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Abstract

Inherent safety aspects are not usually considered as a driving force during the conceptual design stage of chemical plants. Instead, after the selection of the optimal economic flowsheet, safety is added to the design. However, this sequential design approach could reach to inferior designs due to protection devices' cost overrun. The objective of this work is to implement a strategy to simultaneously design a profitable and inherently safer distillation train. Two safety indexes, a disaggregated version of the Safety Weighted Hazard Index and Dow's Fire and Explosion Index, have been adapted to quantify the inherent safety performance. A large-scale multi-objective MILP problem is formulated. Thus, two strategies of objective reduction are utilized: Principal Component Analysis coupled with Deb's algorithm and a method based on the dominance structure. The results prove the suitability of these safety index as inherently safer metrics, and showcase the ability of the objective reduction methods to discriminate among the inherent safety criteria.

Keywords: Multi-objective Optimization, Objective Reduction, Inherent Safety, SWeH Index, Dow's F&E Index.

1. Introduction

Safety must play a key role in the design of a chemical process. Commonly, during the conceptual design stage of a chemical process safety issues are not considered as one of the driving forces, since the main objective controlled is the economic one. In the last decade, the idea of considering a process from a holistic point of view using indicators that cover all the facets of sustainable development[1] has gained

28 wider interest. When the design is under a unique perspective (which is usually the economic one along

29 with some study of the environmental impact), valuable alternatives are discarded. Performing the

30 safety evaluation once the conceptual design is settled, we can only maneuver around that proposed

31 design, which normally results in the addition of control and protective complex equipment to increase

32 the safety of the plant. When we consider safety as one of the core design criteria, the results in the

33 design already account for the inherent safety principles, which tend to diminish the complexity of the

34 protective and control layers required in the last stages of the process design. This highlights the

35 importance of adding Inherently Safer Design (ISD) concepts in the early conceptual design stage[2-4]. ISD

36 is regarded as one of the main future directions for loss prevention in the chemical industries[5].

37 The first definition of Inherent Safety was coined by Kletz[6], where he stated the four main principles of

38 ISD as follows:

39 - Intensification or minimization: reduction of the inventories of a plant is one of the most

40   important steps.

41 - Substitution: there may be occasions when intensification is not a viable procedure. As an

42   alternative, substituting a material with a safer one improves the security of the plant.

43 - Attenuation or moderation: if the usage of hazardous material in non-reduced inventories is

44   mandatory, an alternative is using that material under its less hazardous conditions.

45 - Limitation of effects: design a plant that, if an accident happens, the potential effects (such as

46   the possible number of fatalities) are reduced.

47 While this philosophy seems rather clear, although difficult to quantify, its core could lead to the

48 following recommendation during the conceptual design stage: Incorporate an inherently safer metric

49 as another objective, and not as a constraint[7]. Following this strategy, the protective and control devices

50 would be either removed or reduced in complexity in the subsequent design stages.

51 Therefore, it is required a quantitative method to assess the level of Inherent Safety of a plant. We

52 consider that as long as its analysis can be carried away from a design stage, a safety evaluation metric

53 can be used as an Inherent Safety Index. While this removes some layers of the safety metrics, such as

54 those that account for the control and protective equipment, it provides a quantitative tool to proceed

55 into an initial analysis of the design of a whole plant, a section of a plant, or plant equipment.

56   Safety assessment in chemical processes poses a challenge to be unequivocally quantified. There are

57   many subjective decisions involved in its measurement, leading to different indexes and techniques that

58   try to evaluate safety in the most objective way possible. The most conventional approach to evaluate

59   the hazards present in a system is the Hazard an Operability method (HAZOP). The problem with this

60   approach is that, as we have previously stated, in order to perform this analysis the design of the plant

61   must be already available, which makes it a non-valid technique for inherent safety evaluation. Another

62   main problem of this technique is that it is qualitative. This means that, while alternatives may be

63   discussed upon the results of the method, there will be a certain degree of subjectivity. As stated

64   above, inherent safety as a main approach to assess the safety of a process has been receiving

65   considerably more attention from both industries and researchers[8]. There are various published works

66   that dwell into the incorporation of inherent safety concepts to known chemical processes[9-11]. As an

67   example, Medina-Herrera[10] provided an inherently safer design to different distillation systems

68   implementing quantitative risk analysis (QRA) on competing structures. While that approach provides a

69   good assessment of the inherent safety of the system, it is based on heavily non-linear, non-convex

70   equations, which are very difficult to optimize correctly. It provides nonetheless a good comparative

71   methodology once the number of alternatives has been reduced.

72   In this paper, we base our studies in two safety measures; Dow's Fire and Explosion Index, F&EI [12] and

73   the Safety Weighted Hazard Index, SWeHI[13], as inherently safety indexes (ISI). The reasons behind these

74   choices are various. Dow's F&EI is the most widely used index across the chemical industry, with defined

75   and clear guidelines that allow the user to obtain a simple security score of the process. Moreover, this

76   index has been previously used by other authors[14-15]. One of its limitations is its lack of higher sensitivity

77   to some process variables, such as operation temperature [16]. SWeHI provides more accuracy, although

78   part of it is based on control devices criteria. Thus, we selected the pure equipment-dependent parts of

79   it in order to make the comparison the most universal possible.

80   There exist some inherent safety indicators, such as the Numerical Descriptive Inherent Safety

81   Technique, NuDIST [17] and the Integrated Inherent Safety Index, I2SI [18-19] which are able to calculate an

82   index for the inherent security of a plant. These methods obtain an index for a piece of equipment and

83   then add the result with some metric to provide a general measurement of the safety. However, when

84   trying to optimize a thermally coupled distillation train, the columns are not defined until the final stage,

85   so the concept of separation task is used instead [20-21]. This is also common in the intensification of

86   chemical processes. In those cases, a set of tasks or basic physical principles (reaction, separation,

87   mixing, etc.) can be arranged in different ways to get different intensified alternatives [22-23] (i.e. Divided

88   wall columns, reactive distillation, membrane reactors, etc), and so can the variables as well. For the

89   distillation train case, which sequence should be utilized, how many trays, the volume and other

90   variables, cannot be taken into account by the use of these indexes. Due to this factor, only the

91   previously mentioned SWeHI and Dow's F&EI are considered in this work. A systematic review of

92   inherent safety indicators can be found in the work of Jafari[24].

93   Some of these inherently safer Indexes could produce contradictory results, because they are measuring

94   different aspects of the process: effects of the holdup, temperature or pressure, and could also be in

95   conflict with the economics of the process. In order to assess the system from the perspectives of

96   different safety indexes, a Multi-objective optimization (MOO) is stated. One of the most common

97   approach to obtain the Pareto frontier is the ε-constraint method [25], where all the objectives minus one

98   are transferred to the constraints. However, this MOO method has its drawbacks, being the most

99   prominent one its computational cost, which exponentially increases with the number of objectives.

100   Consequently, high-dimensionality MOO problems demand algorithms to eliminate redundant

101   objectives. Since we are working with more than three objectives, an objective reduction technique is

102   compulsory.

103   A rather traditional approach is to combine all the objectives together into one single objective function

104   by assigning a weight to each of them. In this way, the multi-objective problem is transformed into a

105   single objective problem. However, the weight assignment has always some degree of subjectivity and

106   not always reflects the designer preferences or even the specific and usually important particularities of

107   a given process. In addition, aggregated metrics may overlook some solutions, as illustrated in previous

108   works [26].

109   Another criteria are the utilization of the PCA (Principal Component Analysis) methodology along with

110   Deb's algorithm[27-29] or the methodology based on the works of Brockhoff and Zitzler[30-32], based on the

111   concept of maximum approximation error δ.

112   In this paper, besides comparing the safety indexes and assess their utility as Inherent Safety Index (ISIs),

113   the multi-objective optimization is performed via ε-constraint method once the objectives have been

114   reduced by three different methods for objective reduction. Thus, we aim to compare also these three

115   methods; pure Principal Component Analysis, Deb & Saxena's algorithm [29], and objective reduction

116   based on the maintenance of the dominance structure [33].

117   On the other hand, distillation is the most important operation for the purification and separation in the

118   chemical process industries. It handles more than 90-95% of all the separation and purification

119   processes. Soave and Feliu [34], with the use of data from Mix et al. [35] obtained that the energy

120   consumption in distillation is around 3 % of the total USA energy consumption, being this value

121   approximately $2.87 \cdot 10^{18}$ J per year (which rounds to 54 million tons of crude oil). While distillation is

122   present in almost all chemical engineering processes, safety issues are rarely introduced in the first

123   stage of design, except maybe some rules related to removing toxic or corrosive materials as soon as

124   possible [36-37]. The general separation problem was defined 50 years ago by Rudd and Watson [38] as the

125   separation of several sources mixture into several product mixtures. Today, that general problem has

126   not been completely solved, so we will focus on the much more studied problem of separating a single

127   zeotropic mixture in several products using only distillation columns considering all the possible

128   alternative sequences from conventional columns to fully thermally coupled arrangements (a single

129   condenser and a single reboiler in all the sequence) going through all intermediate alternatives.

130   The major contributions of this paper are:

131   - We consider the inherent safety in the very first stages of the design of complex distillation

132   systems. At the same time we use different indexes -Dow's F&EI and SWeHI together with the

133   economics of the process- and a disaggregation (sub-indexes) included in the SWeHI (B_1, B_2)

134   that take into account different aspects related to the principles of inherent safety designs, like

135   the effect of the hold up, temperatures and pressures without a pre-specified weight in each

136   indicator.

137   - In order to reduce the dimensionality of the multiobjective optimization, we compare different

138   alternatives for rigorous objective reduction. In such a way we can perform a rigorous

139   optimization in the reduced space of objectives with a bounded and known error.

140　　• 　We adapted the MILP algorithm presented by Caballero and Grossmann [39] for the synthesis of

141　　　　thermally coupled distillation sequences, that easily allows the inclusion of ISIs. This algorithm

142　　　　has proved to be very efficient for mixtures with up to six key components, and is able to deal

143　　　　with shortcut or rigorous models and ensures global optimality.

144　　We consider that the method and study here presented has its applications not only in the academic

145　　environment, but in the industrial one as well. While it may require some extra work to add inherent

146　　safety as a core design value, equating it to economic and environmental values, this effort is rewarded

147　　in the possible advantages that derive from not depending completely on control equipment to mitigate

148　　risk and its consequences. Over the last years, the industry has started to consider environmental

149　　damage as a core design principle, which was not that common in the past. It is expected that inherent

150　　safety, and safety in general, will be the next core design principle that will be added to both the

151　　economic and environmental one at an early design stage. The methodology here presented may serve

152　　as a foundation on how to tackle quantitatively inherent safety with the use of safety indexes.

153　　The remainder of this article is organized as follows. First, the problem is formally stated, and then the

154　　MILP approach for the optimal synthesis of thermally coupled distillation sequences is outlined. In the

155　　next section, the methodology is illustrated for the case study presented in this work; the safety of a

156　　distillation train, which is further described in the following paragraph. The following section is devoted

157　　to comparing the selected safety indexes to assess their total or partial utility as Inherent Safety Indexes

158　　for the different design alternatives. Following that, we focus on the comparison of the objective

159　　reduction methods and presenting the results obtained from the optimizations. Finally, we draw some

160　　general conclusions derived from the analysis of the case study.

161　　**2. Problem Statement and theoretical foundations**

162　　The problem addressed in this article can be formally stated as follows. Given is a mixture of M

163　　components that do not form azeotropes. The objective is to obtain the optimal Pareto surface in the

164　　economic (Total Annualized Cost –TAC-) and ISI objectives of sequences of distillation columns, including

165　　conventional and non-conventional sequences to completely separate N (N ≤ M) components. These N

166 components are separated with high recoveries (i.e. sharp separations). The rest are allowed to

167 optimally distribute in all the final streams.

168 As an additional goal, we want to reduce the number of optimization targets if possible. To this aim, the

169 Pareto set will be studied using different objective reduction algorithms, helping the decision-maker to

170 choose which objectives can be eliminated and what consequences would bring that elimination.

171 Before continuing with the methodology it is of interest to introduce a necessarily brief overview of the

172 MILP approach for optimizing complex zeotropic distillation sequences. The interested reader is referred

173 to the original publication [39].

2.1 MILP approach for the synthesis of thermally coupled distillation sequences

175 The design of thermally coupled distillation (TCD) sequences is much more complex than the design of

176 sequences involving only conventional columns (each column has a reboiler and a condenser), for at

177 least two reasons. First, the number of alternatives is larger in TCD and second, when we introduce a

178 thermal couple we are also introducing thermodynamically equivalent configurations (TEC) [40-41]. For

179 example, the total number of column sequences considering also TEC for the separation of a 5

180 component mixture is around 200,000, but two thermodynamically equivalent configurations have the

181 same energy consumption and they only differ in the final arrangement of some column sections in the

182 actual distillation columns. In order to avoid the degeneration created by TEC, is has been proposed to

183 use a task-based approach instead of a column based approach[42-45]. In such a way, all TECs share the

184 same sequence of separation tasks. Continuing with the example, in a 5 component mixture, there are

185 around 5,000 structurally different sequences of separation task (we consider two separation task

186 structurally different if they differ in at least a separation task or in the structure of condensers and

187 reboilers). If we consider only basic configurations (sequences that differ at least in a separation task,

188 without taking into account the structure of internal heat exchangers), the number of sequences for a 5

189 component mixture is 203 [44, 46]. But even using a task-based approach and aggregate or shortcut

190 models, the resulting models are large non-convex MINLPs [41-44, 47-48].

191 Notwithstanding, as noted by Andrecovich and Westerberg[49], when we consider only the sharp

192 separation of consecutive key components using conventional columns, it is possible to, a priori,

193   optimize each possible column in the sequence, and then use a MILP approach to extract the optimal

194   sequence. For example, if we have a mixture of 5 components (A, B, C, D, E) sorted by decreasing

195   volatility, under the assumption of sharp separation the total flow of each component in a sub-mixture

196   is equal to that in the feed stream. (i.e. if we have [25, 30, 35, 15, 20] kmol/h in the feed stream, if the

197   mixture BCD appears in the sequence it would contain 30, 35 and 15 kmol/h of B, C, and D respectively.)

198   Therefore we can optimize the separation task (B/CD) –sharp separate B from CD- or (BC/D) –Separate

199   BC from D- without knowing the rest of the separation sequence. A nice thing about this procedure is

200   that we can use any optimization approach or any level of detail for each one of the separation tasks:

201   from aggregated to rigorous models. Basically, the results of optimization of each separation task are

202   the data for the MILP.

203   The next step consists of generating a superstructure that contains all the separation tasks. Figure 1

204   shows such a superstructure for a 4 component mixture. Finally, from the superstructure, it is necessary

205   to develop a Mixed Integer model that select the best sequence of distillation columns. Taking into

206   account that all tasks in superstructure are completely known the resulting model is a Mixed Integer

207   Linear Programming (MILP) problem.
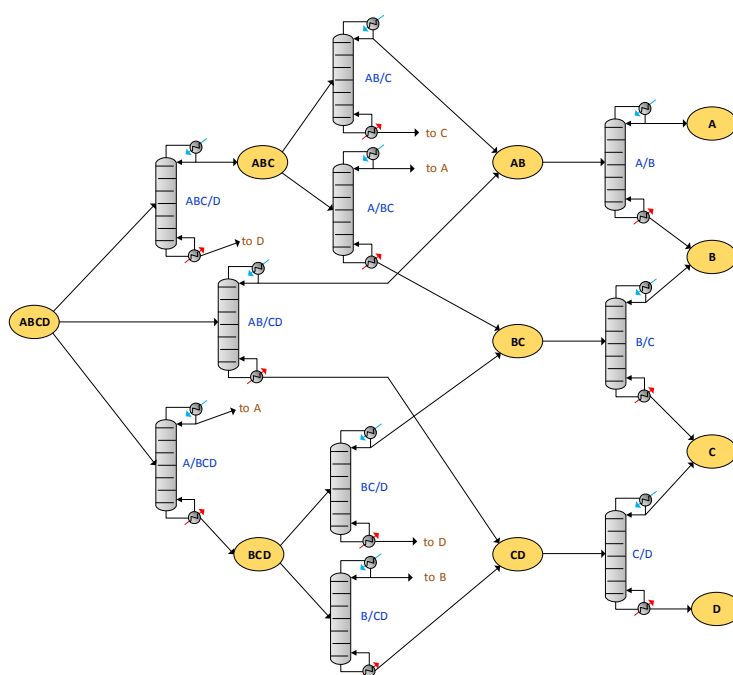
208

209   *Figure 1: Superstructure by Andrecovich and Westerberg for the separation of a zeotropic 4-component mixture*

210 Caballero and Grossmann [39] extended the ideas of Andrecovich and Westerberg [49] to TCD systems.

211 However, the direct extension to thermally coupled configurations is not possible for the following

212 reasons:

213 1. The two side streams that form a thermal couple introduce recycle of information in the

214 system. In a rigorous simulation the numerical solution is usually sensitive to initial values of

215 those streams, and therefore it is not possible a priori to know the flows and compositions of

216 those streams.

217 2. Vapor and liquid transfers between columns. If two columns stacked are optimized

218 independently and there is a transfer of vapor and liquid between those columns it is clear that

219 the column with the largest flow will be the dominant, and it will be necessary to modify the

220 internal flows of the other column and consequently also the diameter and the heat load.

221 3. The performance of a column depends on the feed thermal quality and composition. TCD

222 includes sharp separations of non-consecutive key components. Components with volatilities

223 between the keys are allowed to distribute between distillate and bottoms. Therefore, in

224 general, we do not know the feed composition because it depends on previous separations.

225 Caballero and Grossmann [39] found that the first two issues can be easily solved. According to Carlberg

226 and Westerberg [50-51] in the context of near ideal systems, the two streams that form a thermal coupled

227 are equivalent to a single saturated stream whose flow is the net flow (difference between the vapor

228 and liquid –rectifying section- or Liquid and vapor –stripping section-) and the thermal state is

229 superheated vapor (rectifying section) or subcooled liquid (stripping section). Latter Navarro et al. [52]

230 extended the concept to non-ideal systems and showed that the two streams that form a thermal

231 couple are also equivalent to a single saturated stream plus (rectifying section) or minus (stripping

232 section) and energy stream. With this approach, the resulting system is acyclic.

233 The imbalance in vapor and liquid in the connection points of stacked columns can be easily solved by

234 adding a condenser or a reboiler to compensate the excess or defect of flow.

235 To solve the third issue Caballero and Grossmann [39] proposed to use two superstructure levels. In the

236 upper level, the superstructure includes all the basic sequences of separation tasks. In the lower level,

237 each separation task is divided into as many separation tasks as necessary to explicitly take into account

238 all thermal states and feed compositions that could reach that task. Figure 2 shows the task-based

239 superstructure for a TCD 4 component system. Figure 2 also shows part of the lower level that extends

240 individual separation tasks to take into account differences in composition and thermal state.
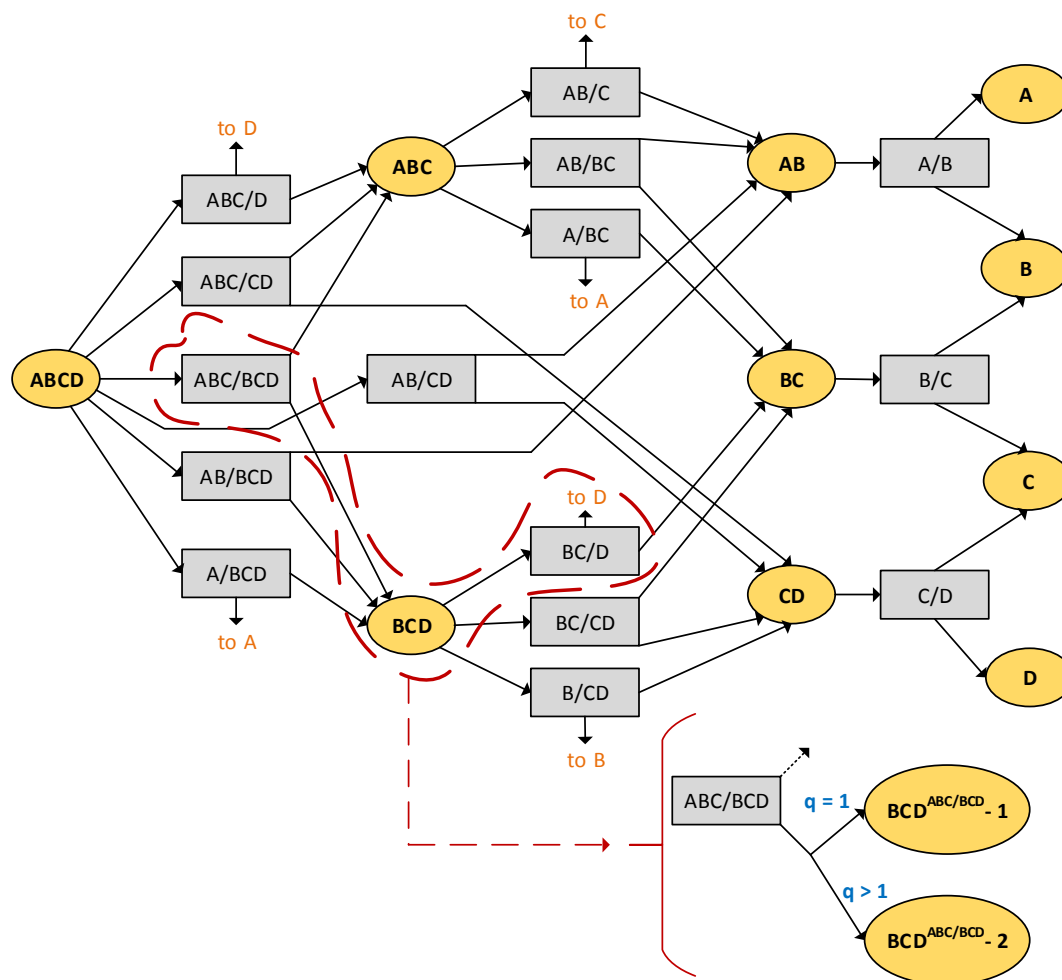
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Figure 2: Task based superstructure for a TCD 4 component system, including a glimpse of the lower level of separation task operating in the superstructure, with q referring to the thermal state of the stream, where we can see how the states are sub-divided in regards to their thermal state and which task they come from (red dashed line)

245 In the extended superstructure, it is possible to optimize a priori all the separation tasks. Note that the

246 number of such a separation tasks could be rather large but much lower than the total number of

247 feasible sequences, and the optimization of a single separation task is a small problem (involves only a

248 column) by comparison with the optimization of a sequence. In the case of using shortcut models, the

249 optimization of a single column becomes a very easy to solve problem and the large number of

250 separation tasks is not a problem. In any case, due to the exponential grow of the number of separation

251 tasks the procedure is limited to mixtures of up to 6 components.

252   Caballero and Grossmann [39] showed that it is possible to generate a MILP model to extract the optimal

253   TCD sequence from the extended superstructure.

254   **3. Methodology**

255   In order to further understand our methodology, a scheme of the procedure, which entails 3 steps, can

256   be seen in Figure 3. In the first step, we generate the superstructure, and optimize each one of the

257   separation tasks. As each separation task could be considered as a pseudo-column comprising a

258   rectifying section and a stripping section [39], we can calculate a separation task using any of the models

259   available for conventional columns. In particular, we modeled each separation task with the Fenske-

260   Underwood-Gilliland shortcut method (implemented in MATLAB) to obtain the optimal values of the

261   following parameters:

262   - The minimum and the actual number of trays

263   - number of trays in each section

264   - vapor and liquid flows in the rectifying and stripping sections

265   - condenser and reboiler duties, the diameter of each column section

266   - the equivalent thermal state of distillate and bottoms if a thermal couple appears

267   - area of the reboilers and condensers

268   From these values, the TAC and the ISI indexes for each separation task are computed.

269   From the second step, MILP optimization, we obtain an optimal sequence of tasks, which then can be

270   arranged into a basic sequence of distillation columns. As an example, Figure 4 shows an output from

271   this step. In particular, it is the optimal sequence of task for the extreme solution corresponding to the

272   minimum value of one of the objectives, the Dow's F&EI. Note also that Figure 4 defines if a task has a

273   condenser/reboiler associated or if it is thermally coupled with the following task.

274   As an optional third step, we apply different objective reduction methodologies in order to find out if
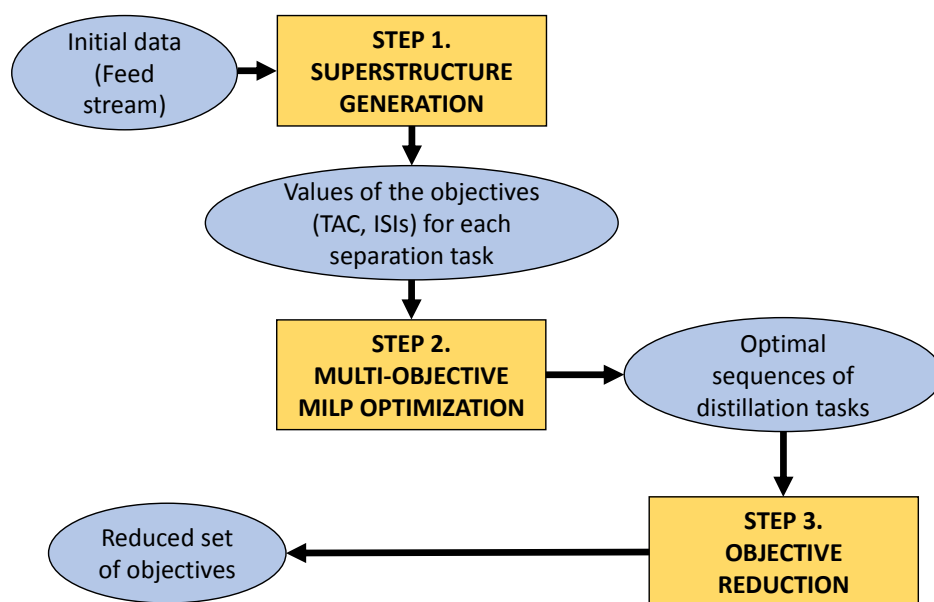
275   some of the safety metrics can be obviated.

276

Figure 3: Methodology utilized in the work

278   For the sequence minimizing the Dow's Index, using a State Task Network (STN) model the resultant

279   separation tasks can be seen in Figure 4. The existence of a condenser/reboiler associated to a task is

280   denoted by a single arrow linking two consecutive tasks whereas a double arrow denotes a task that is
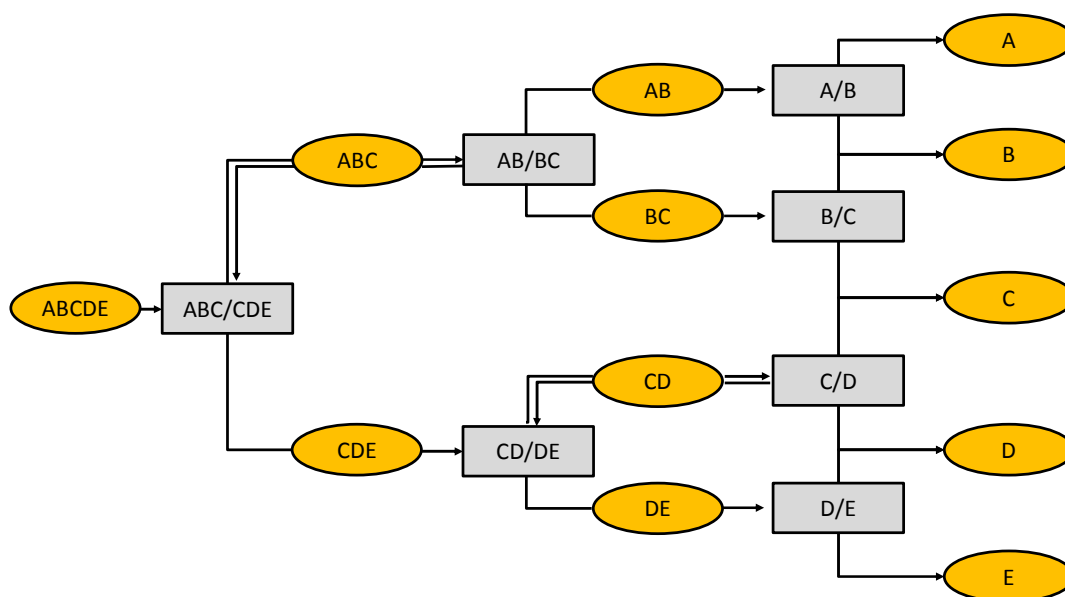
281   thermally coupled with the following.

282

Figure 4: Resulting STN of the mono-optimization problem minimizing the Dow's F&EI

284   These tasks are then converted to a possible sequence, which is shown in Figure 5, following the next

285   assumptions:

286   -   A "pure" product can only be obtained from a distillation column alone.

287   -   Consider only the basic sequences. These being, those with N-1 distillation columns.

288   Thus, since we have to adjoin simple tasks into one column, we must be sure that the index of each task

289   is addable between them, to not incur in an overestimation error.

290   This sequence is not the only possible outcome of this group of tasks. It may not even be the most

291   operable since the working pressures would not allow for some overheated vapor streams to enter the

292   next column without the needing of a compressor. Each task sequence obtained in this optimization will

293   have a number of thermodynamically equivalent column sequences.

294   Since we are not optimizing the final built, but the sequence of distillation tasks that can be ordered in

295   N-1, the sequences represented in this work are only one of the possibilities. A further study, after this

296   first pruning, would be required in order to optimize completely the column sequence. Considering that

297   the objective of the paper is to present different safety indexes, their utility as Inherent Safety Indexes

298   and the minimum number of them needed to obtain a good representation of the safety of the system,

299   the extent of analyzing every thermodynamically equivalent sequence is out of the scope of this work.

300   Additionally, the Safety Indexes studied cannot be added, this meaning, in order to state the safety of a

301   plant is not a valid option to add each Safety Index value of each equipment to the others and give a

302   single number that states the safety. Usually, like in the Dow's F&EI case, an expert committee isolates

303   the dangerous equipment from the safer one of a layout and proceeds to analyze the measurements of

304   each equipment separately. After that, an ordered list is obtained as the output of the analysis, where

305   the equipment is ordered from more to less dangerous. In order to give the plant a safety score, the

306   most dangerous equipment's Dow Index is taken. This philosophy here would be impossible to replicate

307   since we consider separation tasks and not separation equipment. Thus, during this work, the whole

308   sequence will be considered as one system, i.e., one equipment, which is composed of a number of

309   subsystems which would be the separation tasks. The indexes will be calculated for each subsystem,

310   thus the necessity of them being linear with extensive properties such as the amount of material, and

311   the result will provide a number for the whole distillation sequence.

312 This point of view also allows us to not venture into some gray terrain that exists in the field of Safety,

313 such as if only considering the most dangerous of the equipment as the only source of a Global Plant's

314 Index is appropriate, or if it is an oversimplification. Another course of action would be considering only

315 the highest safety index from the sequence, instead of adding them as an equipment, but the former

316 provides us with a much wider range of possible sequences to study and discuss.

317 **4. Case Study**

318 The chosen case study is based on the work of Caballero & Grossmann [39]. It consists of a distillation

319 process of a mixture of five hydrocarbons with zeotropic behavior. Its properties are shown in Table 1.

320 The reason behind the election of this case is to show that the methodology, even when working with

321 similar chemicals, provides a sufficiently different classification of alternatives. Being this the case, it is

322 expected that when the distillation train separates different chemicals, with very different

323 characteristics, this classification will be sharper.

324 The case is solved as a MILP problem. All the characteristics of each separation task are previously

325 calculated in MATLAB using the equations of Fenske-Underwood-Gililland and sent to GAMS in order to

326 perform the linear optimization. Since the optimization is just a sequence of separation tasks and not

327 final columns, all their properties must be additive in order to obtain a possible property of the final

328 built column sequence. Since it is a five-component distillation, the number of columns to form a basic

329 configuration is four.

330 *Table 1: Properties of the feed stream*

Properties	Pentane	Hexane	Heptane	Octane	Nonane
Mole flow [kmol/h]	40	60	60	20	20
Enthalpy of combustion [kJ/kg]	$45.37 \cdot 10^3$	$45.12 \cdot 10^3$	$44.94 \cdot 10^3$	$44.81 \cdot 10^3$	$44.70 \cdot 10^3$
Enthalpy of Vaporization [kJ/mol]	30.77	33.19	35.58	36.83	38.30
Temperature [°C]	85.122				
Pressure [bar]	1				

331

332 Thus, the ISIs chosen must be linear with the volume or the feed mass flowrate of the hypothetical

333 column that would perform the simple separation task, and not account for any independent term.

334 Otherwise, there would be an error in the optimization, since it would choose the sequence of minimum

335   tasks instead of the ones that are the safest. In order to account for this, instead of considering each

336   task separately, we consider as a whole equipment the distillation sequence of tasks provided by the

337   model. This sequence of tasks is latter reorganize in any of the TECs formed by N-1 columns.

338   With these limitations in mind, some of the preselected ISIs must be discarded due to its inability to

339   maintain a linear behavior. Indexes such as the I2SI and the NuDIST are not suited for this case, as

340   explained later in the paper, while other indexes, such as the Dow's F&EI and the SWeHI, can be

341   modified in order to account for their non-linearity. An ISI will be added to every calculation in MATLAB

342   and the optimization will be performed using as objective function the corresponding Eq. (1),

343
$$ISI_{objective} = \sum_{t=1}^{T} ISI_t \, y_t \tag{1}$$

344   where the sub-index t refers to the separation task and T is the total number of separation tasks. The

345   binary y_t takes the value 1 if that task exists and 0 otherwise.

346   According to Turton et al. [53], the cost of a vertical vessel is approximately linear with its volume and

347   certainly, it will be linear with the energy consumption, which will remain unaltered no matter how

348   many tasks are performed in different columns.

349   **5. Studied indexes**

350   **5.1 Dow's Fire and Explosion Index**

351   Its use as an ISI has been studied previously by other authors [14]. It is calculated as shown in Eq. (2).

352
$$F \& EI = MF \cdot F_1 \cdot F_2 \tag{2}$$

353   where:

354   -   *MF* stands as the Material Factor of the chemicals involved. Since the materials that enter the

355   system and the ones that exit it are the same, i.e., not a chemical reaction is involved, this

356   factor will remain constant for the whole system.

357   -   *F₁* stands as the General Process Hazards' factor. Its calculation involves the consideration of a

358   series of penalty factors. In this case study, considering that the core chemicals and equipment

359   will remain relatively unchanged among all the possible alternatives, it is considered that all

360   these penalties will remain the same between the different possible separation tasks. Thus, this

361   factor will also remain constant.

362   - F_2 stands as the Special Process Hazards' factor. Like the General Process Hazards' factor,

363   involves counting a series of penalty factors. Almost every penalty factor included in these

364   calculations will remain constant between the possible separation tasks, except the G item,

365   which involves a penalty to the inventory of the equipment.

366 The inventory in the F&EI stands for the amount of energy in the equipment or stream, and its

367 calculation is shown in Eq. (3)

$$Inventory = \max\left\{W, mf_{\max}\right\} \cdot Hc \tag{3}$$

369 where W stands as the amount of chemical in the equipment. The amount of chemical in one

370 hypothetical column has been defined as a percentage of the volume of that column. While most

371 references recommend a height at the bottom of the column of $1 - 2$ meters, considering the different

372 diameters in the results, plus the different heights and number of trays with both vapor and liquid

373 flowing through them, a value of a 30% of the volume of the column as inventory was assumed in this

374 work. This can be still considered as a pretty conservative value since it is considering only the liquid

375 phase chemical, which despite having the greatest weight when taken into account the inventory of a

376 column, it is not the only factor we need to account for. The parameter mf_{max} refers to the maximum

377 mass of chemical that exits the column in 10 minutes, assuming both a case where the leakage would be

378 produced in the upper stages, with the fluid being mostly vapor or in the lower stages, with the fluid

379 being mostly liquid.

380 As described in Dow's F&EI guide, the G item is calculated using Eq. (4).

$$\log_{10}(G) = 0.17179 + 0.42988 \log_{10}(Inventory) - 0.37244(\log_{10}(Inventory))^2$$
$$+0.17712(\log_{10}(Inventory))^3 - 0.029984(\log_{10}(Inventory))^4 \tag{4}$$

382 While Eq. (4) is clearly non-linear, considering that it is a monotonically increasing function and that the

383 Dow F&EI will be obtained for the whole sequence of tasks instead of obtaining one for each of the

384 tasks, we minimize the total inventory of the sequence, as shown in Eq. (5). It is important to note that

385   this consideration is only possible due to all the other factors being considered equal among the whole

386   spectrum of possibilities, meaning that only this G item will vary among the alternatives.

387
$$ISI_{Dow} = \sum_{t=1}^{T} Inventory_t \, y_t \qquad (5)$$

388   Thus, we would minimize the inventory in a feasible sequence, that then using Eq. (4) will provide the G

389   item for that sequence, which then can be converted into a Dow's F&EI using Eq. (2). It is worth

390   repeating again that the index we are comparing is valid for a sequence of tasks since we are in an early

391   stage. A set of distillation tasks does not mean a set of distillation columns since there are plenty of

392   thermodynamically equivalent options. A detailed discussion about separation tasks, and how to

393   generate basic distillation sequences can be found, for example, in the following references [42-44, 46, 54-55].

394   **5.2 Safety Weighted Hazard Index**

395   Its original equation, as extracted from the original paper by Khan et al. [13], is shown as Eq. (6), where A

396   represents the credit due to control measures and safety arrangements made to counter the

397   undesirable situations and B is the quantitative measure of the damage that the equipment can

398   produce, either by its material charge, chemical leaks, etc. Considering this, we will focus our study in B,

399   since it is only dependent of the properties of the streams, equipment and materials, and that is the

400   data that we have this early in design.

401
$$SWeHI = B \, / \, A \qquad (6)$$

402   Similarly to the actual index, B is also composed of two components; B_1 and B_2. B_1 addresses the damage

403   that can be produced by the equipment due to fire and explosions while B_2 refers to the damage that

404   the equipment can produce due to the toxicity of the possible releases and dispersion of that toxic

405   material in the atmosphere. In their original work, Khan et al.[13] chose the sub-index with the highest

406   value and set B as that one. Since both are measuring different aspects of safety, both are considered as

407   separated indexes here in order to further study its behavior.

408   In the same way as it was considered when evaluating Dow's Index, it is considered that the whole

409   equipment is the distillation train, formed by the different tasks. Hence, that the index remains linear

410 with the mass flow, or with another property that can be translated from separated tasks to final

411 columns, is a must to.

412 Eq. (7) and (8) show how to calculate those parameters, as found in the reference [13].

$$B_1 = 4.76 \cdot ((F_1 \cdot pn_1 + F \cdot pn_2) \cdot pn_3 \cdot pn_4 \cdot pn_5 \cdot pn_6 \cdot pn_7 \cdot pn_8)^{1/3} \qquad (7)$$

$$B_2 = 25.35 \cdot (G \cdot pnr_1 \cdot pnr_2 \cdot pnr_3 \cdot pnr_4 \cdot pnr_5 \cdot pnr_6 \cdot pnr_7)^{0.425} \qquad (8)$$

415 These indexes are clearly non-linear. Thus, for each task, in a similar manner to the treatment given to

416 the Dow's F&EI G item, we consider some changes considering that the index will be obtained for the

417 distillation train and not for each individual column, and thus the exponent can be removed since these

418 are monotonically increasing functions. This change is made by simplifying the equations into linear

419 ones, shown in Eq. (9) and (10).

$$B_{1t} = ((F_1 \cdot pn_1 + F \cdot pn_2) \cdot pn_3 \cdot pn_4 \cdot pn_5 \cdot pn_6 \cdot pn_7 \cdot pn_8) \qquad \forall t \in T \qquad (9)$$

$$B_{2t} = (G \cdot pnr_1 \cdot pnr_2 \cdot pnr_3 \cdot pnr_4 \cdot pnr_5 \cdot pnr_6 \cdot pnr_7) \qquad \forall t \in T \qquad (10)$$

422 Therefore, in order to obtain the objective function for these two indexes, we apply Eq. (11) and (12).

$$ISI_{B_1} = \sum_{t=1}^{T} B_{1t} \, y_t \qquad (11)$$

$$ISI_{B_2} = \sum_{t=1}^{T} B_{2t} \, y_t \qquad (12)$$

425 Notice now that the objective function is calculated with these linear approximations, but the data

426 displayed in this paper has been then modified to have an appropriate value to compare with other

427 processes, i.e., once performed the optimization with our linear modification, the value is then modified

428 as it is intended in the original work, re-adding the exponents.

429 As explained before, in order for (9) and (10) to be linear, all their parameters must be linear either with

430 the volume of the hypothetical column or the mass flows. A brief explanation of their calculation is next

431 provided.

432   **B_1 penalties and core factors**

433   Its core factors are calculated using Eq. (13), (14) and (15).

434
$$F_1 = 0.1 W \cdot Hc \ / \ K \tag{13}$$

435
$$F_2 = 1.304 \cdot 10^{-3} \cdot P \, V \tag{14}$$

436
$$F_3 = \frac{10^{-3}}{T} \cdot (P - VP)^2 V \tag{15}$$

437   where:

438   - W is the amount of chemical in the equipment [kg]

439   - Hc is the enthalpy of combustion of the chemical in the equipment [kJ/kg]

440   - K is a constant that equals 3148

441   - P is the process pressure [kPa]

442   - V is the volume of the chemical in the equipment [m^3]

443   - T is the process temperature [K]

444   - VP is the vapor pressure of the chemical in the equipment [kPa]

445   It is worth remarking that all these parameters are linear with the quantity of chemical in the

446   equipment, which allows us to then add all the tasks into a single B_1 index for the whole sequence.

447   The parameter F is obtained from F_2 and F_3 as a linear combination of the two. Thus, it would be linear

448   as well with the quantity of the chemical.

449   Its first penalty refers to the process temperature. In order to maintain a conservative calculus, we

450   consider as the temperature of the task the higher temperature in the hypothetical column, e.g., the

451   temperature at the bottom. It is obtained from Eq. (16).

$$pn_1 = f(flash, fire, autoignition, process\ temperature)$$

$$
\begin{aligned}
&\text{if (fire point} > \text{process temperature} > \text{ flash point)}\\
&pn_1 = 1.45\\
&\text{else if } (0.75 \text{ autoignition temperature} > \text{ process temperature} > \text{ fire point})\\
&pn_1 = 1.75\\
&\text{or if (process temperature} > 0.75 \text{ autoignition temperature)}\\
&pn_1 = 1.95\\
&\text{else}\\
&pn_1 = 1.10
\end{aligned}
\tag{16}
$$

453   For these, we have to be able of calculating the flash point of a mixture of chemicals [56], although since

454   the penalty is not extremely sensitive to the process temperature, a conservative approach of

455   considering the lowest flash point of the compounds in the mixture as the flash point of the mixture is

456   taken.

457   Its second penalty accounts for the pressure factor. It also decides whether F depends of F_2, F_3 or both of

458   them. It is calculated as shown in Eq. (17). Let AP be the atmospheric pressure in kilopascals:

$$
\begin{aligned}
&\text{if (} VP > AP \ \& \ P > VP)\\
&pn_2 = 1 + ((P - VP)/P) \cdot 0.6\\
&F = F_2 + F_3\\
&\text{otherwise}\\
&pn_2 = 1 + ((P - VP)/P) \cdot 0.4\\
&F = F_2\\
&\text{if (} AP > VP \ \& \ P > AP)\\
&pn_2 = 1 + ((P - VP)/P) \cdot 0.2\\
&F = F_3\\
&\text{otherwise}\\
&pn_2 = 1.1\\
&F = F_3
\end{aligned}
\tag{17}
$$

460   Its third penalty accounts for the weight of the chemical inside the equipment. This penalty is linear with

461   the quantity of the chemical, although it has an independent term that may incur into an

462   overestimation. Nevertheless, considering the ranges of inventories treated in this case study, it can be

463   assumed that the error produced because of that is minimum. It is calculated as shown in Eq. (18)

$$
\begin{aligned}
&\text{if } NF/NR = 1 \\
&pn_3 = 1 + 0.003 * W / 1000 \\
&\text{if } NF/NR = 2 \\
&pn_3 = 1 + 0.005 * W / 1000 \\
&\text{if } NF/NR = 3 \\
&pn_3 = 1 + 0.008 * W / 1000 \\
&\text{if } NF/NR = 4 \\
&pn_3 = 1 + 0.010 * W / 1000
\end{aligned}
\tag{18}
$$

464

465   The effect of the chemicals' reactivity and flammability is assessed in the fourth penalty, as shown in Eq.

466   (19).

467
$$
pn_4 = \max \left\{ 1,\ 0.30 \cdot [NF + NR] \right\}
\tag{19}
$$

468   In both these penalties, the NF and NR parameters come from the National Fire Protection Association

469   (NFPA) American standard [57], which identify the risks posed by the different chemicals that the plant

470   has. Since we have a mixture of different chemicals, a mean between the amounts of each chemical in

471   the total of the column at the feeding point is performed, giving a bit more of sensibility to the index.

472   Penalties from fifth to eighth refer to events that are not accountable this early in design, such as social

473   factors and environmental factors. Besides being unknown at this early stage, they would not vary

474   between the different possible layouts and thus they were given a value of 1.

475   **B_2 penalties and core factors**

476   Its core factor is calculated as shown in Eq. (20)

477
$$
G = S \cdot m_{spill}
\tag{20}
$$

478   where S depends on the released conditions and m_{spill} is the amount of chemical that is expected to be

479   released. Since we are calculating those parameters for every separation task, and the result should be

480   consistent with any arrangement of tasks in a final number of columns, the amount of chemical that will

481   be released has been considered as both the quantity that leaves that task from heads and from

482   bottoms, added together. In doing so, we are considering the worst case scenario, where there are two

483   spills from the most vulnerable points, being these the outlets of the tasks, both heads and bottoms.

484   Thus, it seems obvious that the basic configurations where there are more lateral outputs in the

485   columns will get penalized by this index. The values of *S* can be seen in Table 2.

486   *Table 2: S values*

NH	Liquid	Liquified Gas	Gas	Solid
4	4.00	8.0	13.4	0.1300
3	0.40	0.8	1.34	0.0130
2	0.20	0.4	0.67	0.0060
1	0.07	0.1	0.25	0.0025

487

488   Its first penalty, in the same manner as the B_1 one, refers to the effect of the process temperature. If we

489   are working with a flammable chemical, we use Eq. (16). If it is a toxic or corrosive chemical, Eq.(21). If it

490   is both, which tends to occur in most of the cases, it must be assessed as the highest result of both.

491
$$\text{if (process temperature} > 4 \text{ x ambient temperature)}$$
$$pnr_1 = 1.55$$
$$\text{if (process temperature} > 2 \text{ x ambient temperature)}$$
$$pnr_1 = 1.35 \tag{21}$$
$$\text{else}$$
$$pnr_1 = 1.1$$

492   Likewise, its second penalty refers to the effect of the pressure. Since it only accounts for equipment

493   whose are pressurized, this being, their pressures are higher than 3 atm, it was considered as 1 for all

494   the possible tasks since we are working at atmospheric pressure.

495   Its third penalty accounts for the chemicals that are heavier than air, which take more time to disperse.

496   Thus, the heavier the chemicals, the higher the penalization given to the task and to the final sequence

497   with that task. Its calculation is shown in Eq. (22)

498
$$pnr_3 = 1.2 \cdot vapor\ density\ /\ air\ density \tag{22}$$

499   The fourth penalty is pretty straightforward, assessing the toxicity of the chemical and having a

500   minimum of 1. It is obtained from Eq. (23)

501
$$pnr_4 = \max\left\{1, 0.6 \cdot NH\right\} \tag{23}$$

502   Penalties five to seven, in the same way as the previously mentioned ones in the B_1 calculations, account

503   for issues that are unknown at this design phase. Therefore, they are given a value of 1.

504   **6. Objective reduction and results**

505   For each task sequence, we have the following objectives; *TAC, ISI$_{B1}$, ISI$_{B2}$* and *ISI$_{Dow}$*. A Pareto frontier of

506   these 4 objectives would provide all the information about the interconnection between these

507   indicators, but its computational cost considering 10 values within the range of each objective would

508   escalate to an order of 10^4 optimization problems to be solved, making its computational cost too high

509   to be effective. Instead, we first obtain the sequences that optimize each objective individually. These

510   are shown in Figure 5.

511
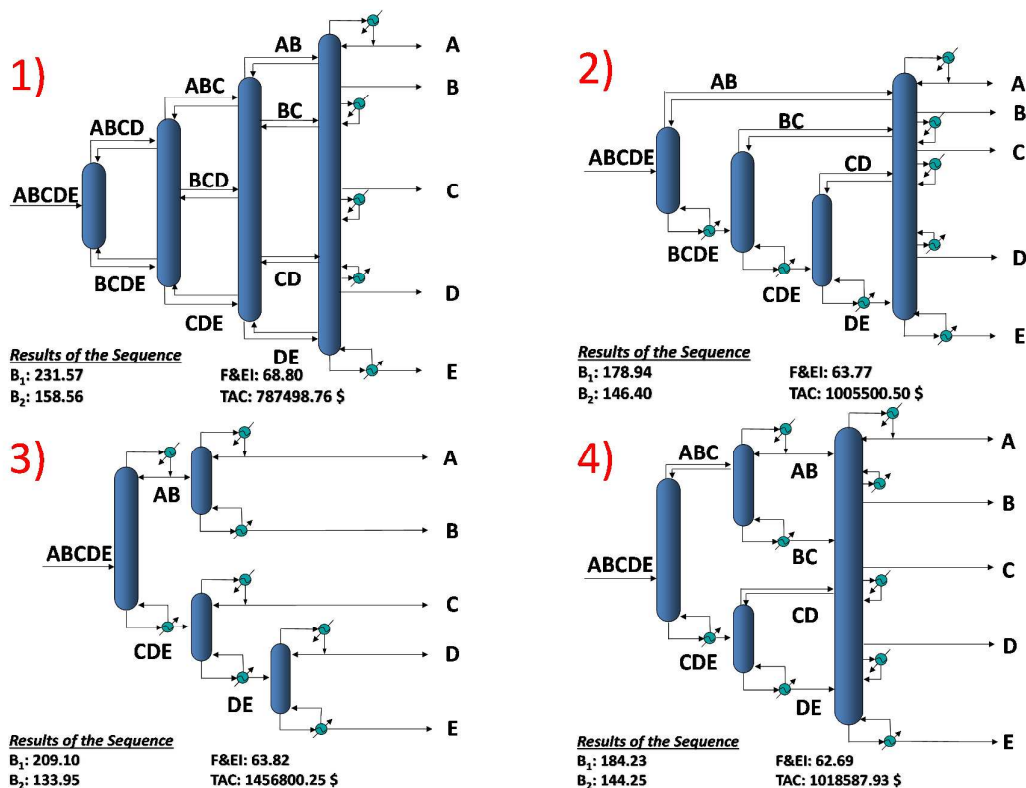
512   *Figure 5: Possible optimal sequences for each mono-objective problem: 1) TAC, 2) B$_1$, 3) B$_2$, 4) F&EI.*

513   It is interesting to note that, as expected, the optimal sequence in regards to the economic objective is

514   the totally thermal coupled sequence, which has the lowest energy consumption. This result was already

515   proven mathematically [58]. In the case of the B_2 component of the SWeHI index, which takes into account

516   toxicity and damage of releases, its optimal sequence is such that no thermal coupled task exists. This

517   agrees with the manner in which we calculated this index. The leakage points, which are considered in

518   this index, are more prone to appear at the bottoms and heads of a column, where the streams exit its

519   vessel. As such, when there exist thermally coupled columns, those have more exit points. In the case of

520   Dow's F&EI and B_1 indexes, as they evaluate the flammability and explosion hazard in the equipment,

521   their corresponding optimal sequences are an intermediate between fully thermally coupled and non-

522   thermally coupled.

523   Next, we solve all the paired bi-objective problems using the ε-constraint method. The number of Pareto

524   paired points are shown in Table 3.

525

526   *Table 3: Number of Pareto Points obtained by solving all the bi-objectives*
527   *optimization problems*

	Number of Pareto Points			
B_1	-	11	3	12
B_2	-	-	9	18
Dow	-	-	-	13
TAC	-	-	-	-
	B_1	B_2	Dow's F&EI	TAC

528

6.1 Principal Component Analysis (PCA) coupled with Deb's algorithm

530   The Principal Component Analysis [59] is a statistical procedure based on the use of an orthogonal

531   transformation to convert a set of points, which are expected to be correlated between them, to a

532   series of uncorrelated linear variables, which are the principal components. The number of principal

533   components is equal to the number of initial variables, in this case, objectives, but the normal praxis

534   includes the consideration of a threshold. Each principal component explains a percentage of the points,

535   so setting a threshold of 90-95 % tends to eliminate at least one of the principal components. This

536   methodology allows the user to remove a number principal component below the threshold and as

537   such, reduce the dimensionality in the space of the principal components. This, however, does not

538   reduce the dimensionality in the original space of objectives, since these reduced principal components

539   still need all the original objectives to be evaluated.

540   In order to analyze the data by PCA, we have to discard all the repeated Pareto values, since some of the

541   resultant task layouts from the paired Pareto optimization could be redundant among the different

542   pairs. The filtered points are shown in Table 4. The results of the Principal Component Analysis is

543   provided in Table 5.

544   The threshold for the PCA is set as 95%, considering that precision will allow for a correct interpretation

545   of the data. Thus, we select the first three PCs, which explain 98.88% of the data. Instead of showing a

546   single 3D image of those PCs, three figures of the paired projections are shown, as well as the original

547   data points projected on the PCs space, which provide more information. These projections can be seen

548   in Figure 6.

549

550

551   *Table 4: Pareto points non-repeated*

B_1	B_2	Dow's F&EI	TAC (k$)	B_1	B_2	Dow's F&EI	TAC (k$)
178.94	146.41	63.77	1005.50	201.37	144.11	63.75	890.26
179.88	150.52	63.55	988.66	202.69	138.39	63.82	1220.45
182.89	150.44	63.70	927.14	203.72	146.75	65.52	839.82
184.23	144.25	62.69	1018.59	203.84	142.04	64.52	962.10
184.88	143.71	63.02	1117.14	205.45	137.83	63.90	1280.88
185.00	148.73	64.82	895.31	209.10	133.95	63.82	1456.80
187.09	144.17	62.86	957.07	210.70	144.75	64.79	866.91
189.52	142.57	64.22	1129.67	211.21	139.34	64.53	1084.28
191.26	142.20	63.79	1027.88	214.75	143.63	64.88	886.58
193.28	163.79	65.64	888.11	216.16	137.43	65.16	1264.30
193.90	163.63	65.82	877.55	218.74	138.98	65.48	1095.87
194.61	140.59	64.20	1140.87	225.67	141.46	65.78	1007.65
194.76	139.92	63.20	1149.89	226.90	165.59	67.76	825.56
195.34	139.35	63.51	1248.44	229.22	140.30	65.86	1027.31
197.14	157.74	66.09	842.62	230.29	159.90	68.05	795.85
197.33	139.83	63.36	1088.37	231.57	158.56	68.81	787.50
197.76	150.39	64.53	860.34	232.34	135.68	65.66	1398.24
198.43	139.88	63.29	1300.73	232.98	154.20	67.53	825.97
198.86	156.36	67.03	831.19	233.36	155.59	68.60	791.90
198.91	144.19	63.60	951.78	236.71	153.83	68.59	803.07
199.16	148.64	65.53	828.65	237.45	153.16	68.50	810.96
200.61	138.20	64.24	1152.05	240.68	151.36	68.48	822.13

552   In order to remove objectives in the original space of objectives, we use Deb's algorithm [29], which

553   provides a procedure to eliminate objectives based on the results of the principal component analysis.

554   Its guidelines are resumed as:

555   1.   Retain the amount of Principal Components that have an accumulated explained variance over

556   a predefined threshold.

557   2.   For those Principal Components, if the eigenvalue is less than 0.10, add to the subset of

558   objectives the objective with the higher absolute value.

559   3.   If the eigenvalue is higher than 0.1:

560   a.   If all the components of the principal component are positive, add to the subset of

561   objectives the objective corresponding to the highest value.

562   b.   If all the components are negative, add all the objectives to the subset of objectives.

563   c.   If none of the previous two cases apply:

564   i.   If the most positive element is smaller than the 90% of the absolute value of

565   the most negative one, add the most negative objective to the subset of

566   objectives.

567   ii.   If the most positive is bigger than the 90% of the absolute value of the most

568   negative one, but smaller than the absolute value of the most negative one,

569   add both the most negative and most positive to the subset of objectives.

570   iii. If the absolute value of the most negative is bigger than the 80% of the most

571   positive, but smaller than the most positive, add to the subset of objectives

572   both the most negative and most positive.

573   iv.   If none of the previous cases apply, add to the subset of objectives the most

574   positive one.

575   4.   If the subset of objectives differs from the original set of objectives, make the subset the new

576   original set and repeat the procedure.

577   Considering the threshold, we first set the initial set of objectives: $F_0 = \{B_1, B_2, Dow's\ F\&EI, TAC\}$ and the

578   new set of objectives as a void set; $F = \{\emptyset\}$. Let mn be the most negative value and mp the most positive

579   of given PC:

580
Table 5: PCA results

PC	B_1	B_2	Dow's F&EI	TAC	% explained
1	0.4032	0.5099	0.5738	-0.4982	66.08
2	0.7096	-0.4514	0.2958	0.4531	27.33
3	-0.1697	0.6156	0.214	0.7393	5.47

| | 4 | -0.5524 | -0.3966 | 0.7331 | -0.0087 | 1.12 |

581   - From the first PC, we add both the most positive and most negative objective to F these being

582   Dow's F&EI and TAC.

583   - From the second PC, since it explains more than 10% of the values, and since $|mn| < 0.8\ mp$,

584   we add the most positive value to F, this being B_1.

585   - From the third PC, since it explains less than 10% of the values, we add the objective with the

586   highest absolute value to F, this being TAC.

587   Since $F \neq F_0$, the PCA analysis must be repeated with the objectives that remain. In this case, $[B_1, Dow's$

588    $F\&EI, TAC]$. Data for this second PCA is shown in Table 6.

589

Table 6. Second PCA results

PC	B_1	Dow's F&EI	TAC	% explained
1	0.5684	0.5886	-0.5748	90.90
2	0.7630	-0.1157	0.6360	6.36
3	-0.3079	0.8001	0.5148	2.74

590   Again, we consider a threshold of 95%, which allows us to obviate again a principal component. Applying

591   again the algorithm, we end with $F = F_0 = \{B_1, Dow's\ F\&EI, TAC\}$. Thus, these are the final chosen

592   objectives. According to Deb's algorithm, the objective B_2 is not necessary when accounting for safety,

593   since it can be explained by the other two inherent safety indexes.

594

595   *Figure 6: Original data points projected into the PC space: a) PCs 1 & 2, b) PCs 1 & 3, c) PCs 2 & 3*

596   **6.2 Elimination of objectives by maintaining the dominance**

597   While Deb's algorithm may provide a good solution when the data is clearly centered on the first

598   Principal Component, it lacks accuracy when the coefficient values of the PCA are similar, e.g.,

599   coefficients of B_2 and Dow's F&EI in the first PCA.

600   In addition, Deb's algorithm does not provide any information of the incurred possible error when an

601   objective is eliminated. In light of this, another method of objective reduction, based upon MILP is

602   studied [33]. While the full-fledged explanation of the model can be seen in the reference, the basic idea

603   is that chooses which objectives must remain to maintain the dominance structure within a given

604   tolerance. The dominance structure can be represented as a parallel plot where we represent on the x –

605   axis the objectives and in the y – axis the value of a number of solutions in these objectives. It allows the

606   user to immediately visualize if there are any dominated solutions, or which objectives are keeping a

607   solution from becoming dominated. It is thus, the relationships among the different solutions and its

608   values on the different objectives.

609   The dominance structure of the case study can be seen in Figure 7. In problems with fewer objectives

610   and fewer Pareto points, it is possible to pinpoint at sight which objective may be redundant and which

611   is necessary. Since this problem has too many Pareto solutions to be this straightforward, the previously

612   mentioned method based on the detection of the redundant objectives and state how much error we

613   are incurring when eliminating one objective is utilized.

614

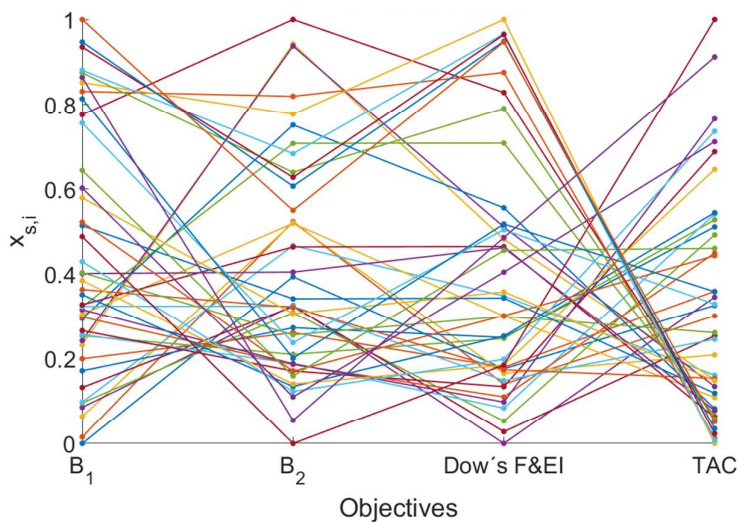*Figure 7: Dominance structure of the case study for 4 objectives and the 44 solutions*

616   Therefore, the concept of min-max δ-error of a dominance structure is utilized. This is the maximum

617   difference between two solutions in a pair that stops being Pareto optimal when one of the objectives is

618   removed. In order to further clarify this concept, it is explained in Figure 8.

619
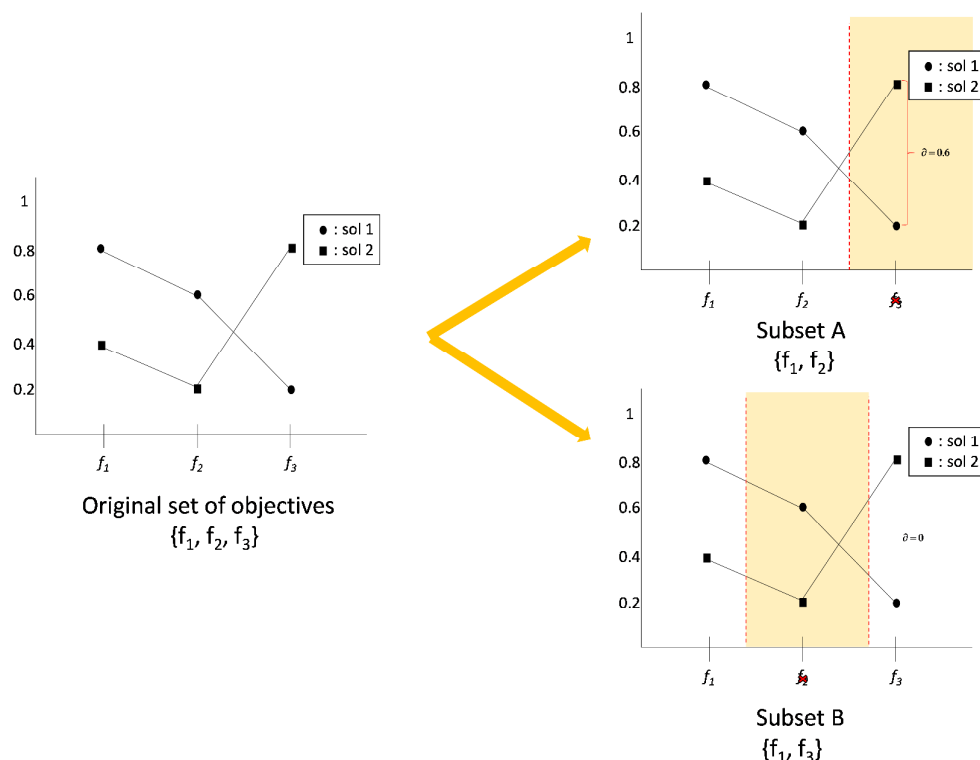
Figure 8: Dominance structure for two solutions and three objectives with normalized data. In the original set of objectives, both solutions are Pareto optimal. In subset A, objective f_3 is removed and solution 2 dominates completely solution one, with an error of δ=0.6. In subset B, objective f_2 is removed but the dominance structure remains unchanged

624   Thus, we minimize the greatest error that we obtain in the dominance structure when we eliminate an

625   objective. Using a binary cut strategy we obtain more solutions for that number of pruned objectives.

626   Identically to the PCA strategy, we only need the data from Table 4 to solve the model. The output of

627   the MILP provides the objectives maintained and the δ-error incurred when removing the rest of

628   objectives. As it is expected, the solution with the lower δ-error is the one that breaks the least the

629   dominance structure.

630   The results are shown in Table 7.

631   *Table 7: Results of the objective reduction based on the dominance structure*

Number of pruned objectives	Objectives maintained	Maximum Error δ (%)
1	B_1, B_2, TAC	6.8
1	B_2, Dow's, TAC	41.6
1	B_1, Dow's, TAC	88.9
2	B_2, TAC	76.8

632   Thus, while a 6.8% of error is considered an acceptable approximation, if we want to let the system be

633   reduced to 2 objectives we may incur into an error of a maximum of a 76.8%. From this perspective, we

634   could only eliminate one objective, Dow's F&EI, without altering severely the dominance structure.

635   **6.3 Results**

636   Considering the difference between the methods utilized, it is considered that the reduction by

637   dominance structure is the most reliable, since it includes a measure of the error resultant from

638   removing an objective. As commented above, Deb's algorithm works very well when the data is heavily

639   directed to one of the principal components. However, it is still a heuristic method. This means that

640   when there are similar values in the principal components, as those shown in Tables 5 and 6, which

641   objective gets removed is a less clear subject. Due to these two observations; the ability to obtain an

642   error when removing objectives and the non-heuristic characteristic, it is decided to keep the reduced

643   set of objectives that results from the δ-error model, instead of those which Deb's algorithm maintains.

644   Whereas for Deb's algorithm the removed objective would be B_2, for the δ-error model it would be

645   Dow's F&EI. In this case study, Deb's algorithm shows clearly that the TAC can never be obviated, since

646   there is a clear trade-off between it and any ISI, but it fails at recognizing which ISI should be removed.

647   On the other hand, the method based on the dominance structure eliminates the Dow's F&EI objective,

648   which does not change the dominance structure in an impactful manner, and as such it is considered as

649   the best course of action.

650   These results can be explained by the maner in which these ISIs are calculated. Both for Dow's F&EI and

651   B_1, the amount of chemical in the equipment is a core factor. In the case of the Dow's, it is actually the

652   whole differentiating factor among different alternatives, while the B_1 considers penalties and other

653   parameters depending on various data, such as vapor pressure, temperature, etc. For this, it seems

654   appropriate that B_1 acts as a more precise ISI and would not be removed in favor of the Dow's. B_2's core

655   factor is G, which is calculated from the streams exiting the columns. Thus, it will provide a different

656   result than both B_1 and Dow's F&EI, which explains why it should not be eliminated in order to maintain

657   the dominance structure.

658   Therefore, the reduced set of objectives is formed by the objectives B_1, $B_2,$ and TAC. Once only three

659   objective remains, the computational cost of calculating a new Pareto set of solutions is reduced. The

660   model is evaluated again with an epsilon constraint method in order to obtain all the Pareto optimal

661   solutions. The results are shown in Figure 9. Every point in these graphs showcases an equally "good"

662   different optimal solution. It is up to the designer to weight those three objectives in order to come with
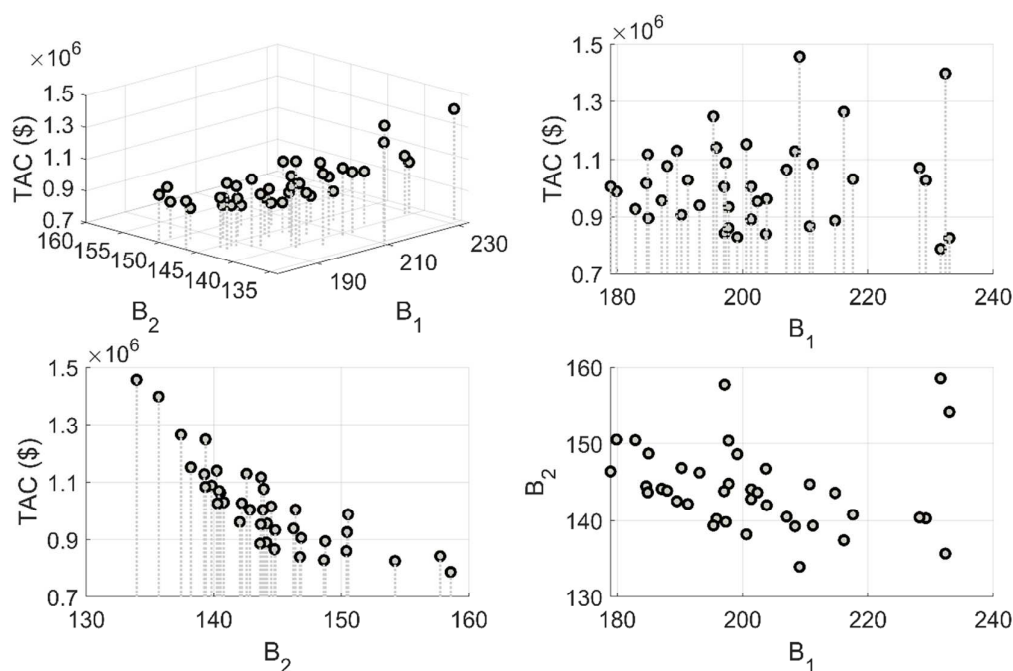
663   the desired design.

665   *Figure 9: Pareto frontier for three objectives, as well as its 2D projections*

666   **7. Conclusions**

667   An alternative method to assess the inherent safety of a distillation train design is introduced. While the

668   indexes here studied tend to be calculated for a piece of equipment, a consideration of the whole

669   distillation train sequence as a unique piece of equipment whose economic and inherent safety

670   performance is assessed.

671   From the results it can be extracted that it is possible to utilize some Safety Indexes as Inherent Safety

672   Indexes, having enough data to perform the analysis at an early stage of the design. Some

673   simplifications have been made into the case study, but the results allow the user to choose among

674   alternative sequences of tasks with significant differences in the studied objectives.

675   Three methods to deal with the multi-objective optimization are compared. The PCA, which forms new

676   objectives from the initial ones by lineal combination of those; Deb & Saxena's algorithm, which bases

677   the choice of objectives in the data obtained from the PCA; and our method based on the dominance

678   structure, which aims to maintain and minimize the higher error produced in the structure when one

679   objective is eliminated.

680   Results show that it is possible to apply those Safety Indexes in an early stage in design, acting then as

681   Inherent Safety Indexes. In addition, the method based on the dominance structure shows that the

682   inherent safety level of the design can be assessed with a unique safety index, with the considerations

683   previously explained in the paper, this being the Safety Weighted Hazard Index. Notwithstanding, its

684   consideration of choosing only the highest value between B_1 and B_2 could be argued, since they lead to

685   noticeably different results.

686   While in this problem the need of maintaining a linear index was required due to the case study, it is

687   recommended as a good practice for every other problem. Some of the indexes have strongly nonlinear,

688   nonconvex calculations, that would diminish their utility as inherent safety indexes since its inclusion in

689   the model would make the problem much more difficult to solve. Since the majority of Safety Indexes

690   are applied only when all the information is given, i.e., the plant is finally built, they tend to not be

691   additive, like Dow's F&EI. That is why in this work we adapt the safety indexes into a global index for the

692   sequence and not one for each column.

693   It is worth mentioning that even with the number of objectives reduced, the amount of equally good

694   Pareto solutions is pretty large. There are other strategies, such as the concept of Pareto efficiency of

695   order k [60] which can help the decision maker to diminish the number of options. Since that is not a

696   reduction of objectives, but of solutions, it is out of the scope of this work.

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Nomenclature

Abbreviations and Acronyms

F&EI	Dow's Fire and Explosion Index
SWeHI	Safety Weighted and Hazard Index
I2SI	Integrated Inherently Safety Index
ISI	Inherently Safety Index
TAC	Total Annualized Cost

Sets

t	Set of tasks
objective	Set of safety indexes evaluated

Parameters

δ	Maximum δ-error
$Inventory_t$	Inventory of a task t
B_{1t}	B_1 from the SWeHI of a task t
B_{2t}	B_2 from the SWeHI of a task t

Variables

$ISI_{objective}$	Value of the ISI objective in a sequence
y_t	Binary variable. 1 if task t exists, 0 otherwise

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Acknowledgments

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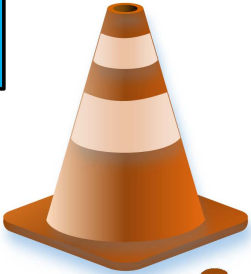852 **1999,** *18* (1), 30-35.

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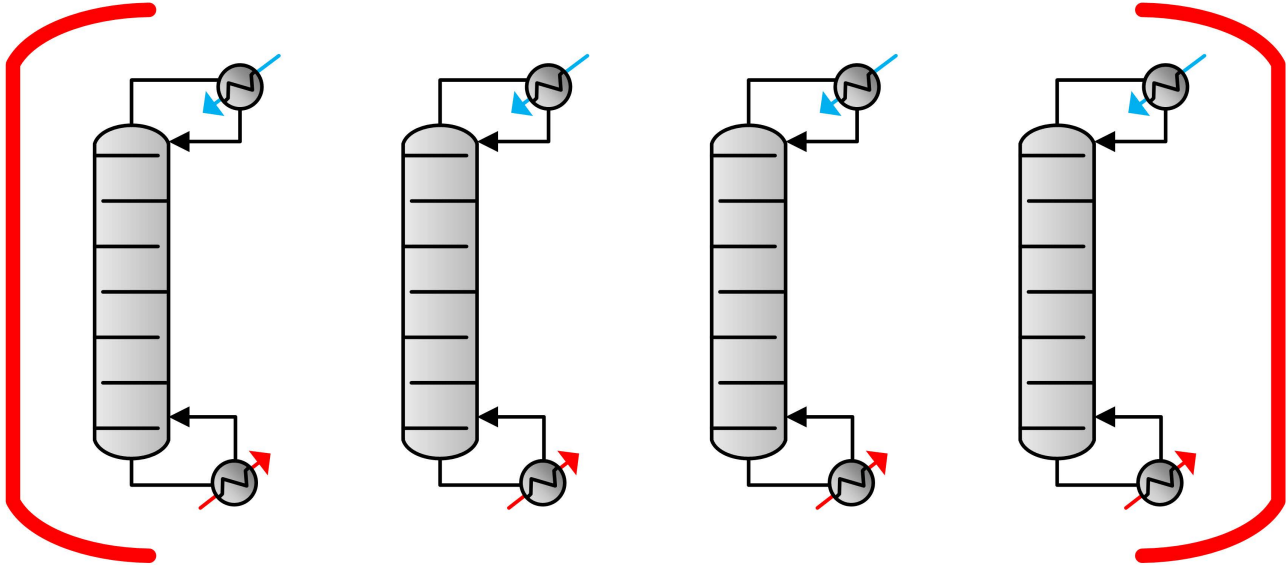
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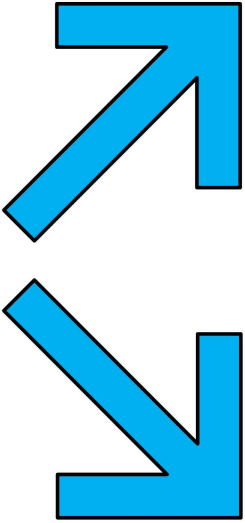
Economic objective

Safety objective