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Intensification for the Silane Production Involving Economic and Safety Objectives

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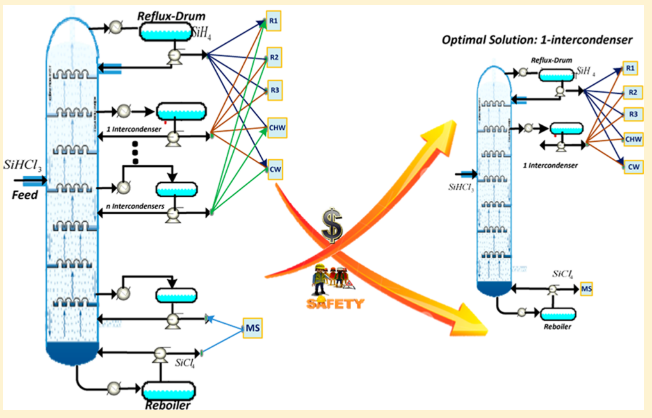
ABSTRACT: The use of conventional reactive distillation columns for silane production has the disadvantage of large consumption of refrigerant because the silane is produced in the dome of the column and this must be condensed at about −78 °C. The incorporation of intercondensers may improve the cost and safety of the system; however, a proper study for the system is needed to determine the associated effects. Therefore, in this paper is presented an optimization approach for the silane production accounting simultaneously for economic and safety issues incorporating intercondensers. The presented approach is based on a software link between Microsoft Excel (for implementing the optimization algorithm based on differential evolution), Aspen Plus (for simulating the process), and SCRI (for quantifying the associated risk). The results show that the addition of intercondensers minimizes the total annual cost, because the amount of needed refrigerant is reduced. The safety analysis also shows that the use of intercondensers improves the risk of the system.



1. INTRODUCTION

Nowadays the energy demands have been satisfied through fossil and nuclear fuels; however, the intensive use of these resources has damaged significantly the environment. Furthermore, the enormous population growth has increased the energy demand, which cannot be satisfied with only fossil resources to yield a sustainable process. This way, several renewable energy resources have arisen to currently represent 22.1% of global energy.[1] In this context, solar energy has gained a lot of attention because of the availability of this resource[2] as well as the improvement for the solar technologies.[3] The use of photovoltaic cells has been one of the most used technologies for concentrating solar energy. These systems are made of cells that have a covering of silicon (i.e., silane).[4,5] The research has focused on finding the optimal technologies for the production of silane. The most widely used process for the production of silane is the Siemens process; this has as its main disadvantage excessive energy consumption.[6] Reactive distillation (RD) has become an important option for the production of silane;[7] this alternative represents energy savings and the associated cost is reduced, because in the conventional process the use of a reaction-separation system is required whereas the RD process only requires the use of a single vessel.[8] The reduction of number of process units decreases the needed substances that present a hazard to cause accidents related to fire, explosion and toxic release. Minimizing inventories depicts an inherent safety strategy; this is also called process intensification. RD represents a clear example of this strategy. To simplify, substitution and moderation are other strategies that use inherent safety to reduce or eliminate the hazard. The simplification improves the process design, avoiding unnecessary complexity and reducing the opportunity to present errors.[9,10] Substitution refers to replacing hazardous substances to provide a lower risk.[11] Finally, moderation refers to the use of substances under conditions that prevent a high hazard;[12] an example is the use of diluted substances, low temperatures, and low pressures. When a conventional process is modified, it is necessary to know the involved risk through the implementation of an inherent safety approach. In this case, the addition of intercondensers in a reactive distillation column for the production of silane is a modification to the conventional process that may help to decrease the cost;[13,14] however, we also need to know the effect of this modification in the associated risk. The existing methodologies do not consider the effect of this change in risk, these only assess the economic

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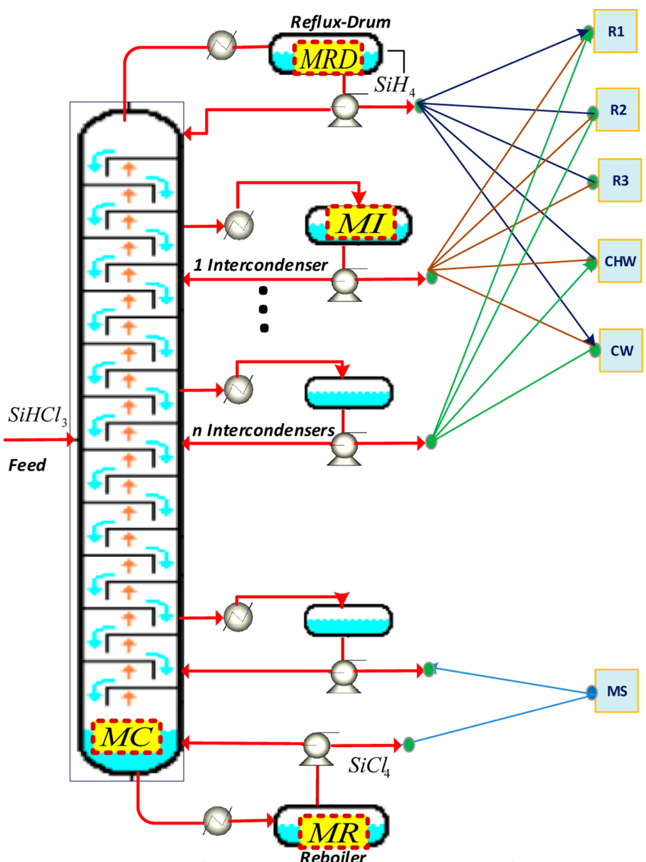
impact. Because the silane as well as their chemical precursors have flammable and explosive properties, it is attractive to know the effect on risk due to the addition of intercondensers in the production process. Thus, in this paper is presented an approach to determine the optimal number of intercondensers, as well as the optimization of the reactive distillation column and heat integration, involving a quantitative risk analysis (QRA). Furthermore, an inherent analysis is performed[15] to determine the inherent strategy that reflects the addition of intercondensers due to the behavior of the optimization variables.

2. PROBLEM STATEMENT

The addressed problem consists in determining the impact of the addition of intercondensers in the reactive distillation for the silane production on safety and cost,[14] Figure 1 shows the



$$TotalRisk = f\left(MC, MRD, MR, \sum_{n} MI_n \right)$$

Figure 1. Superstructure associated with column optimization and selection of refrigeration system.

proposed superstructure, where it is possible to see that pure trichlorosilane is fed, which is converted in silane through three reaction steps (eqs 1, 2, and 3). The silane then leaves the column at the top, while in the bottom the unreacted chlorosilane is removed. The removed silane must be condensed at about −78 °C, which implies the use of a refrigeration system that allows cooling the silane at temperatures below −78 °C. Conventional columns require high amounts of refrigerant, this leads to a great disadvantage in the cost. Thus, in the superstructure shown in Figure 1 is possible to see a conventional column, where are added intercondensers and interreboilers, this with the purpose of reducing excessive cooling costs. There are three cooling systems that can be used (R1, R2, and R3) in addition to CHW and cooling water (CW). For heating, medium pressure steam (MS) is available. Table 1 contains inlet and outlet temperatures as well as the

Table 1. Utilities Used for Cooling and Heating

utility	inlet/outlet temp (°C)	utility cost ($/MWh)
R1	−88/−88	151.94
R2	−30/−30	34.67
R3	−20/−20	28.4
CHW	5/15	15.95
CW	30/40	1.274
MS	160/160	50.58

cost of MS and cooling systems. This way, the optimization problem consists in finding the optimal number of intercondensers to add to the conventional column to minimize the cost; the column design and the selection of refrigeration systems are also objectives to consider in the optimization. Silane (SiH_4), dichlorosilane (SiH_2Cl_2), monochlorosilane (SiH_3Cl), and the precursor compound ($SiHCl_3$) exhibit hazard properties, which can result in accidents related to fire and explosion. The involved reactions are the following:

$$2SiHCl_3 \rightleftarrows SiH_2Cl_2 + SiCl_4 \quad (1)$$

$$2SiH_2Cl_2 \rightleftarrows SiH_3Cl + SiHCl_3 \quad (2)$$

$$2SiH_3Cl \rightleftarrows SiH_4 + SiH_2Cl_2 \quad (3)$$

Based on the analysis of the temperature profile for the column, it is possible to determine the best utilities for heat integration and the possible location of the intercondensers. Two important criteria are considered to determine the heat integration.[14] First, the heat removed or added at a stage in a rectifying or stripping section is not equal to the net condenser or reboiler duty reduction. Also, the heat removed or added at stages alters the vapor−liquid equilibrium composition; thus the temperature profile changes in the column. With this information, in Figure 2 it is possible to appreciate the case where 100 kW is removed at stage 16 and 300 kW at stage 18. It can be seen that despite that the CHW seems a candidate for using cooling utility at stage 16, actually it cannot be used to remove 100 kW because the temperature difference between the stage 3 and the CHW is lower than the ΔT_{min}. Similarly, CW cannot be used to remove 300 kW because the temperature difference between stage 18 and CW is lower than the ΔT_{min}. In addition, it is demonstrated that despite 400 kW being removed in the stripping section, only 384 kW is successfully removed at the condenser. It can be said that 16 kW is inefficiently removed at the condenser and it results in an increment in the reboiler duty. This way, a parametric study was performed prior to the thermodynamic optimization; in this study we performed an analysis for the temperature profiles in the column, allowing us to know the most appropriate stages in which intercondensers must be placed. When intercondensers are added, inventories of these compounds as well as the operating conditions can change depending on the number of added intercondensers, resulting in different levels of risk. Thus, the addressed problem involves the application of a quantitative risk analysis to the solutions obtained from optimization.

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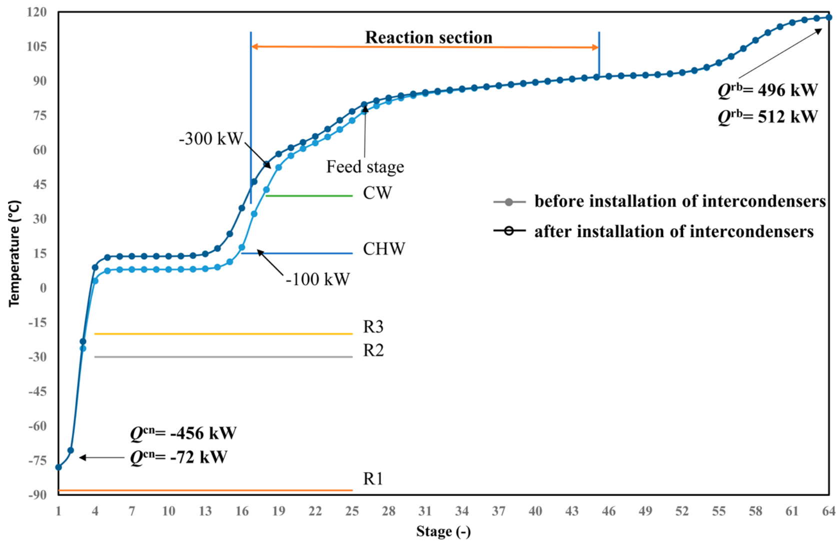

Figure 2. Temperature profile for the column with two heat-integrated stages.

3. OPTIMIZATION FORMULATION

Optimization Problem. The problem was formulated as a mono-objective optimization problem, where the objective is to minimize the operating cost (OC). Equation 4 shows the objective function; this takes into account the cooling ($C_j^{cool}Q_{i,j}^{ex}$) and heating costs ($C_i^{heat}Q_{i,j}^{ex}$). REC and STR are the set of stages in the rectifying and stripping subject to the installation of intercondensers and interreboilers, respectively. CU is the set of cooling utilities, and HU is the set of heating utilities. C^{cool} represents the cost of cooling utilities and C^{heat} corresponds to cost of heating utilities. $Q_{i,j}^{ex}$ is the amount of heat exchanged between heat sources HSO (i.e., HSO = REC ∪ HU) and heat sinks HSI (i.e., HSI = STR ∪ CU). OH represents the annual operating hours. Changes in the condenser and reboiler duties, due to heat integration at stages in a column, can be calculated through expressions that relate the heat removed or added at a stage and the effective condenser and reboiler duty reduction (eqs 5 and 6). Q_0^{cn} and Q_0^{rb} are the condenser and reboiler duties before any heat integration, finally Q^{cn} and Q^{rb} are those values resulted from heat integration at the different stages. Q^{SX} is the heat removed or supplied at stages i (rectifying) or j (stripping) by side exchangers, whereas ΔQ^{SX} is the respective compensation term at a given stage subject to heat integration. ΔQ^{SX} represents an indicator for the inefficiency in the condenser and reboiler duty reduction resulted from heat integration.

$$\min OC = OH\left(\sum_{\substack{i\in REC\\ j\in CU}} C_j^{cool}Q_{i,j}^{ex} + \sum_{\substack{i\in HU\\ j\in STR}} C_i^{heat}Q_{i,j}^{ex}\right) \tag{4}$$

$$Q^{cn} = Q_0^{cn} - \sum_{i\in REC}(Q_i^{SX} + \Delta Q_i^{SX}) - \sum_{j\in STR}(\Delta Q_j^{SX}) \tag{5}$$

$$Q^{rb} = Q_0^{rb} - \sum_{j\in STR}(Q_j^{SX} - \Delta Q_j^{SX}) + \sum_{j\in REC}(\Delta Q_i^{SX}) \tag{6}$$

The removed (rectifying section) or added heats (stripping section) result in an increase in the reboiler and condenser duties, respectively. The compensation terms, in the rectifying and stripping sections, due to the removed and added heats are calculated as follows:

$$\Delta Q_i^{SX} \approx \Delta\hat{Q}_i^{SX} = \max_{k\in PW}\{a_{k,i}\delta_i + b_{k,i}Q_i^{SX}\} \qquad i \in REC \tag{7}$$

$$\Delta Q_j^{SX} \approx \Delta\hat{Q}_j^{SX} = \max_{k\in PW}\{a_{k,j}\delta_j + b_{k,j}Q_j^{SX}\} \qquad j \in STR \tag{8}$$

PW is the set of segments in the piecewise linear function. $\Delta\hat{Q}^{SX}$ is a piecewise linear function that approximates ΔQ^{SX}. δ is a dummy variable, which is zero when Q^{SX} is zero, whereas a and b are parameters in the linear functions. The heat integration network between stages and heat sources is represented in the following equations. The removed heat through cooling utilities in the rectifying section is obtained by eq 9, whereas the added heat through heating utilities in the stripping section is represented by eq 10.

$$\sum_{j\in CU} Q_{i,j}^{ex} = -Q_i^{SX} \qquad i \in REC \tag{9}$$

$$\sum_{i\in HU} Q_{i,j}^{ex} = Q_j^{SX} \qquad j \in STR \tag{10}$$

The energy balances for the condenser and reboiler are obtained by eqs 11 and 12.

$$Q_1^{SX} = Q_0^{cn} - \sum_{i\in REC}(Q_i^{SX} + \Delta Q_i^{SX}) - \sum_{j\in STR'}(\Delta Q_j^{SX}) \tag{11}$$

$$Q_N^{rb} = Q_0^{rb} - \sum_{j\in STR'}(Q_j^{SX} - \Delta Q_j^{SX}) + \sum_{j\in REC'}(\Delta Q_i^{SX}) \tag{12}$$

where REC′ is the set of stages in the rectifying section excluding the condenser and STR′ is the set of stages in the stripping section excluding the reboiler. Because the stages are numerated from the top to bottom, the subscript 1 means the condenser location (top) and N is the reboiler location (bottom).

The logarithmic mean temperature difference (ΔT_{LM}) is used to determine the temperature driving force for heat

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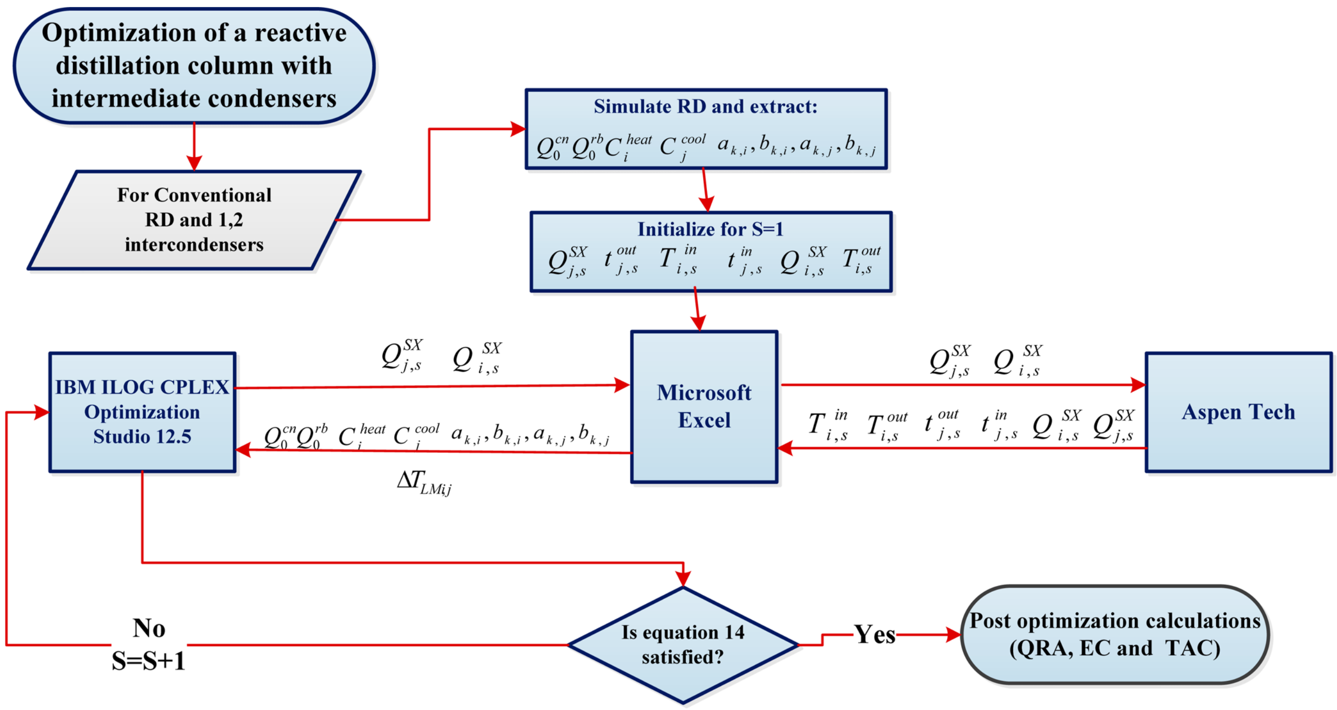

Figure 3. Solution algorithm.

transfer in heat exchangers, and it is used as a feasibility criterion for heat integration. Equation 13 represents the ΔT_{LM} between heat sources and sinks whereas eq 14 shows the feasibility criterion based on the "Big-M" formulation.

$$\Delta T_{\mathrm{LM}i,j} = \left\{ \frac{(T_i^{\mathrm{out}} - t_j^{\mathrm{in}}) - (T_i^{\mathrm{out}} - t_j^{\mathrm{in}})}{\ln[(T_i^{\mathrm{in}} - t_j^{\mathrm{out}})/(T_i^{\mathrm{out}} - t_j^{\mathrm{in}})]} \right. \quad \text{if} \quad \left. \begin{matrix} T_i^{\mathrm{in}} - t_j^{\mathrm{out}} \\ T_i^{\mathrm{out}} - t_j^{\mathrm{in}} \end{matrix} \quad i \in \mathrm{HSO},\ j \in \mathrm{HSI} \right\} \tag{13}$$

T^{in} and T^{out} are inlet and outlet temperatures of the heat source i whereas t^{in} and t^{out} are inlet and outlet temperatures of the heat sink j. ΔT_{min} is the minimum allowed temperature difference, and M is a big positive value. It is necessary to add an equation that eliminates all infeasible heat exchanges (eq 14).

$$Q_{i,j}^{\mathrm{ex}} - M\Delta T_{\mathrm{LM}i,j} \le 0 \qquad i \in \mathrm{HSO},\ j \in \mathrm{HSI} \tag{14}$$

An additional constraint to enforce a determined number of heat exchangers in the rectifying and stripping sections is needed:

$$\sum_{\substack{i\in \mathrm{HSO}\\ j\in \mathrm{HSI}}} Y_{i,j}^{\mathrm{ex}} \le N^{\mathrm{ex}} \tag{15}$$

In the above constraint, $Y_{i,j}^{\mathrm{ex}}$ is a binary variable, which becomes 1 if a heat exchanger is installed between a heat source i and sink j, and 0 otherwise. N^{ex} is a parameter that limits the maximum number of heat exchangers to be installed.

Equation 16 allows determining the optimal location of the exchangers in feasible heat exchanges.

$$Q_{i,j}^{\mathrm{ex}} - Y_{i,j}^{\mathrm{ex}} Q_{\mathrm{max}}^{\mathrm{ex}} \ge 0 \qquad i \in \mathrm{HSO},\ j \in \mathrm{HSI} \tag{16}$$

Solution Strategy. The model was solved using the software Aspen Plus V.8 and the optimization software IBM ILOG CPLEX Optimization Studio 12.5. Microsoft Excel was used to link these software. Figure 3 shows the optimization block, where the algorithm starts with the simulation of the RD in Aspen Plus. From this simulation, the values extracted are Q_0^{cn}, Q_0^{rb},C_i^{heat}, C_j^{cool}, $a_{k,i}$, $b_{k,i}$, $a_{k,j}$, and $b_{k,j}$, and these values are used to propose the initial values for optimization in IBM ILOG CPLEX Optimization Studio 12.5. $\Delta T_{\mathrm{LM}i,j}$ is obtained in Microsoft Excel. Equation 17 (where ϕ is a small number) represents the convergence criterion used; if this is not satisfied, the values obtained from the optimization are converted into the input data of the simulation. The process is repeated until it reaches convergence. Table 2 shows the parameters required for the optimization and postoptimization calculations.

$$\sqrt{\sum_{i\in \mathrm{REC}} (Q_{i,s}^{\mathrm{SX}} - Q_{i,s+1}^{\mathrm{SX}})^2 + \sum_{i\in \mathrm{REC}} (Q_{j,s}^{\mathrm{SX}} - Q_{j,s+1}^{\mathrm{SX}})^2} \le \phi \tag{17}$$

Equations 18 and 19 represent the temperature reduction in the rectifying section due to the installation of intercondensers by taking the minimum temperature value at each stage through all the iterations, whereas eqs 20 and 21 represent the temperature increase in the stripping section due to the installation of interreboilers by taking the maximum temperature value at each stage through all the iterations.

$$T_i^{\mathrm{in}} = \min\{T_{i,s}^{\mathrm{in}}\} \qquad i \in \mathrm{REC} \tag{18}$$

$$T_i^{\mathrm{out}} = \min\{T_{i,s}^{\mathrm{out}}\} \qquad i \in \mathrm{REC} \tag{19}$$

$$t_j^{\mathrm{in}} = \max\{t_{j,s}^{\mathrm{in}}\} \qquad j \in \mathrm{STR} \tag{20}$$

$$t_j^{\mathrm{out}} = \max\{t_{j,s}^{\mathrm{out}}\} \qquad j \in \mathrm{STR} \tag{21}$$

The risk and the cost of equipment are calculations that are performed at the postoptimization stage. The cost calculations

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Table 2. Optimization and Postoptimization Parameters

concept	value[a]
M (−)	50
OH (h/year)	8500
PB (year)	10
U^{cn} [kW/(m^2 K)]	0.568
U^{rb} [kW/(m^2 K)]	0.454
A^{cn}_{min} (m^2)	3
A^{rb}_{min} (m^2)	10
ΔT_{min} (K)	8
$Q^{ex}_{maxi,j}$	450
N^{ex} (−)	[2, 3, 4]

[a]The values of $Q^{ex}_{max1,j}$ $j \in CU$ and $Q^{ex}_{maxi,N}$ $i \in HU$ were set to 1000 to warranty feasibility in the condenser and reboiler of the conventional reactive distillation column.

were based on the Guthrie method.[16] Equations 22 and 23 are used to calculate the condenser, intercondensers, reboiler, and interreboilers.

$$A^{cn}_{i,j} = \frac{Q^{ex}_{i,j}}{U^{cn}(\Delta T_{LMi,j} + \varepsilon)} \qquad i \in \text{REC}, j \in \text{CU} \tag{22}$$

$$A^{rb}_{i,j} = \frac{Q^{ex}_{i,j}}{U^{rb}(\Delta T_{LMi,j} + \varepsilon)} \qquad i \in \text{HU}, j \in \text{STR} \tag{23}$$

A^{cn}_{ij} and A^{rb}_{ij} are the heat transfer area for condensers and reboilers, U^{cn} and U^{rb} are the overall heat transfer coefficients for condensers and reboilers, and ε is a small value to avoid a division by zero if the heat exchange is infeasible.

The equipment cost is computed by using eq 24, which takes into account the cost of the column C^{col}, tray cost C^{tray}, and cost of heat exchangers including the top condenser and bottom reboiler. The total annual cost (TAC) (eq 25) represents the sum of the cost of the equipment plus operating costs, in this equation PB is the payback time.

$$\text{EC} = C^{col} + C^{tray} + \sum_{\substack{i \in \text{HSO} \\ j \in \text{HSI}}} C^{ex}_{i,j} \tag{24}$$

$$\text{TAC} = \text{EC}/\text{PB} + \text{OC} \tag{25}$$

4. QUANTITATIVE RISK ANALYSIS

It is necessary to mention that the QRA is a postoptimization calculation. Figure 4 shows the steps of the QRA. The computation of QRA starts with the identification of potential incidents, for this step HAZOP[17] is applied. The potential incidents that may occur in a RD are instantaneous and continuous release (an incident is the loss of matter and energy). The second step aims to define the conditions under which the incident occurs as well as potential accidents that may occur. The consequence is evaluated as a function of accidents. Each incident may evolve in different accidents. The event tree provides the expected accidents from an incident (Figure 5). In accordance with the event tree, potential accidents that may occur are boiling liquid expanding vapor explosion (BLEVE), unconfined vapor cloud explosion (UVCE), jet fire, and flash fire. For calculations of physical variables caused by accidents (overpressure and radiation), it is considered the total mass of the column (MC), the mass in the reflux drum (MRD) and the reboiler (MR). For RD, if intercondensers are included, it is necessary to consider the mass of these (MI) in calculating the physical variables of accidents (Figure 1). The calculation of the physical (radiation and overpressure) and dispersion variables were performed with the software SCRI.[18] The worst scenario was considered for calculating the dispersion, as well as a wind speed of 1.5 m/s^2 and atmospheric stability type F.

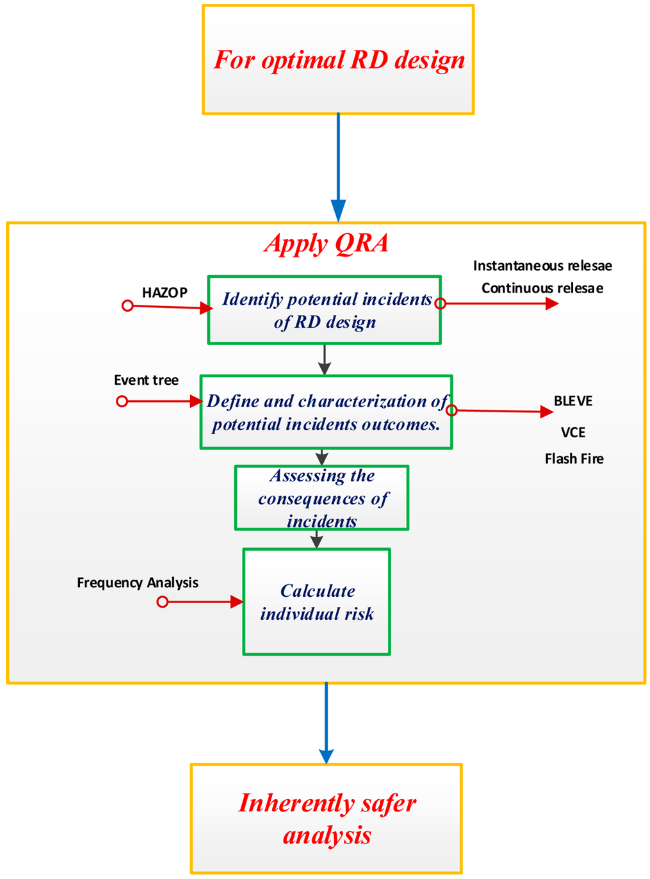

Figure 4. Implemented quantitative risk analysis.

The consequence assessment consists in finding the probability of damage that these accidents cause to other facilities or personnel. To calculate the damage that the physical variables cause, a vulnerability Probit model is used. In this work, the damage to people was considered and Probit functions related to death from container hemorrhage were used due to overpressure and deaths from third degree burns due to radiation.[19] The probability of damage is obtained by substituting Probit values in eq 28:

$$Y = -77.1 + 6.91 \ln(p^{\circ}) \tag{26}$$

$$Y = -14.9 + 2.56 \ln(t_e I^{4/3}/10^4) \tag{27}$$

$$P_{x,y,i} = 50\left[1 + \frac{Y+5}{|Y-5|} \operatorname{erf}\left(\frac{|Y-5|}{\sqrt{2}}\right)\right] \tag{28}$$

For the frequency and probability analysis, an event tree is used. The initial frequencies were extracted from the purple book.[20] The risk quantification is done in terms of individual risks. Individual risk is the risk that a person has based on its position, which represents a damage of a given magnitude and frequency due to the effects of physical variables, caused by the

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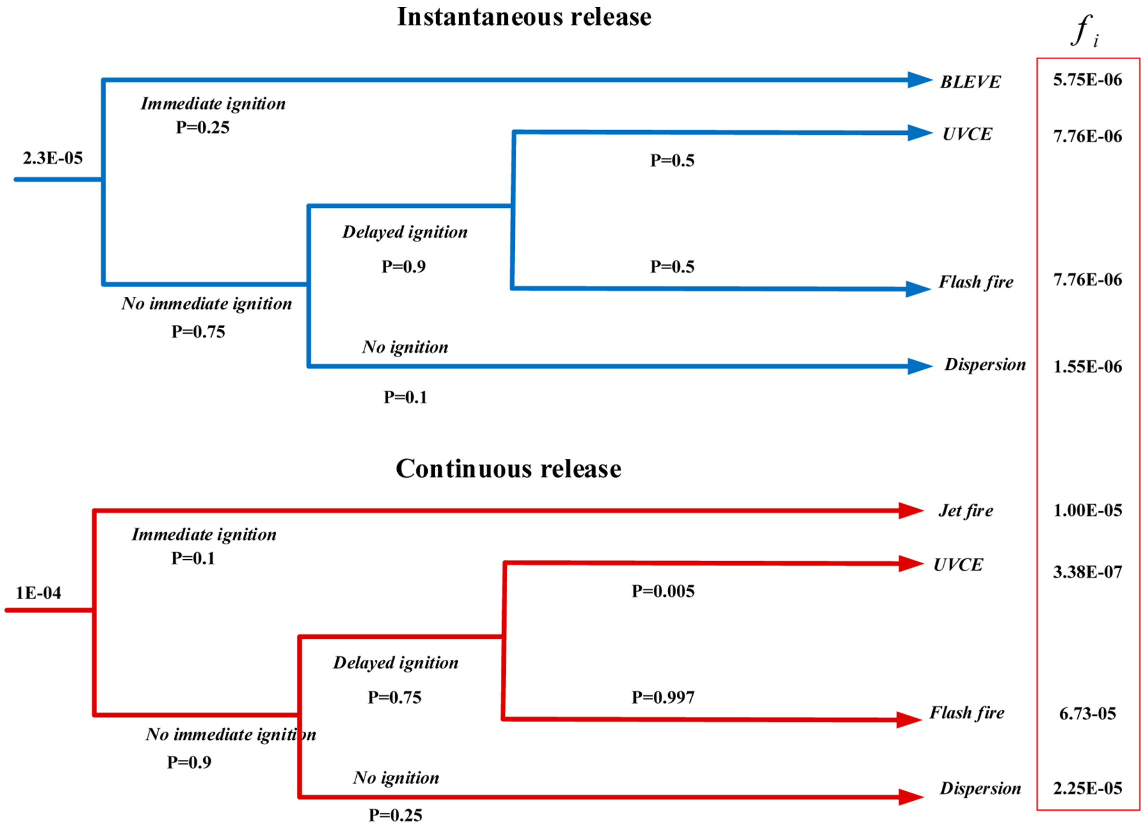

Figure 5. Event tree for reactive distillation.

occurrence of an accident. This risk is independent of the number of people exposed. According to eq 29, the individual risk in the position (x, y) is determined by multiplying the probability of affectation caused by an accident $(P_{x,y,i})$ and the frequency of an accident f_i. Three columns were analyzed, a conventional reactive distillation column RD, an intercondenser and two intercondensers. The characteristics of these columns are shown in Table 3 (reflux ratio, mass flows to the condenser, reboiler, and intercondensers). To calculate the reboiler inventories and condensers, holdups of 6 and 12 min were considered, respectively.[21]

Table 3. Column Design Conditions

column	feed flow rate (kg/s)		reflux ratio
conventional RD	condenser	1.24	54.47
	reboiler	3.52	
1 intercondenser	condenser	0.06	1.80
	reboiler	3.52	
	1 intercondenser	1.15	
2 intercondenser	condenser	0.11	3.80
	reboiler	4.51	
	1 intercondenser	0.29	
	2 intercondenser	2.12	

$$\mathrm{IR}_{x,y} = \sum_{i=1}^{n} f_i P_{x,y,i} \tag{29}$$

5. RESULTS

The optimization results show that the addition of an intercondenser reduces the TAC 54% due to the reduction in cold utility cost. A second intercondenser in the conventional column results in a TAC of 68.921 \$/year, which involves a saving in the TAC of 472 052 \$/year compared with the conventional column, in which the cost is 840 973 \$/year. When intercondensers are added to the conventional column, the equipment cost (EC) decreases (as it is shown in Table 4);

Table 4. Optimal Results

solution	costs	value	total individual risk (year^{-1})
$N^{ex} = 2$	EC (\$)	390 980	1.06×10^{-05}
conventional RD	$\sum_{i \in REC, i \in CU} C_j^{cool} Q_{i,j}^{ex}$	588 613	
	TAC (\$/year)	840 973	
$N^{ex} = 3$	EC (\$)	387 988	1.02×10^{-06}
1 intercondenser	$\sum_{i \in REC, i \in CU} C_j^{cool} Q_{i,j}^{ex}$	134 173	
	TAC (\$/year)	386 234	
$N^{ex} = 4$	EC (\$)	429 375	4.46×10^{-06}
2 intercondensers	$\sum_{i \in REC, i \in CU} C_j^{cool} Q_{i,j}^{ex}$	60 012	
	TAC (\$/year)	368 921	

this is due to the reduction in the cold utility cost, where the conventional column has a cooling of 588.613 \$/year, for the column with an intercondenser this value decreases by 77%. The column with two intercondensers is the most attractive from the economic point of view. For the risk assessment, the associated radiation, overpressure, and dispersion were determined for each column. The results show that radiation

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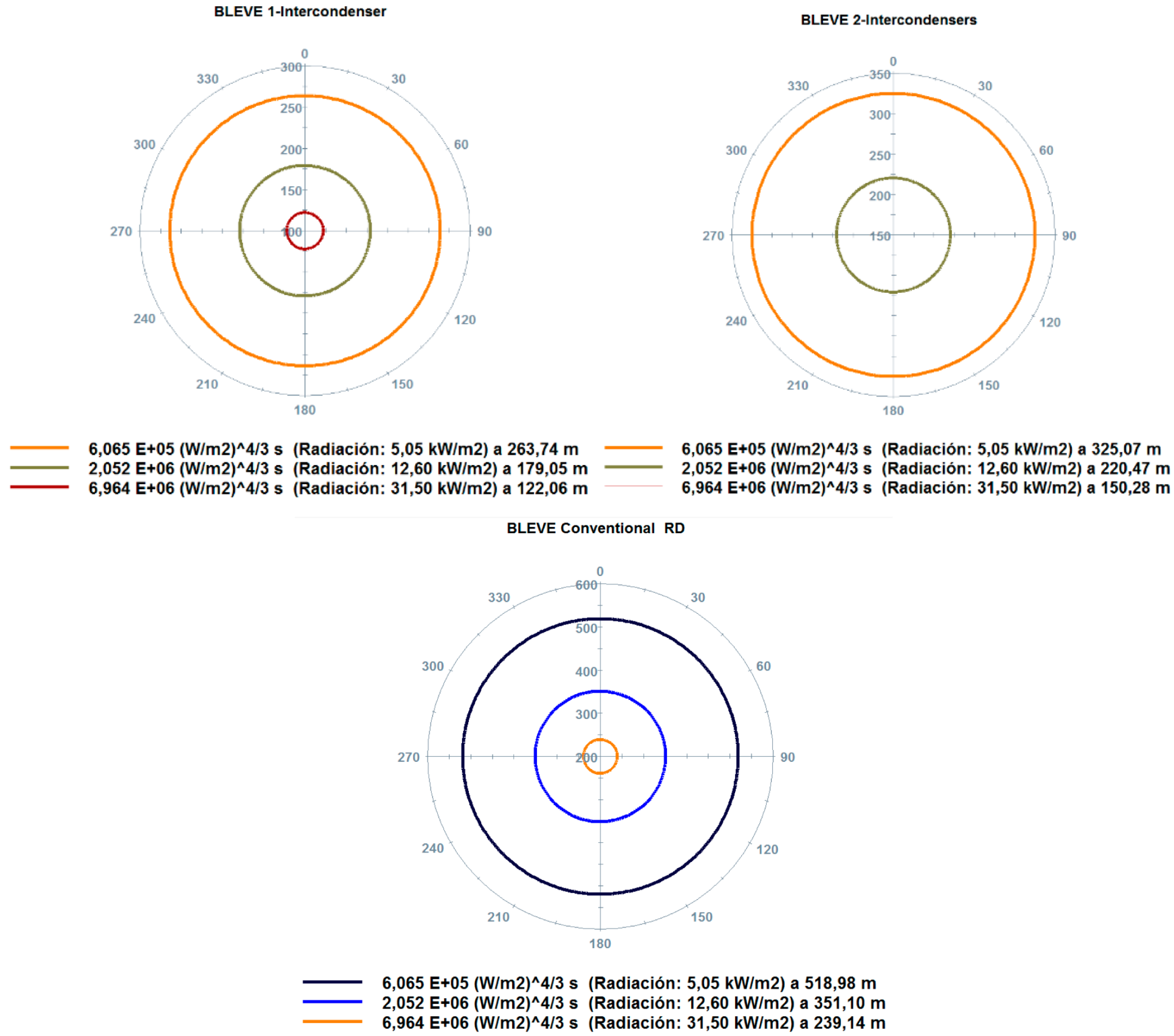

Figure 6. Isoradiation curves due to BLEVE.

has a significant impact on the affected area, which is shown in Figure 6, where the isoradiation curves due to BLEVE are shown for each column. Each curve represents a value of radiation for a probability of death by100%, 50%, and 0%, due to the radiation exposure. Moreover, overpressure has a lower impact. Figure 7 shows that the overpressure profile for a distance of 61.33 m has a probability of 90%; this result is due to operating pressures of the columns, which operate at 5 atm. The individual risk was calculated at a distance of 100 m for the three columns, with respect to just one isorisk value.

The results for the total individual risk are presented in Figure 8, where the total annual cost and the total individual risk are plotted. The column that resulted with the greatest risk was the conventional one (RD). At a value of 1.06×10^{-05}, this column also presents the greatest cost. The reason for the increased risk is due mainly to the value of the reflux ratio, which yields a greater column and consequently a greater amount of inventories. When an intercondenser is added to the conventional column, the reflux ratio and the flow to the main condenser decrease; thus the risk decreases to a value of 1.02×10^{-6}. As shown in Figure 1, the total mass in an instant release considers the sum of the mass of the column, reboiler, condenser, and all intercondensers; this way, in the column where the intercondenser is added, there is 828 kg of flammable mass. Even with the added mass, due to the addition of an intercondenser, the risk of the column with an intercondenser is lower with respect to the conventional one; the reason is associated with the value of the reflux ratio.

If two intercondensers are added, the reflux ratio decreases to 3.8 related to the reactive distillation column (54.47); however, this value is still higher than the column with an intercondenser (1.8), proving a higher risk compared with an intercondenser column.

The effect of the addition of intercondensers in the column is reflected in the risk and cost, which decrease simultaneously. The reflux ratio is one of the main optimization variables involved in the cost and risk; high values imply a greater risk, whereas low reflux ratios represent low risks. Furthermore, low reflux ratios impact the formation of silane.

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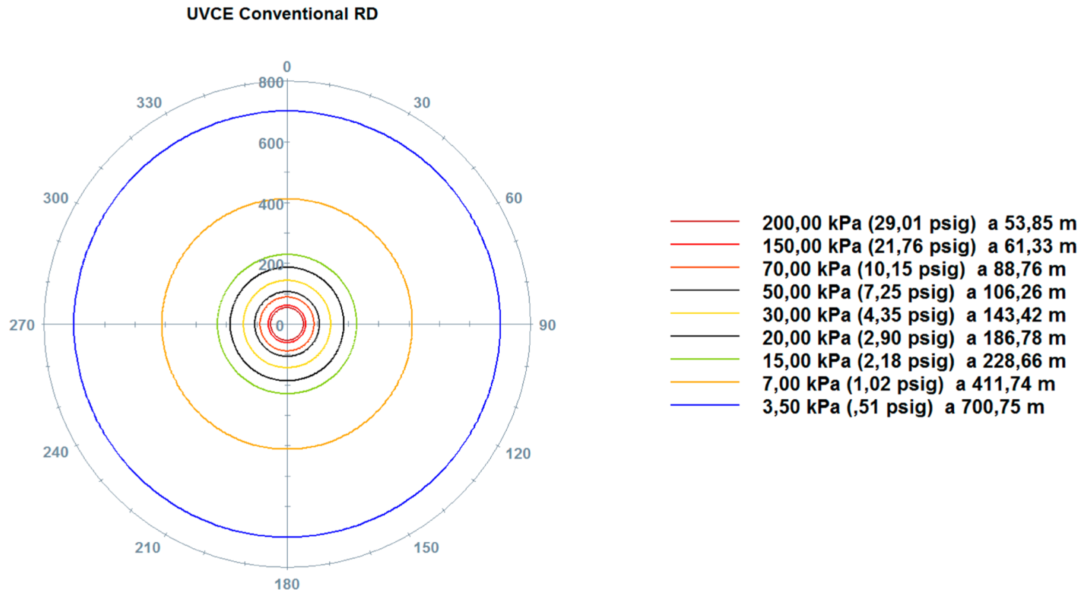

Figure 7. Overpressure curves for RD.

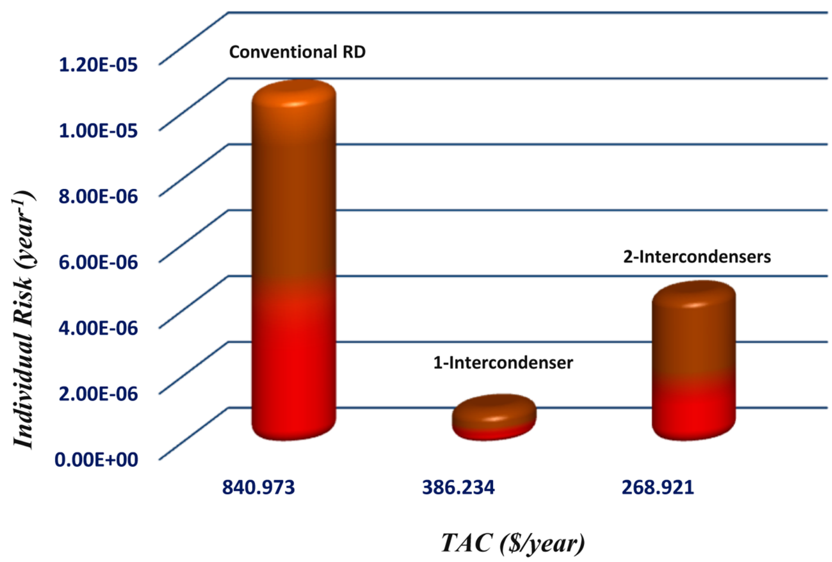

Figure 8. Total individual risk and TAC.

As mentioned earlier, inherent safety strategies involve minimization, moderation, substitution, and simplification. The addition of intercondensers represents an application of the minimization strategy, because the reflux ratio decreases (Table 3); if this ratio decreases, the size of the column also decreases, thus giving smaller inventories.

6. CONCLUSIONS

This paper has presented a study for the optimal production of silane involving different intensified designs, which include conventional columns, reactive distillation columns, and columns with intercondensers, where the operating conditions are optimized, and simultaneously includes a quantitative risk analysis for determining the associated risk. The results have shown that the addition of intercondensers to conventional columns for the production of silane impacts a higher proportion the cooling cost. The proposed approach has shown that the addition of two intercondensers is the optimal economic option; however, the quantitative risk analysis shows that the addition of an intercondenser is the safest option. However, the risks for the columns with one and two intercondensers are lower than for the conventional one. Adding the intercondensers decreases the size of the column and consequently the risk, thereby minimizing the inventory. This strategy corresponds to the inherent safety approach being a clear example of the application of the minimization strategy. The application of the quantitative risk analysis represents an additional selection criterion, ensuring balanced designs for cost and risk.

It is recommended to implement an entropy minimization and an exergy analysis in a future work. In addition, the implemented process is general and it can be applied to other cases, where only the data for the inventories, operating conditions, and the properties of the substances involved in the process (toxicity, flammability and explosiveness) are needed for the safety analysis. Furthermore, the optimization approach can be applied to other cases for a fixed flowchart and with a

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low number of manipulated continuous variables for the proper use of the heuristic search algorithm.

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Notes

The authors declare no competing financial interest.

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