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Multi-objective early design of complex distillation sequences considering economic and inherent safety criteria.

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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 development¹ 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 stage²⁻⁴. ISD
36 is regarded as one of the main future directions for loss prevention in the chemical industries⁵.

37 The first definition of Inherent Safety was coined by Kletz⁶, 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 constraint⁷. 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.

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3 56 Safety assessment in chemical processes poses a challenge to be unequivocally quantified. There are
4
5 57 many subjective decisions involved in its measurement, leading to different indexes and techniques that
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7 58 try to evaluate safety in the most objective way possible. The most conventional approach to evaluate
8
9 59 the hazards present in a system is the Hazard and Operability method (HAZOP). The problem with this
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11 60 approach is that, as we have previously stated, in order to perform this analysis the design of the plant
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13 61 must be already available, which makes it a non-valid technique for inherent safety evaluation. Another
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15 62 main problem of this technique is that it is qualitative. This means that, while alternatives may be
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17 63 discussed upon the results of the method, there will be a certain degree of subjectivity. As stated
18
19 64 above, inherent safety as a main approach to assess the safety of a process has been receiving
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21 65 considerably more attention from both industries and researchers⁸. There are various published works
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23 66 that dwell into the incorporation of inherent safety concepts to known chemical processes⁹⁻¹¹. As an
24
25 67 example, Medina-Herrera¹⁰ provided an inherently safer design to different distillation systems
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27 68 implementing quantitative risk analysis (QRA) on competing structures. While that approach provides a
28
29 69 good assessment of the inherent safety of the system, it is based on heavily non-linear, non-convex
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31 70 equations, which are very difficult to optimize correctly. It provides nonetheless a good comparative
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33 71 methodology once the number of alternatives has been reduced.

34 72 In this paper, we base our studies in two safety measures; Dow's Fire and Explosion Index, F&EI¹² and
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36 73 the Safety Weighted Hazard Index, SWeHI¹³, as inherently safety indexes (ISI). The reasons behind these
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38 74 choices are various. Dow's F&EI is the most widely used index across the chemical industry, with defined
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40 75 and clear guidelines that allow the user to obtain a simple security score of the process. Moreover, this
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42 76 index has been previously used by other authors¹⁴⁻¹⁵. One of its limitations is its lack of higher sensitivity
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44 77 to some process variables, such as operation temperature¹⁶. SWeHI provides more accuracy, although
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46 78 part of it is based on control devices criteria. Thus, we selected the pure equipment-dependent parts of
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48 79 it in order to make the comparison the most universal possible.

49 80 There exist some inherent safety indicators, such as the Numerical Descriptive Inherent Safety
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51 81 Technique, NuDIST¹⁷ and the Integrated Inherent Safety Index, I2SI¹⁸⁻¹⁹ which are able to calculate an
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53 82 index for the inherent security of a plant. These methods obtain an index for a piece of equipment and
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55 83 then add the result with some metric to provide a general measurement of the safety. However, when

trying to optimize a thermally coupled distillation train, the columns are not defined until the final stage, so the concept of separation task is used instead²⁰⁻²¹. This is also common in the intensification of chemical processes. In those cases, a set of tasks or basic physical principles (reaction, separation, mixing, etc.) can be arranged in different ways to get different intensified alternatives²²⁻²³ (i.e. Divided wall columns, reactive distillation, membrane reactors, etc), and so can the variables as well. For the distillation train case, which sequence should be utilized, how many trays, the volume and other variables, cannot be taken into account by the use of these indexes. Due to this factor, only the previously mentioned SWeHI and Dow's F&EI are considered in this work. A systematic review of inherent safety indicators can be found in the work of Jafari²⁴.

Some of these inherently safer Indexes could produce contradictory results, because they are measuring different aspects of the process: effects of the holdup, temperature or pressure, and could also be in conflict with the economics of the process. In order to assess the system from the perspectives of different safety indexes, a Multi-objective optimization (MOO) is stated. One of the most common approach to obtain the Pareto frontier is the ϵ -constraint method²⁵, where all the objectives minus one are transferred to the constraints. However, this MOO method has its drawbacks, being the most prominent one its computational cost, which exponentially increases with the number of objectives. Consequently, high-dimensionality MOO problems demand algorithms to eliminate redundant objectives. Since we are working with more than three objectives, an objective reduction technique is compulsory.

A rather traditional approach is to combine all the objectives together into one single objective function by assigning a weight to each of them. In this way, the multi-objective problem is transformed into a single objective problem. However, the weight assignment has always some degree of subjectivity and not always reflects the designer preferences or even the specific and usually important particularities of a given process. In addition, aggregated metrics may overlook some solutions, as illustrated in previous works²⁶.

Another criteria are the utilization of the PCA (Principal Component Analysis) methodology along with Deb's algorithm²⁷⁻²⁹ or the methodology based on the works of Brockhoff and Zitzler³⁰⁻³², based on the concept of maximum approximation error δ .

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3 112 In this paper, besides comparing the safety indexes and assess their utility as Inherent Safety Index (ISIs),
4 113 the multi-objective optimization is performed via ϵ -constraint method once the objectives have been
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6 114 reduced by three different methods for objective reduction. Thus, we aim to compare also these three
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8 115 methods; pure Principal Component Analysis, Deb & Saxena's algorithm ²⁹, and objective reduction
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10 116 based on the maintenance of the dominance structure ³³.

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13 117 On the other hand, distillation is the most important operation for the purification and separation in the
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15 118 chemical process industries. It handles more than 90-95% of all the separation and purification
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17 119 processes. Soave and Feliu ³⁴, with the use of data from Mix et al. ³⁵ obtained that the energy
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19 120 consumption in distillation is around 3 % of the total USA energy consumption, being this value
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21 121 approximately $2.87 \cdot 10^{18}$ J per year (which rounds to 54 million tons of crude oil). While distillation is
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23 122 present in almost all chemical engineering processes, safety issues are rarely introduced in the first
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25 123 stage of design, except maybe some rules related to removing toxic or corrosive materials as soon as
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27 124 possible ³⁶⁻³⁷. The general separation problem was defined 50 years ago by Rudd and Watson ³⁸ as the
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29 125 separation of several sources mixture into several product mixtures. Today, that general problem has
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31 126 not been completely solved, so we will focus on the much more studied problem of separating a single
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33 127 zeotropic mixture in several products using only distillation columns considering all the possible
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35 128 alternative sequences from conventional columns to fully thermally coupled arrangements (a single
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37 129 condenser and a single reboiler in all the sequence) going through all intermediate alternatives.

38 130 The major contributions of this paper are:

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40 131 • We consider the inherent safety in the very first stages of the design of complex distillation
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42 132 systems. At the same time we use different indexes -Dow's F&EI and SWeHI together with the
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44 133 economics of the process- and a disaggregation (sub-indexes) included in the SWeHI (B_1 , B_2)
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46 134 that take into account different aspects related to the principles of inherent safety designs, like
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48 135 the effect of the hold up, temperatures and pressures without a pre-specified weight in each
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50 136 indicator.
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52 137 • In order to reduce the dimensionality of the multiobjective optimization, we compare different
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54 138 alternatives for rigorous objective reduction. In such a way we can perform a rigorous
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56 139 optimization in the reduced space of objectives with a bounded and known error.

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3 140 • We adapted the MILP algorithm presented by Caballero and Grossmann³⁹ for the synthesis of
4 141 thermally coupled distillation sequences, that easily allows the inclusion of ISIs. This algorithm
5 142 has proved to be very efficient for mixtures with up to six key components, and is able to deal
6 143 with shortcut or rigorous models and ensures global optimality.
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11 144 We consider that the method and study here presented has its applications not only in the academic
12 145 environment, but in the industrial one as well. While it may require some extra work to add inherent
13 146 safety as a core design value, equating it to economic and environmental values, this effort is rewarded
14 147 in the possible advantages that derive from not depending completely on control equipment to mitigate
15 148 risk and its consequences. Over the last years, the industry has started to consider environmental
16 149 damage as a core design principle, which was not that common in the past. It is expected that inherent
17 150 safety, and safety in general, will be the next core design principle that will be added to both the
18 151 economic and environmental one at an early design stage. The methodology here presented may serve
19 152 as a foundation on how to tackle quantitatively inherent safety with the use of safety indexes.
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28 153 The remainder of this article is organized as follows. First, the problem is formally stated, and then the
29 154 MILP approach for the optimal synthesis of thermally coupled distillation sequences is outlined. In the
30 155 next section, the methodology is illustrated for the case study presented in this work; the safety of a
31 156 distillation train, which is further described in the following paragraph. The following section is devoted
32 157 to comparing the selected safety indexes to assess their total or partial utility as Inherent Safety Indexes
33 158 for the different design alternatives. Following that, we focus on the comparison of the objective
34 159 reduction methods and presenting the results obtained from the optimizations. Finally, we draw some
35 160 general conclusions derived from the analysis of the case study.
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45 161 **2. Problem Statement and theoretical foundations**

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47 162 The problem addressed in this article can be formally stated as follows. Given is a mixture of M
48 163 components that do not form azeotropes. The objective is to obtain the optimal Pareto surface in the
49 164 economic (Total Annualized Cost –TAC-) and ISI objectives of sequences of distillation columns, including
50 165 conventional and non-conventional sequences to completely separate N ($N \leq M$) components. These N
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components are separated with high recoveries (i.e. sharp separations). The rest are allowed to optimally distribute in all the final streams.

As an additional goal, we want to reduce the number of optimization targets if possible. To this aim, the Pareto set will be studied using different objective reduction algorithms, helping the decision-maker to choose which objectives can be eliminated and what consequences would bring that elimination.

Before continuing with the methodology it is of interest to introduce a necessarily brief overview of the MILP approach for optimizing complex zeotropic distillation sequences. The interested reader is referred to the original publication³⁹.

2.1 MILP approach for the synthesis of thermally coupled distillation sequences

The design of thermally coupled distillation (TCD) sequences is much more complex than the design of sequences involving only conventional columns (each column has a reboiler and a condenser), for at least two reasons. First, the number of alternatives is larger in TCD and second, when we introduce a thermal couple we are also introducing thermodynamically equivalent configurations (TEC)⁴⁰⁻⁴¹. For example, the total number of column sequences considering also TEC for the separation of a 5 component mixture is around 200,000, but two thermodynamically equivalent configurations have the same energy consumption and they only differ in the final arrangement of some column sections in the actual distillation columns. In order to avoid the degeneration created by TEC, it has been proposed to use a task-based approach instead of a column based approach⁴²⁻⁴⁵. In such a way, all TECs share the same sequence of separation tasks. Continuing with the example, in a 5 component mixture, there are around 5,000 structurally different sequences of separation task (we consider two separation task structurally different if they differ in at least a separation task or in the structure of condensers and reboilers). If we consider only basic configurations (sequences that differ at least in a separation task, without taking into account the structure of internal heat exchangers), the number of sequences for a 5 component mixture is 203^{44, 46}. But even using a task-based approach and aggregate or shortcut models, the resulting models are large non-convex MINLPs^{41-44, 47-48}.

Notwithstanding, as noted by Andreovich and Westerberg⁴⁹, when we consider only the sharp separation of consecutive key components using conventional columns, it is possible to, a priori,

optimize each possible column in the sequence, and then use a MILP approach to extract the optimal sequence. For example, if we have a mixture of 5 components (A, B, C, D, E) sorted by decreasing volatility, under the assumption of sharp separation the total flow of each component in a sub-mixture 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 mixture BCD appears in the sequence it would contain 30, 35 and 15 kmol/h of B, C, and D respectively.) Therefore we can optimize the separation task (B/CD) –sharp separate B from CD- or (BC/D) –Separate BC from D- without knowing the rest of the separation sequence. A nice thing about this procedure is that we can use any optimization approach or any level of detail for each one of the separation tasks: from aggregated to rigorous models. Basically, the results of optimization of each separation task are the data for the MILP.

The next step consists of generating a superstructure that contains all the separation tasks. Figure 1 shows such a superstructure for a 4 component mixture. Finally, from the superstructure, it is necessary to develop a Mixed Integer model that select the best sequence of distillation columns. Taking into account that all tasks in superstructure are completely known the resulting model is a Mixed Integer Linear Programming (MILP) problem.

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

210 Caballero and Grossmann³⁹ extended the ideas of Andreovich and Westerberg⁴⁹ 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 Grossmann³⁹ found that the first two issues can be easily solved. According to Carlberg
226 and Westerberg⁵⁰⁻⁵¹ 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 Grossmann³⁹ 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

all thermal states and feed compositions that could reach that task. Figure 2 shows the task-based superstructure for a TCD 4 component system. Figure 2 also shows part of the lower level that extends individual separation tasks to take into account differences in composition and thermal state.

241

242 *Figure 2: Task based superstructure for a TCD 4 component system, including a glimpse of the lower level of*
 243 *separation task operating in the superstructure, with q referring to the thermal state of the stream, where we can*
 244 *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 Grossmann³⁹ 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 section³⁹, 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.

Figure 3: Methodology utilized in the work

For the sequence minimizing the Dow's Index, using a State Task Network (STN) model the resultant separation tasks can be seen in Figure 4. The existence of a condenser/reboiler associated to a task is denoted by a single arrow linking two consecutive tasks whereas a double arrow denotes a task that is thermally coupled with the following.

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

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

This point of view also allows us to not venture into some gray terrain that exists in the field of Safety, such as if only considering the most dangerous of the equipment as the only source of a Global Plant's Index is appropriate, or if it is an oversimplification. Another course of action would be considering only the highest safety index from the sequence, instead of adding them as an equipment, but the former provides us with a much wider range of possible sequences to study and discuss.

4. Case Study

The chosen case study is based on the work of Caballero & Grossmann³⁹. It consists of a distillation process of a mixture of five hydrocarbons with zeotropic behavior. Its properties are shown in Table 1. The reason behind the election of this case is to show that the methodology, even when working with similar chemicals, provides a sufficiently different classification of alternatives. Being this the case, it is expected that when the distillation train separates different chemicals, with very different characteristics, this classification will be sharper.

The case is solved as a MILP problem. All the characteristics of each separation task are previously calculated in MATLAB using the equations of Fenske-Underwood-Gilliland and sent to GAMS in order to perform the linear optimization. Since the optimization is just a sequence of separation tasks and not final columns, all their properties must be additive in order to obtain a possible property of the final built column sequence. Since it is a five-component distillation, the number of columns to form a basic configuration is four.

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]	45.37·10 ³	45.12·10 ³	44.94·10 ³	44.81·10 ³	44.70·10 ³
Enthalpy of Vaporization [kJ/mol]	30.77	33.19	35.58	36.83	38.30
Temperature [°C]	85.122				
Pressure [bar]	1				

Thus, the ISIs chosen must be linear with the volume or the feed mass flowrate of the hypothetical column that would perform the simple separation task, and not account for any independent term. Otherwise, there would be an error in the optimization, since it would choose the sequence of minimum

tasks instead of the ones that are the safest. In order to account for this, instead of considering each task separately, we consider as a whole equipment the distillation sequence of tasks provided by the model. This sequence of tasks is latter reorganize in any of the TECs formed by N-1 columns.

With these limitations in mind, some of the preselected ISIs must be discarded due to its inability to maintain a linear behavior. Indexes such as the I2SI and the NuDIST are not suited for this case, as explained later in the paper, while other indexes, such as the Dow's F&EI and the SWeHI, can be modified in order to account for their non-linearity. An ISI will be added to every calculation in MATLAB and the optimization will be performed using as objective function the corresponding Eq. (1),

$$ISI_{objective} = \sum_{t=1}^T ISI_t y_t \quad (1)$$

where the sub-index t refers to the separation task and T is the total number of separation tasks. The binary y_t takes the value 1 if that task exists and 0 otherwise.

According to Turton et al.⁵³, the cost of a vertical vessel is approximately linear with its volume and certainly, it will be linear with the energy consumption, which will remain unaltered no matter how many tasks are performed in different columns.

5. Studied indexes

5.1 Dow's Fire and Explosion Index

Its use as an ISI has been studied previously by other authors¹⁴. It is calculated as shown in Eq. (2).

$$F \text{ \& } EI = MF \cdot F_1 \cdot F_2 \quad (2)$$

where:

- MF stands as the Material Factor of the chemicals involved. Since the materials that enter the system and the ones that exit it are the same, i.e., not a chemical reaction is involved, this factor will remain constant for the whole system.
- F_1 stands as the General Process Hazards' factor. Its calculation involves the consideration of a series of penalty factors. In this case study, considering that the core chemicals and equipment will remain relatively unchanged among all the possible alternatives, it is considered that all

these penalties will remain the same between the different possible separation tasks. Thus, this factor will also remain constant.

- F_2 stands as the Special Process Hazards' factor. Like the General Process Hazards' factor, involves counting a series of penalty factors. Almost every penalty factor included in these calculations will remain constant between the possible separation tasks, except the G item, which involves a penalty to the inventory of the equipment.

The inventory in the F&EI stands for the amount of energy in the equipment or stream, and its calculation is shown in Eq. (3)

$$Inventory = \max \{W, mf_{\max}\} \cdot Hc \quad (3)$$

where W stands as the amount of chemical in the equipment. The amount of chemical in one hypothetical column has been defined as a percentage of the volume of that column. While most references recommend a height at the bottom of the column of 1 – 2 meters, considering the different diameters in the results, plus the different heights and number of trays with both vapor and liquid flowing through them, a value of a 30% of the volume of the column as inventory was assumed in this work. This can be still considered as a pretty conservative value since it is considering only the liquid phase chemical, which despite having the greatest weight when taken into account the inventory of a column, it is not the only factor we need to account for. The parameter $mf_{\max}$ refers to the maximum mass of chemical that exits the column in 10 minutes, assuming both a case where the leakage would be produced in the upper stages, with the fluid being mostly vapor or in the lower stages, with the fluid being mostly liquid.

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

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

While Eq. (4) is clearly non-linear, considering that it is a monotonically increasing function and that the Dow F&EI will be obtained for the whole sequence of tasks instead of obtaining one for each of the 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
$$ISI_{Dow} = \sum_{t=1}^T Inventory_t y_t \tag{5}$$

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
$$SW eHI = B / A \tag{6}$$

402 Similarly to the actual index, B is also composed of two components; B₁ and B₂. B₁ addresses the damage
403 that can be produced by the equipment due to fire and explosions while B₂ 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

with the mass flow, or with another property that can be translated from separated tasks to final columns, is a must to.

Eq. (7) and (8) show how to calculate those parameters, as found in the reference¹³.

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

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

These indexes are clearly non-linear. Thus, for each task, in a similar manner to the treatment given to the Dow's F&EI G item, we consider some changes considering that the index will be obtained for the distillation train and not for each individual column, and thus the exponent can be removed since these are monotonically increasing functions. This change is made by simplifying the equations into linear ones, shown in Eq. (9) and (10).

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

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

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

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

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

Notice now that the objective function is calculated with these linear approximations, but the data displayed in this paper has been then modified to have an appropriate value to compare with other processes, i.e., once performed the optimization with our linear modification, the value is then modified as it is intended in the original work, re-adding the exponents.

As explained before, in order for (9) and (10) to be linear, all their parameters must be linear either with the volume of the hypothetical column or the mass flows. A brief explanation of their calculation is next provided.

432 **B₁ penalties and core factors**

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

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

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

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

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 [m³]
- 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 B₁ 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).

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

if (fire point > process temperature > flash point)

$$pn_1 = 1.45$$

else if (0.75 autoignition temperature > process temperature > fire point)

$$pn_1 = 1.75$$

or if (process temperature > 0.75 autoignition temperature)

$$pn_1 = 1.95$$

else

$$pn_1 = 1.10$$

(16)

For these, we have to be able of calculating the flash point of a mixture of chemicals⁵⁶, although since the penalty is not extremely sensitive to the process temperature, a conservative approach of considering the lowest flash point of the compounds in the mixture as the flash point of the mixture is taken.

Its second penalty accounts for the pressure factor. It also decides whether F depends of F_2 , F_3 or both of them. It is calculated as shown in Eq. (17). Let AP be the atmospheric pressure in kilopascals:

if (VP > AP & P > VP)

$$pn_2 = 1 + ((P - VP) / P) \cdot 0.6$$

$$F = F_2 + F_3$$

otherwise

$$pn_2 = 1 + ((P - VP) / P) \cdot 0.4$$

$$F = F_2$$

if (AP > VP & P > AP)

$$pn_2 = 1 + ((P - VP) / P) \cdot 0.2$$

$$F = F_3$$

otherwise

$$pn_2 = 1.1$$

$$F = F_3$$

(17)

Its third penalty accounts for the weight of the chemical inside the equipment. This penalty is linear with the quantity of the chemical, although it has an independent term that may incur into an overestimation. Nevertheless, considering the ranges of inventories treated in this case study, it can be assumed that the error produced because of that is minimum. It is calculated as shown in Eq. (18)

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if $NF / NR = 1$
 $pn_3 = 1 + 0.003 \cdot W / 1000$
if $NF / NR = 2$
 $pn_3 = 1 + 0.005 \cdot W / 1000$
if $NF / NR = 3$
 $pn_3 = 1 + 0.008 \cdot W / 1000$
if $NF / NR = 4$
 $pn_3 = 1 + 0.010 \cdot W / 1000$

(18)

The effect of the chemicals' reactivity and flammability is assessed in the fourth penalty, as shown in Eq. (19).

$pn_4 = \max \{ 1, 0.30 \cdot [NF + NR] \}$

(19)

In both these penalties, the NF and NR parameters come from the National Fire Protection Association (NFPA) American standard ⁵⁷, which identify the risks posed by the different chemicals that the plant has. Since we have a mixture of different chemicals, a mean between the amounts of each chemical in the total of the column at the feeding point is performed, giving a bit more of sensibility to the index.

Penalties from fifth to eighth refer to events that are not accountable this early in design, such as social factors and environmental factors. Besides being unknown at this early stage, they would not vary between the different possible layouts and thus they were given a value of 1.

B₂ penalties and core factors

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

$G = S \cdot m_{spill}$

(20)

where S depends on the released conditions and m_{spill} is the amount of chemical that is expected to be released. Since we are calculating those parameters for every separation task, and the result should be consistent with any arrangement of tasks in a final number of columns, the amount of chemical that will be released has been considered as both the quantity that leaves that task from heads and from bottoms, added together. In doing so, we are considering the worst case scenario, where there are two spills from the most vulnerable points, being these the outlets of the tasks, both heads and bottoms.

Thus, it seems obvious that the basic configurations where there are more lateral outputs in the columns will get penalized by this index. The values of S can be seen in Table 2.

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

Its first penalty, in the same manner as the B_1 one, refers to the effect of the process temperature. If we are working with a flammable chemical, we use Eq. (16). If it is a toxic or corrosive chemical, Eq.(21). If it is both, which tends to occur in most of the cases, it must be assessed as the highest result of both.

$$\begin{aligned}
 &\text{if (process temperature } > 4 \times \text{ ambient temperature)} \\
 &\quad pnr_1 = 1.55 \\
 &\text{if (process temperature } > 2 \times \text{ ambient temperature)} \\
 &\quad pnr_1 = 1.35 \\
 &\text{else} \\
 &\quad pnr_1 = 1.1
 \end{aligned} \tag{21}$$

Likewise, its second penalty refers to the effect of the pressure. Since it only accounts for equipment whose are pressurized, this being, their pressures are higher than 3 atm, it was considered as 1 for all the possible tasks since we are working at atmospheric pressure.

Its third penalty accounts for the chemicals that are heavier than air, which take more time to disperse. Thus, the heavier the chemicals, the higher the penalization given to the task and to the final sequence with that task. Its calculation is shown in Eq. (22)

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

The fourth penalty is pretty straightforward, assessing the toxicity of the chemical and having a minimum of 1. It is obtained from Eq. (23)

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

Penalties five to seven, in the same way as the previously mentioned ones in the B_1 calculations, account for issues that are unknown at this design phase. Therefore, they are given a value of 1.

6. Objective reduction and results

For each task sequence, we have the following objectives; TAC , ISI_{B1} , ISI_{B2} and ISI_{Dow} . A Pareto frontier of these 4 objectives would provide all the information about the interconnection between these indicators, but its computational cost considering 10 values within the range of each objective would escalate to an order of 10^4 optimization problems to be solved, making its computational cost too high to be effective. Instead, we first obtain the sequences that optimize each objective individually. These are shown in Figure 5.

511

Figure 5: Possible optimal sequences for each mono-objective problem: 1) TAC, 2) B_1 , 3) B_2 , 4) F&EI.

It is interesting to note that, as expected, the optimal sequence in regards to the economic objective is the totally thermal coupled sequence, which has the lowest energy consumption. This result was already proven mathematically⁵⁸. In the case of the B_2 component of the SWeHI index, which takes into account toxicity and damage of releases, its optimal sequence is such that no thermal coupled task exists. This

agrees with the manner in which we calculated this index. The leakage points, which are considered in this index, are more prone to appear at the bottoms and heads of a column, where the streams exit its vessel. As such, when there exist thermally coupled columns, those have more exit points. In the case of Dow's F&EI and B_1 indexes, as they evaluate the flammability and explosion hazard in the equipment, their corresponding optimal sequences are an intermediate between fully thermally coupled and non-thermally coupled.

Next, we solve all the paired bi-objective problems using the ϵ -constraint method. The number of Pareto paired points are shown in Table 3.

Table 3: Number of Pareto Points obtained by solving all the bi-objectives 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

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

The Principal Component Analysis⁵⁹ is a statistical procedure based on the use of an orthogonal transformation to convert a set of points, which are expected to be correlated between them, to a series of uncorrelated linear variables, which are the principal components. The number of principal components is equal to the number of initial variables, in this case, objectives, but the normal praxis includes the consideration of a threshold. Each principal component explains a percentage of the points, so setting a threshold of 90-95 % tends to eliminate at least one of the principal components. This methodology allows the user to remove a number principal component below the threshold and as such, reduce the dimensionality in the space of the principal components. This, however, does not reduce the dimensionality in the original space of objectives, since these reduced principal components still need all the original objectives to be evaluated.

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

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:

1. Retain the amount of Principal Components that have an accumulated explained variance over a predefined threshold.
2. For those Principal Components, if the eigenvalue is less than 0.10, add to the subset of objectives the objective with the higher absolute value.
3. If the eigenvalue is higher than 0.1:
 - a. If all the components of the principal component are positive, add to the subset of objectives the objective corresponding to the highest value.
 - b. If all the components are negative, add all the objectives to the subset of objectives.
 - c. If none of the previous two cases apply:
 - i. If the most positive element is smaller than the 90% of the absolute value of the most negative one, add the most negative objective to the subset of objectives.
 - ii. If the most positive is bigger than the 90% of the absolute value of the most negative one, but smaller than the absolute value of the most negative one, add both the most negative and most positive to the subset of objectives.
 - iii. If the absolute value of the most negative is bigger than the 80% of the most positive, but smaller than the most positive, add to the subset of objectives both the most negative and most positive.
 - iv. If none of the previous cases apply, add to the subset of objectives the most positive one.
4. If the subset of objectives differs from the original set of objectives, make the subset the new original set and repeat the procedure.

Considering the threshold, we first set the initial set of objectives: $F_0 = \{B_1, B_2, \text{Dow's } F\&EI, TAC\}$ and the new set of objectives as a void set; $F = \{\emptyset\}$. Let mn be the most negative value and mp the most positive of given PC:

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

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

6.2 Elimination of objectives by maintaining the dominance

While Deb's algorithm may provide a good solution when the data is clearly centered on the first Principal Component, it lacks accuracy when the coefficient values of the PCA are similar, e.g., coefficients of B₂ and Dow's F&EI in the first PCA.

In addition, Deb's algorithm does not provide any information of the incurred possible error when an objective is eliminated. In light of this, another method of objective reduction, based upon MILP is studied³³. While the full-fledged explanation of the model can be seen in the reference, the basic idea is that chooses which objectives must remain to maintain the dominance structure within a given tolerance. The dominance structure can be represented as a parallel plot where we represent on the x-axis the objectives and in the y-axis the value of a number of solutions in these objectives. It allows the user to immediately visualize if there are any dominated solutions, or which objectives are keeping a solution from becoming dominated. It is thus, the relationships among the different solutions and its 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.

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.

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 $\delta=0.6$. In subset B, objective f_2 is removed but the dominance structure remains unchanged

Thus, we minimize the greatest error that we obtain in the dominance structure when we eliminate an objective. Using a binary cut strategy we obtain more solutions for that number of pruned objectives. Identically to the PCA strategy, we only need the data from Table 4 to solve the model. The output of the MILP provides the objectives maintained and the δ -error incurred when removing the rest of objectives. As it is expected, the solution with the lower δ -error is the one that breaks the least the dominance structure.

The results are shown in Table 7.

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

Thus, while a 6.8% of error is considered an acceptable approximation, if we want to let the system be reduced to 2 objectives we may incur into an error of a maximum of a 76.8%. From this perspective, we could only eliminate one objective, Dow's F&EI, without altering severely the dominance structure.

6.3 Results

Considering the difference between the methods utilized, it is considered that the reduction by dominance structure is the most reliable, since it includes a measure of the error resultant from removing an objective. As commented above, Deb's algorithm works very well when the data is heavily directed to one of the principal components. However, it is still a heuristic method. This means that when there are similar values in the principal components, as those shown in Tables 5 and 6, which objective gets removed is a less clear subject. Due to these two observations; the ability to obtain an error when removing objectives and the non-heuristic characteristic, it is decided to keep the reduced set of objectives that results from the δ -error model, instead of those which Deb's algorithm maintains. Whereas for Deb's algorithm the removed objective would be B_2 , for the δ -error model it would be Dow's F&EI. In this case study, Deb's algorithm shows clearly that the TAC can never be obviated, since there is a clear trade-off between it and any ISI, but it fails at recognizing which ISI should be removed. On the other hand, the method based on the dominance structure eliminates the Dow's F&EI objective, which does not change the dominance structure in an impactful manner, and as such it is considered as the best course of action.

These results can be explained by the maner in which these ISIs are calculated. Both for Dow's F&EI and B_1 , the amount of chemical in the equipment is a core factor. In the case of the Dow's, it is actually the whole differentiating factor among different alternatives, while the B_1 considers penalties and other parameters depending on various data, such as vapor pressure, temperature, etc. For this, it seems 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 factor is G, which is calculated from the streams exiting the columns. Thus, it will provide a different result than both B_1 and Dow's F&EI, which explains why it should not be eliminated in order to maintain the dominance structure.

Therefore, the reduced set of objectives is formed by the objectives B_1 , B_2 , and TAC. Once only three objective remains, the computational cost of calculating a new Pareto set of solutions is reduced. The

model is evaluated again with an epsilon constraint method in order to obtain all the Pareto optimal solutions. The results are shown in Figure 9. Every point in these graphs showcases an equally “good” different optimal solution. It is up to the designer to weight those three objectives in order to come with the desired design.

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

7. Conclusions

An alternative method to assess the inherent safety of a distillation train design is introduced. While the indexes here studied tend to be calculated for a piece of equipment, a consideration of the whole distillation train sequence as a unique piece of equipment whose economic and inherent safety performance is assessed.

From the results it can be extracted that it is possible to utilize some Safety Indexes as Inherent Safety Indexes, having enough data to perform the analysis at an early stage of the design. Some simplifications have been made into the case study, but the results allow the user to choose among alternative sequences of tasks with significant differences in the studied objectives.

Three methods to deal with the multi-objective optimization are compared. The PCA, which forms new objectives from the initial ones by lineal combination of those; Deb & Saxena's algorithm, which bases

the choice of objectives in the data obtained from the PCA; and our method based on the dominance structure, which aims to maintain and minimize the higher error produced in the structure when one objective is eliminated.

Results show that it is possible to apply those Safety Indexes in an early stage in design, acting then as Inherent Safety Indexes. In addition, the method based on the dominance structure shows that the inherent safety level of the design can be assessed with a unique safety index, with the considerations previously explained in the paper, this being the Safety Weighted Hazard Index. Notwithstanding, its consideration of choosing only the highest value between B_1 and B_2 could be argued, since they lead to noticeably different results.

While in this problem the need of maintaining a linear index was required due to the case study, it is recommended as a good practice for every other problem. Some of the indexes have strongly nonlinear, nonconvex calculations, that would diminish their utility as inherent safety indexes since its inclusion in the model would make the problem much more difficult to solve. Since the majority of Safety Indexes are applied only when all the information is given, i.e., the plant is finally built, they tend to not be additive, like Dow's F&EI. That is why in this work we adapt the safety indexes into a global index for the sequence and not one for each column.

It is worth mentioning that even with the number of objectives reduced, the amount of equally good Pareto solutions is pretty large. There are other strategies, such as the concept of Pareto efficiency of order k^{60} which can help the decision maker to diminish the number of options. Since that is not a 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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5 compounds

Train of distillation tasks

Economic objective

Safety objective