673 nature. Therefore, the inherent safety level of a process should be assessed not only in the steady
674 state condition but also in dynamic mode and the future researches should address the dynamic
675 aspects of ISD strategies. Furthermore, there is a strong interaction between involved materials
676 and process inherent safety (Ten et al., 2015). Therefore, there are great opportunities for
677 integrating ISD concepts during product design stage using computer-aided molecular design
678 (CAMD) techniques. Based on CAMD techniques, it is possible to select or design new materials
679 that meet specific thermophysical properties. Consequently, CAMD can be used as a good tool in
680 order to design new molecules that feature desirable safety indicators such as moderated
681 flammability, toxicity, and etc. This leads to implementation of the substitution strategy of
682 inherent safety.

683 **6. Nomenclature /Abbreviations**

684

$f^{\text{non-ideal}}$	non-ideal solution vector on Pareto front
C_{total}	total cost of the accident [accident cost, for example, \$]
f^{ideal}	ideal solution vector on Pareto front
P_{ch}	chiller (evaporator) pressure [kPa]
P_{cond}	condenser pressure [kPa]

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P_{nf}	probability of occurrence of an accident as an independent event
$C_{(x,y)_i}$	consequence of scenario i in the risk receptor location (x, y) [accident cost]
F_{ij}	solution i of j th objective on the Pareto front
P_{econ}	optimum drum operating pressure [kPa]
$R_{(x,y)_i}$	risk level associated with an accident scenario i in the risk receptor location (x, y) [accident cost* time ⁻¹]
$R_{(x,y)}$	risk level associated with all scenarios in the (x, y) location [accident cost* time ⁻¹]
R_{nf}	risk associated with the simultaneous explosion of “ n_f ” drums [accident cost* time ⁻¹]
$R_{overall}$	overall risk [accident cost* time ⁻¹]
Y_i	assessment parameter in decision-making
$C_n^{n_f}$	number of accident combinations that can occur when n_f units suffer an occurrence out of “ n ”
d_{i-}	distance of each solution (i) from the non-ideal solution
d_{i+}	distance of every solution (i) on the Pareto front from the ideal solution
$f_{BLEVE/FIREBALL}$	frequency of a BLEVE/fireball outcome [time ⁻¹]
f_i	frequency of scenario i [time ⁻¹]
$f_k(\vec{x})$	objective function number k (x is a vector of decision variables)
n_f	number of drums that suffer an occurrence
ALARP	As Low As Reasonably Practicable
BLEVE	Boiling Liquid Expanding Vapor Explosion
CAMD	Computer-Aided Molecular Design
CRF	Capital Recovery Factor
ETA	Event Tree Analysis
FTA	Fault Tree Analysis
ISD	Inherently Safer Design
ISEOD	Inherently Safer and Economically Optimal Design
LINMAP	Linear Programming Technique for Multidimensional Analysis of Preference
MOO	Multi-Objective Optimization
n	the total number of drums in the cycle

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NPP	Number Of Parallel Paths
NSGA	Non-Dominated Sorting Genetic Algorithm
QRA	Quantitative Risk Assessment
TAC	Total Annualized Cost
TOPSIS	Technique for Order Preference by Similarity to an Ideal Solution
VCE	Vapor Cloud Explosion
VCF	Vapor Cloud Fire

685

686 7. Reference

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