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Simultaneous structural and operating optimization of process flowsheets combining process simulators and metaheuristic techniques: The case of solar-grade silicon process

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ABSTRACT

This paper presents a new optimization approach for the simultaneous structural optimization of process flowsheets with the operating conditions through combining process simulators with metaheuristic techniques. The proposed approach allows optimization of a superstructure in process simulators and reduce the computation time. A superstructure for different configurations for producing solar-grade silicon is considered, which includes three different configurations for solar-grade silicon production (Siemens Process, Intensified FBR Union Carbide Process, and Hybrid Process). The operating conditions with major impact in the performance of each of the proposed configuration were considered as decision variables. The improved multi-objective differential evolution (I-MODE) algorithm was selected as search method from others metaheuristic techniques because its efficiency to solve multi-objective problems in a short central process unit (CPU) time. The optimization algorithm consists in linking the process simulator software Aspen Plus^{TM} with the metaheuristic technique. The results offered attractive options for the considered objective functions in the addressed case study.

1. Introduction

The proper use of natural and energy resources has gained a fundamental relevance to satisfy the demands of the modern lifestyle in current population growth (Pérez-Lombard, 2008). Therefore, it is necessary to propose optimization strategies where it is guaranteed that the limited resources are used in the best possible way (Pimentel et al., 1994). Many alternative solutions have been proposed to reduce the environmental problem through the study of different industrial processes (Bamufleh et al., 2013), supply chains (Domínguez-García et al., 2017), habitational complexes (Núñez-López et al., 2018), solid waste management (Diaz-Barriga-Fernandez, 2018), distributed multiproduct biorefineries (Santibañez-Aguilar et al, 2014) and water, food and power grids (González-Bravo et al., 2018), among others.

The traditional optimization for the production processes usually involves the simultaneous selection of the flowsheet as well as the corresponding operating conditions (González-Bravo et al., 2017). The optimization techniques that are currently used in all these studies are based on mathematical programing (Ponce-Ortega et al., 2008) and deterministic optimization (Ponce-Ortega & Santibañez-Aguilar, 2019), whose formulation usually corresponds to mixed-integer non-linear programming problems (Costa &Oliveira, 2001) that are formulated based on a superstructure (Yeomans & Grossmann, 1999) through disjunctive programming formulations (Grossmann & Ruiz, 2012).

Mathematical programming techniques have as main limitation the availability to produce optimal solutions in non-convex problems (Coello-Coello et al., 2002), and frequently is not possible even to find a feasible solution (Devillers, 1996). The involved relationships in simulating the units in chemical and process industries frequently involve high non-linear and non-convex formulations (Harjunkoski et al., 1998); therefore, process simulators have included alternative solution approaches through sequential modular strategies (Sandler, 2015), where the involved units are simulated sequentially to find a feasible solution (Biegler et al., 1997).

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Nomenclature

CF	Crossover Fraction
ChiTC	Chi-square Termination Criteria
CPU	Central Process Unit
DE	Differential Evolution
EP	Entire Production
F	Mutation Fractions
F1	Emissions Factor (1.3 lb/btu)
F2	Efficiency Factor (0.85)
I-MODE	Improved Multi Objective Differential Evolution
MIDACO	Mixed Integer Distributed Ant Colony Optimization
MINLP	Mixed-Integer Non-Linear Programming
MNG	Maximum Numbers of Generations
MOEA/D	Multi-Objective Evolutionary Algorithm based on Decomposition.
NA	Not apply
PS	Population Size
SP	Sale Price
SSTC	Steady State Termination Criteria
TE	Entire CO_2 Emissions
TI	Total Income
TLS	Taboo List Size
TP	Total Profit
TR	Taboo Radius
VBA	Visual Basic for Applications

This way, very powerful process simulators are available to simulate different types of processes (Dimian, 2003) including chemical processes (Husain, 1986); however, the main limitation of these process simulators is that only a specific process (specific units and their interconnections) can be analyzed but the optimization is not allowed (Martin-Martin, 2019) because the involved units are considered as black-boxes (Capitanescu et al., 2015), whose relationships cannot be manipulated. Recently, process simulators have incorporated optimization tools, where in addition to a sensitivity analysis it is possible to establish some objective functions. However, these optimization tools incorporated in commercial simulation software are usually very limited (Segovia-Hernández & Gómez-Castro, 2017) because allow the manipulation of a single degree of freedom, mono-objective and local optimization (limited optimization tools) and the main disadvantage implies that the structural optimization is not allowed (Gutiérrez-Antonio & Briones-Ramírez, 2010).

To improve the performance of the used optimization tools in the commercial process simulators (Najim et al., 2004), the use of metaheuristic algorithms (Sharma & Rangaiah, 2016), nature inspired cooperative strategies (González et al., 2010) and nature-inspired optimization algorithms (Yang, 2014) through external links with process simulators has been proposed (Hernández-Pérez et al., 2019); this way, several metaheuristic approaches have been considered such as genetic/quadratic search algorithm (Jang et al., 2005) and parallelization strategies for rapid and robust evolutionary multi-objective optimization (Tang et al., 2007) together with different process simulators (Lim et al., 1999).

Differential Evolutionary (DE) is an evolutionary algorithm that was developed to handle optimization problems. DE algorithm has been used for solving chemical engineering problems (Dragoi & Curteanu, 2016). For example, Errico et al. (2017) integrated synthesis and differential evolution in a methodology for design and optimization of distillation processes, Miranda-Galindo et al. (2014) used stochastic multi-objective optimization algorithms to hydrodesulfurization process of diesel, Quiroz-Ramírez et al. (2017) applied a multi-objective stochastic optimization to a hybrid process production-separation in the production of biobutanol, Wong et al. (2016) used elitist non-dominated sorting genetic algorithm with termination criteria to design of shell-and-tube heat exchangers for multiple objectives, Ho-Huu (2018) reported an improved Multi-Objective Evolutionary Algorithm based on Decomposition (MOEA/D) for bi-objective optimization problems with complex Pareto fronts applicated to structural optimization. Hernandez-Perez et al. (2020) optimized the methanol production process from shale gas using an evolutionary algorithm. However, the main limitation that only the operating conditions are optimized still remind.

Simultaneous optimization of discrete structures with process operating conditions is well-studied in literature. For example, Grooss and Roosen (1998) proposed process optimization using evolutionary algorithms; however, hybrid optimization algorithms based on differential evolution have been developed to be more efficient in solving problems in which conventional metaheuristic tools can be trapped in a local optimum or consumed too much computing time. On the other hand, the direct search methods mentioned by Lang and Biegler (1987), such as SQP (Successive Quadratic Programing), are a class of methods for finding a local optimum to nonlinear constrained optimization problems, but nonlinear programming does not guarantee the solution of highly non-convex problems. Likewise, the metaheuristic design framework by Geraili et al. (2014) presented a modeling approach for designing energy systems applicated to biorefineries; however, it did not include a strategy for the optimization of multiple simulations in which different configurations of the process flowsheet is possible.

Zhao et al. (2018) proposed a superstructure optimization within ProSimPlus simulator using an external metaheuristic optimizer called Mixed Integer Distributed Ant Colony Optimization (MIDACO). ProSimPlus is a process engineering software that performs rigorous mass and energy balance calculations for a wide range of industrial steady-state processes (prosim.net). However, it is a little known and less used commercial simulator compared to Aspen Plus. MIDACO is a global optimization software (Schlueter, 2009) based on extended ant colony optimization (Schlüter et al., 2009) for non-convex Mixed-Integer Non-Linear Programming (MINLP). On the other hand, Improved Multi-objective Differential Evolution (I-MODE) is a new approach to solve multi-objective optimization based on basic DE (Sharma and Rangaiah, 2013). DE is a simple algorithm, but it has been successfully applied to selected real world multi-objective problems (Fan et al., 2008). The I-MODE algorithm is equipped with contour line to select candidate individuals, and combines with the crowding distance sorting and Pareto-based ranking, and epsiv dominance. The I-MODE code is developed in Visual Basic for Application (VBA), so it can be easily manipulated since Micosoft™ Excel.

One important point is that the linking between process simulators usually allows optimizing the operating conditions, and the main contribution of the present optimization approach is to combining process simulators with metaheuristic techniques for simultaneous optimization of process flowsheets with the corresponding operating conditions. This paper proposes a method through which it is possible to analyze simultaneously multiple configurations of the same process; this way, it can find the optimal solution without the need of simulating each case with every set of values. This implies a considerable saving in the computational time since only the configurations with the best performance will take part in next generations displacing the configurations with the worst objective function values. In a conventional way to search an optimal solution, it is necessary to simulate each configuration with possible sets of values until a termination criterion is reached, which consumes a considerable computational time. However, with the method proposed here, it is possible to find the best operating val-

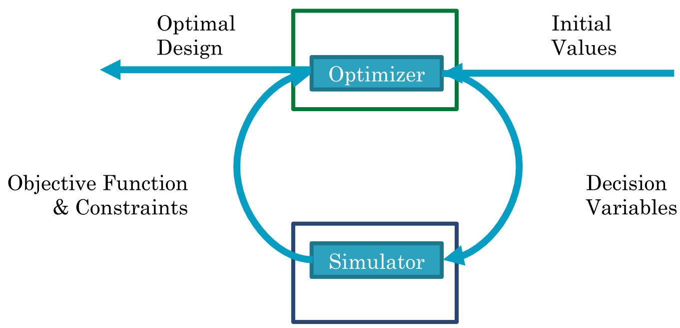

Fig. 1. Conventional single-case optimization framework.

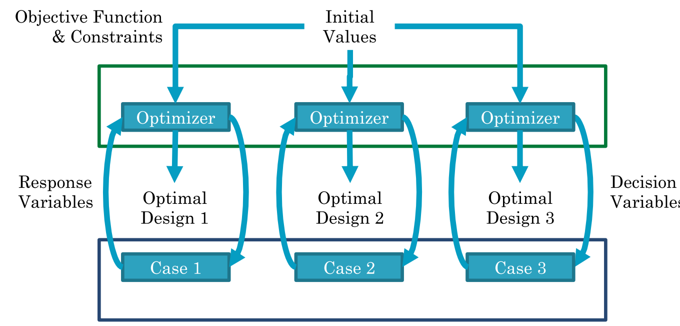

Fig. 2. Optimization framework where multiple configurations are possible.

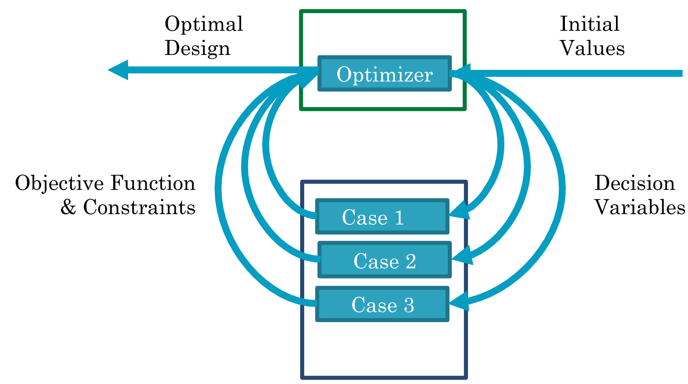

Fig. 3. Multi-case optimization framework.

ues in the best configuration in the equivalent computation time to perform the search in a single case.

The Solar-Grade Silicon Process (SGSP) was selected as case study to use the proposed optimization method, where different configurations of the same process can be optimized simultaneously to determine the optimal structure and operating conditions. The case of the solar-grade silicon production process is not very large in terms of the number of possible configurations; however, it is very useful to explain the proposed methodology and follow the manipulation of the variables and present the necessary code for the call of the files that contain the simulation. The difference between each configuration depends on the order for units, the connection for streams and the used technology. The SGSP involves different stages and there are several alternatives for the production of this silicone. The most important ones are the Siemens Process, the Intensified FBR Union Carbide Process, and the Hybrid Process, each of which has been analyzed and previously reported (Ramírez-Márquez et al., 2019). However, these previous works have focused on the design part of the separation columns without considering the search for the best operating conditions of the involved reactors. Although the SGSP has been previously addressed, in this work the simultaneous structural and operating conditions for the considered process are optimized to reduce the computational time and improve the obtained solutions through a new methodology.

2. General optimization approach

In a general way, the reported optimization approaches for process flowsheets through metaheuristic strategies consist in linking a process flow diagram previously specified in a commercial simulation program, and subsequently, using a controller program, search variable values are exported to the simulator and the response variable values are imported after running the simulation (as shown in Fig. 1). A search variable (also called a decision variable) is one whose specification exhausts a degree of freedom in the mathematical model in the process simulator, the value will be randomly changed by the algorithm in order to explore better solutions. A response variable is one that is obtained as a result of the operations that correspond to the mathematical model of the process simulator and its value is dependent on the value of the search variables. The strategy of a stochastic optimization algorithm is to manipulate the value of the search variables and evaluate the performance (through objective functions) of the corresponding value of the response variables.

If exists more than one configuration option in the process, that is, if it is possible to choose between different configurations, it is necessary to optimize each of these options separately and then compare them to choose the one that best meets the considered objectives (see Fig. 2). This strategy leads to problems inherent in the manipulation of different cases or configurations since each of them requires the algorithm specifications and the creation of a code for linking the process simulator with the optimization algorithm. Therefore, it is inevitable to infer that the computation time is greater in at least as many times as different configurations of the process exist.

The simulation would fail in some operating condition but success in others, this is determined which continues and which is discarded by evaluating the performance of the objective functions. Each evaluation corresponds to a particular set of values of the decision variables proposed randomly by the optimization algorithm. The performance of each set of values is evaluated and, in the way that an evolutionary algorithm proceeds, only the best performing solutions can generate offspring. As in any evolutionary algorithm, part of the values that make up the proposed solution set, will be used to generate a new set of values and be evaluated again in the next iteration.

In this paper, a new optimization strategy is proposed for the selection of the best process flowsheet when multiple configurations are possible. This strategy simultaneously optimizes the structural configuration for the flowsheet and the operating conditions (Fig. 3). This optimization method is based on the use of different cases to find the optimum values for the selected decision variables and, at the same time, the selection of the best process configuration. In this method, the case number of the process configuration (simulation case) is treated as a decision variable. In this way, the simulation case takes part in the solution vector as a chromosome. It is possible using a code instruction in which part of the simulation file path is a number. This number is declared in the algorithm as an integer variable (Fig. 4). An integer variable is one that can only acquire a value of an integer number, that is, defined without including decimals or fractions (for example, one, two, three, etc.).

The optimization problem presented in this new strategy is a multi-objective one, this way, it can be implemented the optimization to obtain a pareto solution in the stipulated optimization

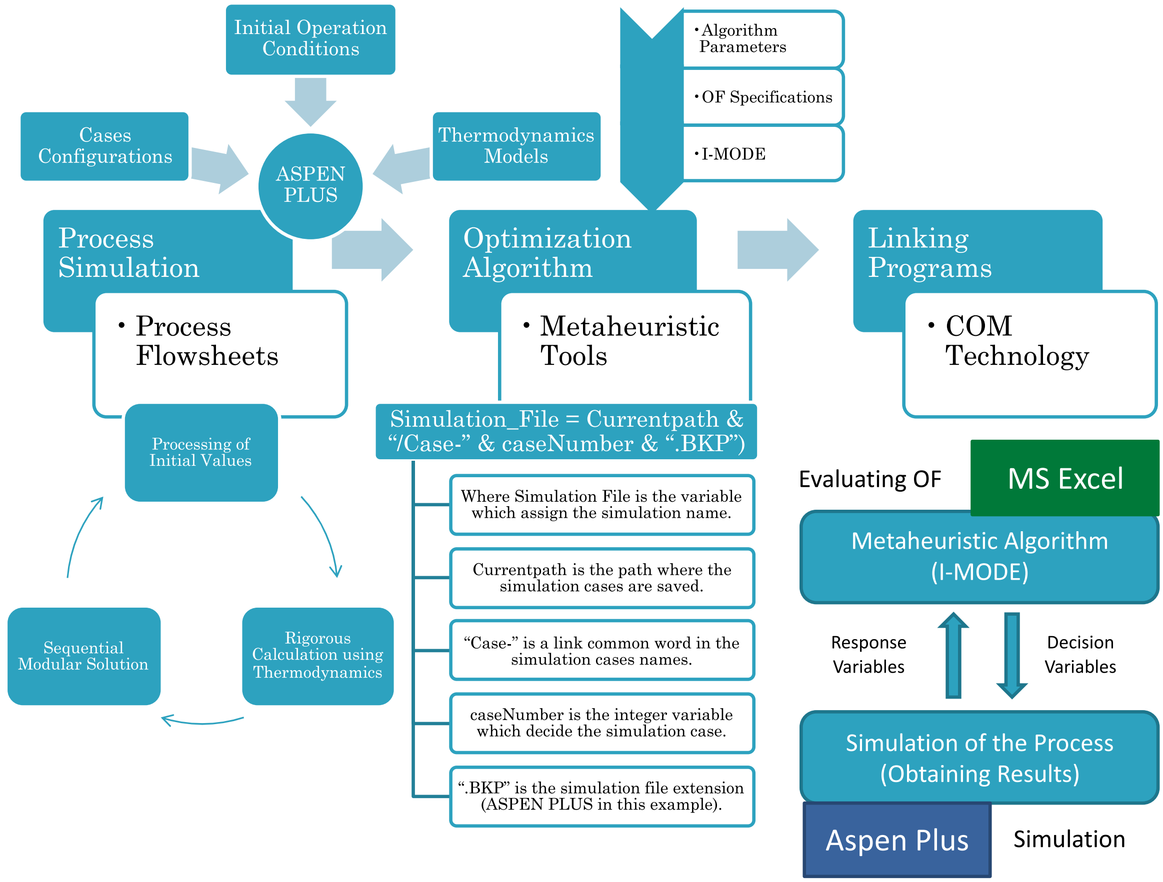

Fig. 4. Multi-case optimization solution.

range; however, this solution strategy corresponds to the classical approaches for addressing these types of problems, the above leads to the inherent complications in these methodologies, which as explained, involve excessive computing time and complicated manipulation of both the optimization algorithm and the necessary codes to link the programs. The reason why different cases are specified (Case 1 to Case 3) is not because this is the number of optimal solutions, but that each of these configurations corresponds to a different alternative solution to the process flowsheet configuration. However, it is not known which of these options represents the best performance of the objective functions, and which is the best value of the variables that can be manipulated in the process. That is why the proposed strategy addresses the selection of the process configuration and simultaneously searches for the optimal values of the operating conditions (search variables).

Using the code shown in Fig. 4, the algorithm will randomly propose a case number to be solved, and will export the values of the search variables to it. If this is a successful configuration, it will simulate a greater number of times than cases that are not. In this way, a selection of the best process flow diagram is obtained in less computation time.

3. Solar-grade silicon process

The main contribution consists in a general optimization strategy based on metaheuristic tools and commercial process simulators. The reason why the details of the case study (solar-grade silicon process) are exhaustively addressed is because it is necessary to understand the nature and impact of the search variables selected for the optimization model. In this way, it would be possible to associate equally relevant variables for the performance of the objective functions established in other case studies.

The alternatives to produce solar-grade silicon are the Siemens process, the intensified FBR Union Carbide process, and the hybrid process. These processes are described as follows.

3.1. Siemens process

This process uses SiO_2 as raw material. The first stage is to produce metallurgic silicon via SiO_2 reduction with coal. An electric arc furnace is the unit used for this transformation (Ranjan et al., 2011). The purity achieved for metallurgic grade silicon, Si(MG), is around 98-99%. Si(MG), H_2 and HCl are fed to a fluidized bed for the production of chlorosilanes. The exit stream is fractionated. Hydrogen (H_2) and hydrogen chloride (HCl) are removed when chlorosilanes condense. Then, a distillation column is used to split the liquid stream of $SiHCl_3$ and $SiCl_4$. The bottoms, $SiCl_4$, consist of a byproduct of the process while from the top a stream 99.99% $SiHCl_3$ is obtained (Díez et al., 2013). This revision is sufficient to feed the stream to the chemical vapor deposition reactor of the Siemens Process. The production of solar grade silicon uses $SiHCl_3$ and hydrogen via chemical vapor deposition. U shape bars of ultrapure silicon are used as seed. These bars are heated up using electric energy. After silicon deposition, byproducts of HCl, H_2 and $SiCl_4$ are obtained. Silicon is cooled down with an exchanger to ambient temperature and the gases are separated by a set of process units to be recycled to the process. The siemens process flowsheet is shown in Fig. 5.

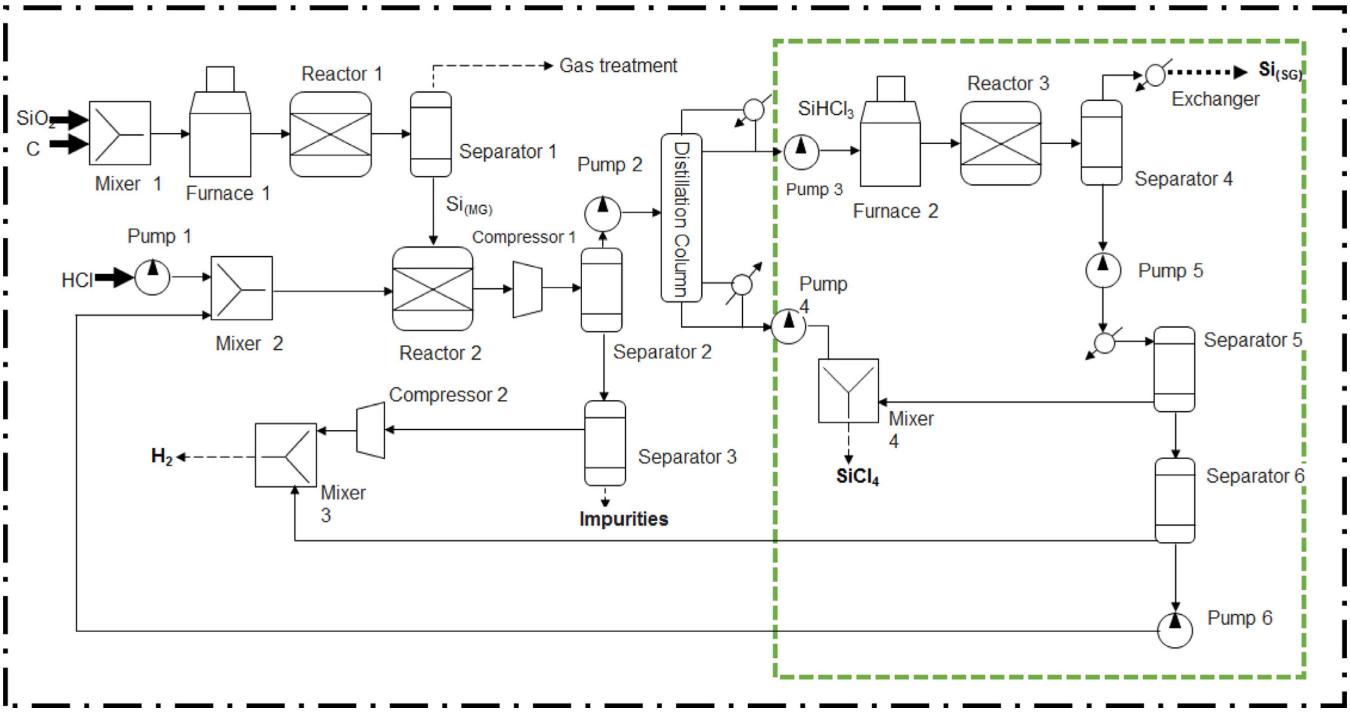

Fig. 5. Solar-grade silicon production process.Siemens Process Flowsheet.

3.2. Intensified FBR union carbide process

The stage to obtain Si(MG) is the same as for the Siemens Process. The Si(MG) is hydrogenated together with $SiCl_4$ in a fluidized bed reactor. The stream of products is separated using a flash module to remove the chlorosilanes. Afterwards, the stream consisting mainly of trichlorosilane and tetrachlorosilane is fed to a system of two distillation columns. A high purity stream of $SiCl_4$ is obtained from the bottoms of the first column, which is recycled. From the other column, a high purity trichlorosilane stream is obtained from the bottoms that are fed to a reactive distillation column. Next, trichlorosilane disproportion reactions are carried out in a reactive distillation column. High purity trichlorosilane is fed to the new intensified process, the reactive distillation system. The column produces high purity silane over the top that is fed to the chemical vapor deposition reactor to produce high purity silicon and hydrogen (Farrow, 1974). It is modeled on a stoichiometric reactor where the silane conversion reaches 80% (Tejero-Ezpeleta, 2004). The product stream is separated to isolate the polysilicon from the gases. Polysilicon is solidified while the gases, mainly H_2 and HCl, are recycled. The intensified FBR union carbide process flowsheet is shown in Fig. 6.

3.3. Hybrid process

The production of Si(MG) is carried out, as in previous cases, by means of the carboreduction of SiO_2. Then, an FBR is used for the hydrogenation of Si(MG) and $SiCl_4$ to obtain a mixture of di, tri and tetrachlorosilane. Next, two distillation columns are used to separate the mixture of chlorosilanes. From the top of the first column, there is obtained di and trichloro silane, while from the bottoms a mixture of tetrachlorosilane with traces of $SiHCl_3$ is obtained. $SiHCl_3$ is removed and the tetrachlorosilane is recycled to the process. The second column separates the mixture of $SiHCl_2$ and $SiHCl_3$, and obtained from the bottom $SiHCl_3$ of high purity. After that, $SiHCl_3$ is used as feed for the chemical Siemens vapor deposition reactor. Next of the deposition, HCl and hydrogen are separated from the Si(SG). Then, both streams are cooled down. The hybrid process flowsheet is shown in Fig. 7.

4. Computational model formulation

A model formulation based on a process simulation software was implemented in this methodology to obtain the best values for the selected decision variables. The different configurations for flowsheets of the process were introduced to the process simulator platforms. Likewise, the initial values of the decision variables, the thermodynamic models, and units were specified, and the absence of errors or warnings were corroborated running every simulation. The proposed methodology can solve this type of problems where it is necessary to choose from different options for the configuration of the same process and at the same time find the best operating conditions or design specifications.

The performance of every set of values in each configuration is determined by objective functions. The objective function is expressed in an equation whose value is maximized or minimized depending on its "desirability". This equation is calculated using the values of the response variables that are obtained from the process simulator after running a simulation with the given values of the search variables, that is, the optimizer program will propose values for the decision variables according to its algorithm until the best possible value of the objective functions is obtained.

In the case study that was selected to apply this optimization strategy, two objective functions were selected, an economic objective function (in order to be maximized) and an environmental objective function (in order to be minimized). These two objective functions are conflicting with each other, so as will be seen in the discussion of results, the best solution of one offers the worst alternative of the other.

4.1. Simulated process configuration

The addressed processes by Ramírez-Márquez et al., 2018a were the Siemens, Intensified FBR Union Carbide Process and Hybrid

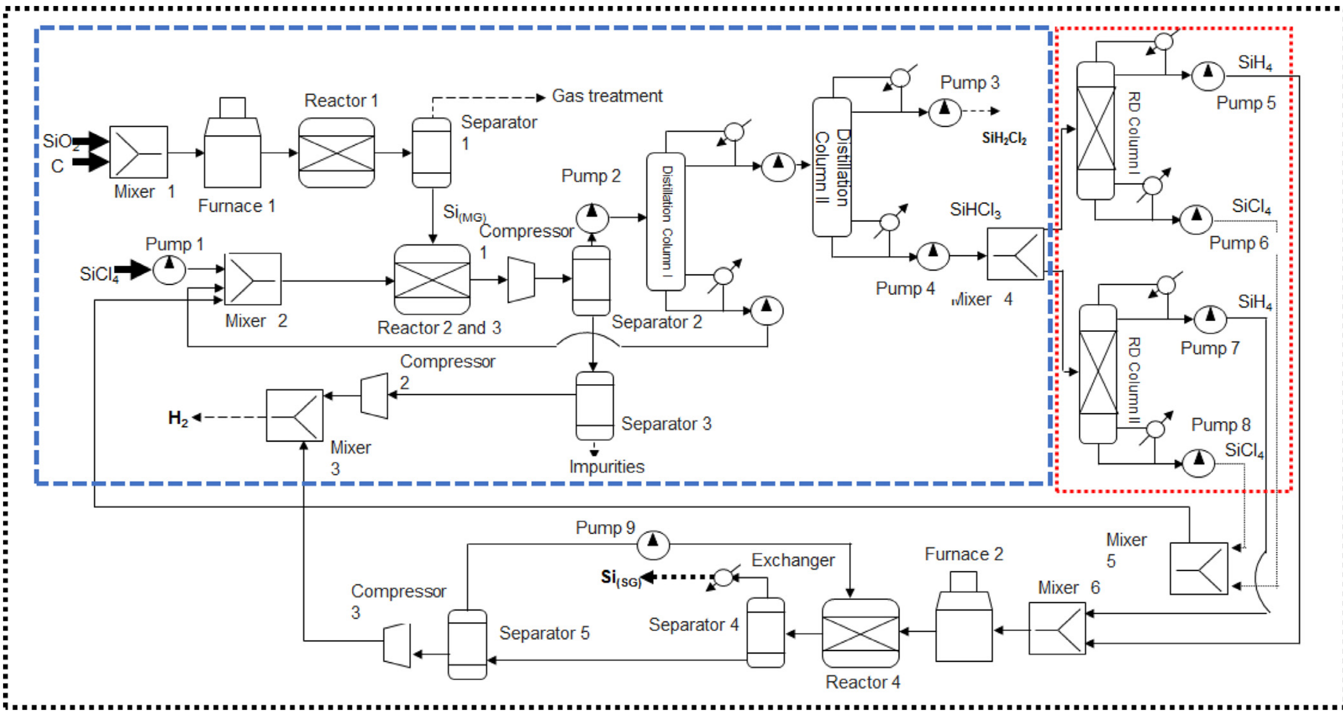

Fig. 6. Solar-grade silicon production process. Intensified FBR union carbide process Flowsheet.

Process. The procedure to construct the corresponding process flowsheets was described by Ramírez-Márquez et al., 2018b, and these initial flowsheets are used in this paper to construct the corresponding superstructure to simultaneously optimize the structure and operating conditions for the process. These flowsheets were implemented in the process simulator Aspen Plus^{TM} V8.8, this because the available units required in the simulation, the thermodynamic models as well as the rigorous solution approach for analyzing processes. Aspen Plus^{TM} is a commercial process simulator widely used for simulation processes, were the implemented approach considers zero degrees of freedom and sequential modular simulations are implemented to analyze processes. Aspen Plus^{TM} works in a "closed box" procedure resolving the problem of process simulation without offering the user the possibility of manipulating the used equations to obtain the presented results.Likewise, this process simulator has some optimization options, however it consists of a very basic single variable optimization tool, and the main limitation is that this does not allow the structural optimization. Due to the above, in this paper is proposed an optimization strategy that allows the linking of both search variables and response variables as data that is used in an external metaheuristic optimization algorithm able to work with black box models like the ones of Aspen Plus^{TM} or any other modular sequential process simulator. This way, a superstructure that consists of these three processes for solar-grade silicon production was implemented in Aspen Plus^{TM}, this consists of the Siemens Process, the Intensified FBR Union Carbide Process, and the Hybrid Process. All degrees of freedom were exhausted as data requested by the process simulator program in an initial run, such values are designated as current values.

After the simulation of each of the processes with proposed values, some of the degrees of freedom (data requested by the process simulator software) were selected as search optimization variables or decision variables, that is, data that would be manipulated by the optimization algorithm until finding the values with which the best results of two objective functions would be obtained, which are described below.

4.2. Total profit objective function

The economic objective function consists in maximizing the total profit (TP), which is defined as the entire gain that is obtained after subtracting what is necessary to invest a profit. TP can be calculated with the total income (TI) minus the total cost (TC), Eq. 1. TI means the profits in a year obtained by selling the product and can be directly calculated from the total annual production (TP) multiplying by a sale price (SP), Eq. 2. TP is calculated using a response variable, the silicon production expressed in lb/h and multiplying by operating hours in a day (24 hours) and the labored days in a year (360 days). A SP value of 0.72 US$/lb is assumed based on what is reported in digital databases.

$$TP = Total\ Profit = TI - TC \tag{1}$$

$$TI = Total\ Income = TP \cdot SP \tag{2}$$

Where $EP = Total\ Production = Production\ (\frac{kg}{h}) \cdot 24(\frac{h}{d}) \cdot 360(\frac{d}{yr})$ and $SP = Sale\ Price = 0.72(\frac{US}{kg})$.

$$TC = Total\ Cost = Utilities + Depreciations \tag{3}$$

TC represents the sum of the costs involved in the production of the product, in this study two mainly were considered: the cost of the utilities and the depreciations for each process. The depreciation considers equipment costs. Table 1 shows the capital cost, the cost of utilities and depreciations. Depreciations were calculated considering a utile life of ten years for the plant in each process. The values presented in Table 1 were obtained by the Aspen Process Economic Analyzer (APEA) at current values for each case.

The economic objective function TP is calculated by the set of Eqs. 1 to 3 starting with the response variables (EP) obtained by Aspen Plus^{TM}. TP is expressed in millions of US$ per year (MUS$/yr), which is obtained multiplying the production by 1×10^{-6} $/M$.

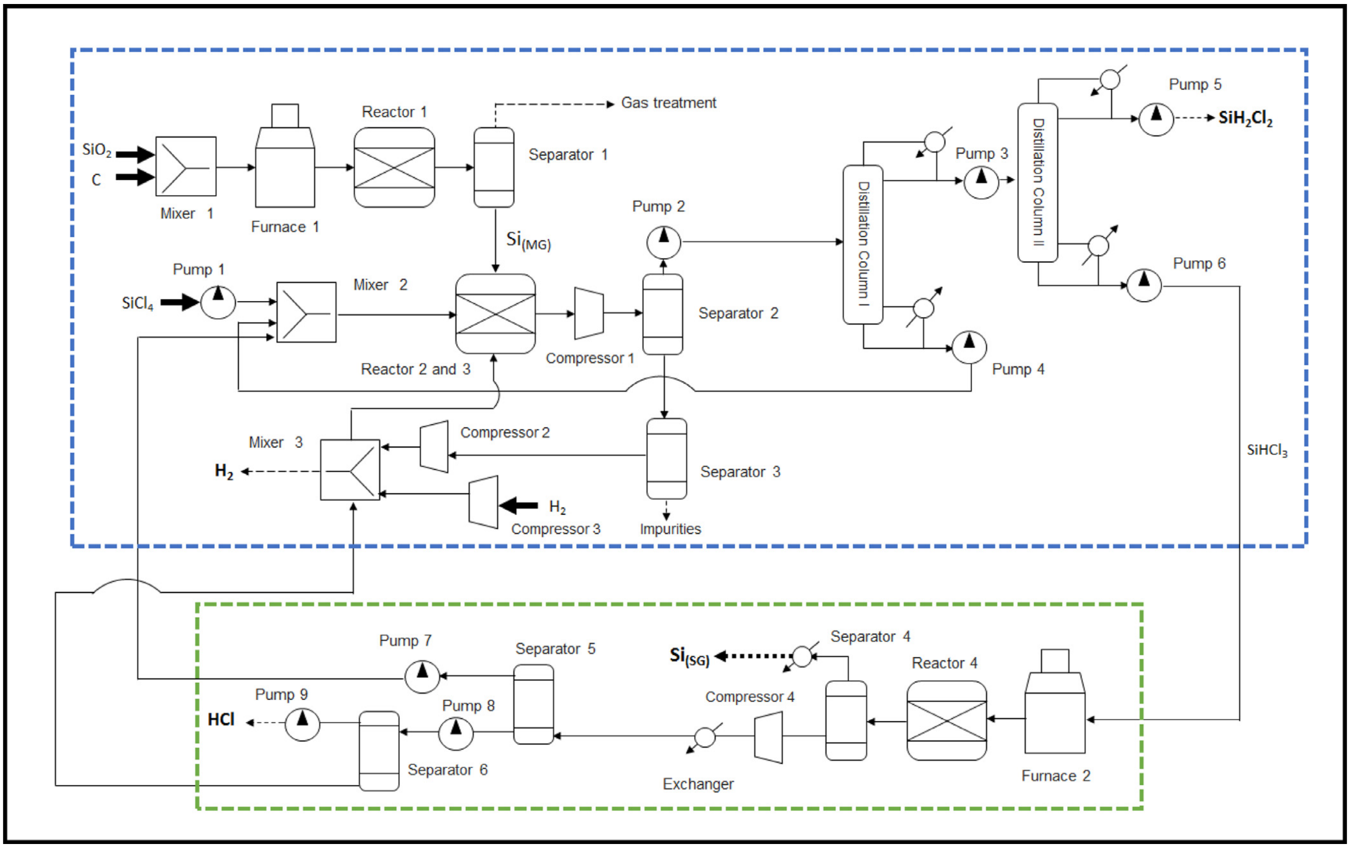

Fig. 7. Solar-grade silicon production process.Hybrid Process Flowsheet.

Table 1
Results for the total annual cost.

Process	Capital (MMUS$)	Utilities (MMUS$/YR)	Depreciation (MMUS$/YR)
Siemens	4.73886	0.427862	0.473886
Intensified FBR Union Carbide	20.7769	1.36862	2.07769
Hybrid	6.09487	0.893691	0.609487

4.3. Total emissions objective function

A second objective function has been considered, which involves environmental aspects. Environmental objective function consists in minimizing the total CO_2 emissions (TE) (Eq. 4) associated with the heating (btu/h) needed in the reactors of each proposed configuration, which acts as a response variable.

$$TE = Total\ Emissions = \sum_{n=1}^{5} R_n \left(\frac{kg}{h}\right) \cdot 24 \left(\frac{h}{d}\right) \cdot 360 \left(\frac{d}{yr}\right) \quad (4)$$

Where R_n corresponds to CO_2 emissions by Reactor «n» (lb/h).

It was used the US-EPA-Rule-E9-5711 as CO_2 emission factor data source (F1) with a value of 2.34 $\times 10^{-7}$ kg/cal for Natural Gas as ultimate fuel source. The CO_2 energy source efficiency factor (F2) is of 0.85, which corresponds to CO_2 emissions associated with the fuel needed to obtain high temperature by a fired heat. The CO_2 emissions are directly proportional to the needed heat (Q) associated to reactor «n» obtained by the simulator calculations. The R value is calculated using Eq. 5.

$$R = CO_2\ \text{emissions} = \sum_{n=1}^{3} Q_n \left(\frac{cal}{h}\right) \cdot F1 \left(\frac{kg}{cal}\right) \cdot F2 \cdot 24 \left(\frac{h}{d}\right) \cdot 360 \left(\frac{d}{yr}\right) \quad (5)$$

TE is expressed in millions of Tons per year (MTon/yr) multiplying the TE (kg/yr) by 1 $\times$ 10^{-6} MTon/kg.

5. Optimization strategy

Metaheuristic optimization methods are attractive for solving complex, high nonlinear and potentially nonconvex problems (Ramírez-Márquez et al., 2018a). In this paper, it has been proposed a new methodology of multi-objective optimization that allows to simultaneously analyze a set of different configurations of the same process in order to find the best one while finding the optimal operating conditions. This strategy is based on adding the case number of a process configuration as an entire variable, in this way the case number participates in the evolutionary process of selecting the best conditions. Analyzing the configurations at the same time that the operating conditions and design specifications have multiple advantages, the main one is that the evolutionary algorithm will gradually discard the less successful process configurations for given objective functions and thus consume less computational resources in simulating configurations in which the optimum is not found.

5.1. Optimization algorithm

Due to the nature of this problem, which involves many equations for the rigorous simulation of processes, a metaheuristic op-

Table 2
Current values in each case and limits for decision variables in all cases.

Value	Case	Units					
		Reactor 1		Reactor 2		Reactor 3	
		Temp (K)	Press (MPa)	Temp	Pres (MPa)	Temp (K)	Press (MPa)
Current	1	533	0.5	NA	NA	1373	0.1
	2	773	3.6	773	3.86	973	4
	3	773	3.6	773	3.86	1373	0.1
Min	1 to 3	520	0.4	750	3.6	950	0.05
Max	1 to 3	780	3.7	800	4	1400	4.5

timization algorithm is necessary. The multi-objective optimization hybrid method I-MODE (Sharma & Rangaiah, 2013) works with three different termination criteria: Chi-squared termination criterion (ChiTC), Steady State termination criterion (SSTC) and Maximum Number of Generations (MNG). The I-MODE algorithm has been successfully used in a general methodology (Ponce-Ortega & Hernández-Pérez, 2019)in order to optimize previously established process flow diagrams. That methodology consists in linking a commercial software of process simulation with a metaheuristic optimization algorithm.

5.2. Decision variables

The selected decision variables are listed in Table 2. In general, each reactor can be modified in two operating conditions, temperature and pressure, these aspects impact in both objective functions and they were selected as decision variables. The current values for all decision variables corresponding to the reaction units are presented in Table 2. In the same way, Table 2 shows the values for boundaries, upper (Max) and lower (Min) limits.

In Table 2, there are some cells corresponding to the Reactor 2 in Case 1 (Siemens Process), in which the current value does not apply (NA), which means that it has no current assigning values because there is no "Reactor 2" device in this configuration. The strategy used in this methodology in order to avoid mistakes in the process of exporting and importing variables consists in creating a "fictitious unit" within the simulation. This means that a unit (Reactor) with the name of "Reactor 2" was assigned to which the random values of the selected variables in the metaheuristic optimization algorithm are assigned, however, the streams of said unit are not connected to other block within the simulation, so that it does not affect with the obtained results.This strategy was chosen because this is the best way to assign these values to a variable call without creating a conflict in the export of data with the process simulator. The costs corresponding to the unit were calculated before the creation of the "fictitious unit" and the calculation of any utility cost is not ensured, so it is not involved in the calculation of carbon dioxide emissions.

The initial value for the optimization metaheuristic algorithm in each process was the half between the minimum and the maximum possible value.

5.3. Constraints

The constraints in this case study are implicit, it is that the possible restrictions are specified in the limits presented as minimum and maximum values in Table 2. In such a way that the restrictions of this case study can be formulated as expressed in Eq. 6:

$$Val_{Min} \leq x_i \ \leq Val_{Max} \tag{6}$$

Where i is the number of the decision variables, which can take a value since 1 up to 7 considering x_1 (which corresponds to case number or configuration process).

5.4. Parameters associated to the used algorithm

For the optimization process, in this study the values for the parameters associated to the used I-MODE algorithm are the following: population size (PS): 10 individuals, maximum number of generations (MNG): 30, taboo list size (TLS): 5 individuals, taboo radius (TR): 0.01, crossover fraction (CF): 0.8, mutation fraction (F): 0.8.

With respect to evolutionary algorithms, these heuristic rules are one of the main disadvantages, there is no exact way to determine the best values of the algorithm parameters. However, there are many bibliographical references to choose a good value (for example Sharma & Rangaiah, 2013). In this manuscript, the way in which they were selected incudes a sensitivity analysis, which consists in the following: a number is proposed for each parameter (number of individuals, number of generations, etc.) separately, then the result is analyzed after running the optimization, it is proposed to double that value for the same parameter, if it improves significantly it means that the proposed value is not enough, then the procedure is repeated by doubling the value again until the solution does not change in a considered way. Once an appropriate value for a parameter has been found, the same procedure is followed to find a suitable value for another parameter. For more details see Sharma & Rangaiah (2013).

6. Results and discussion

This section presents the results of the multi-objective optimization method. The simulation was performed on an Intel^{TM} Core ^{TM} i7-6700HM CPU @ 2.6 GHz, 32 GB computer, the computing time required to obtain the Pareto optimal solutions was of 16.24 min. The I-MODE optimization approach has demonstrated to be a superior metaheuristic technic for different applications (Sharma and Rangaiah, 2016), because it requires lower computation time than other approaches. The complexity of the addressed problem only is related to the computation time, and the implemented approach can address such problems. Finally, but the most important, if the simulations are optimized separately and each one specifies the same values for the use of the I-MODE (PS: 10 individuals, MNG: 30 generations) this consumes the computing time equivalent to the number of configurations to analyze. For this case study, it was found that the total computation time required to explore all possible configurations separately was 48.72 min, which is too much greater than 16.24 min that correspond to the computation time consumed using the proposed approach.

6.1. Results after Maximum Number of Generations (MNG)

The proposed strategy yields the Pareto sets shown in Fig. 8, where there can be seen the optimal solutions generated according to the stochastic procedure of this method corresponding to the solutions for cases 1 to 3. Due to the methodological strategy proposed in this paper, only a Pareto graph is obtained after running the metaheuristic optimization process. This Pareto plot is

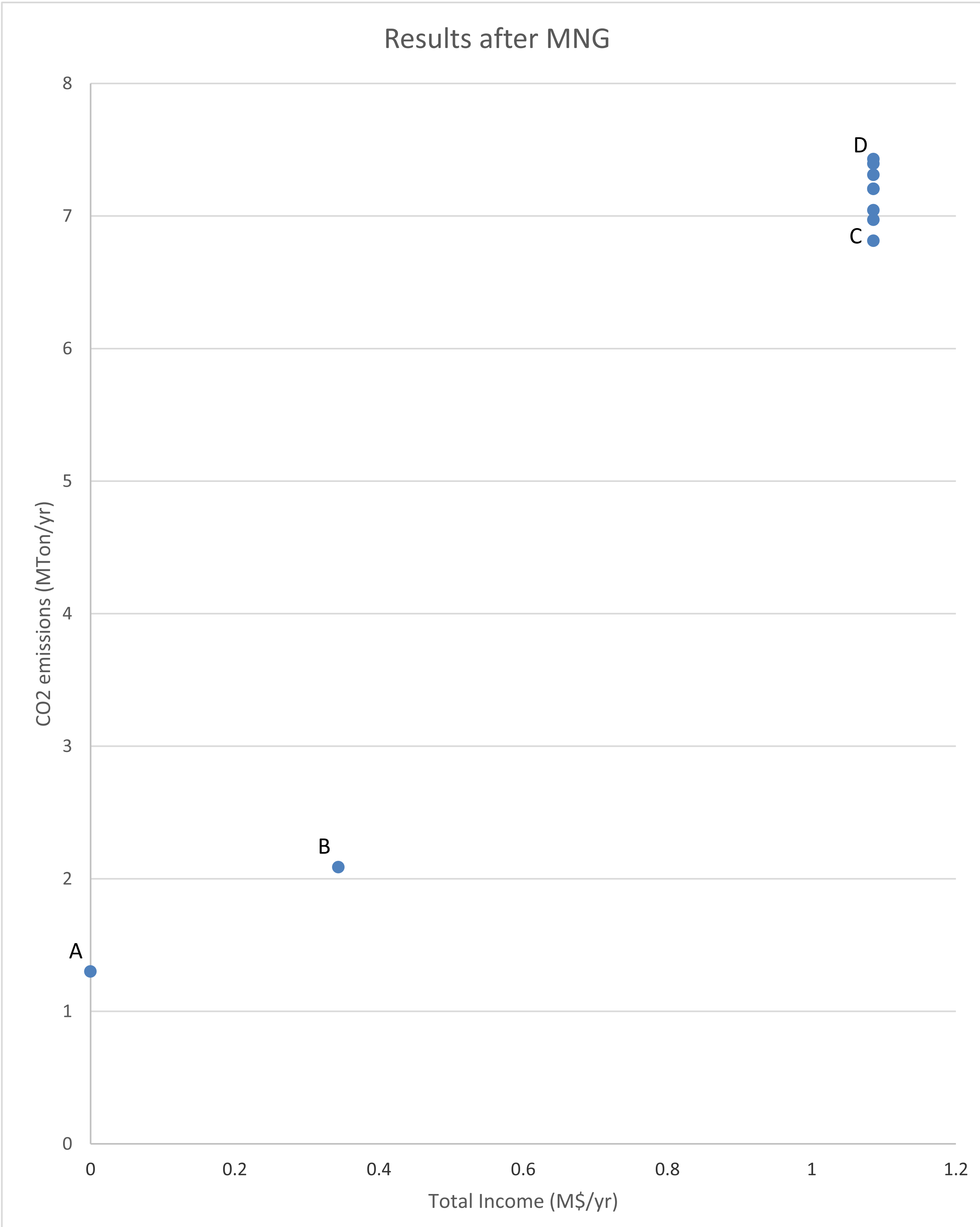

Fig. 8. Results after maximum number of generations for Cases 1 to 3.

obtained starting with the selected decision variables, their values for the lower and upper bounds and the values for the parameters associated to the used I-MODE algorithm.

The termination criterion shown in Fig. 8 corresponds to the results after Maximum Number of Generations (MNG), which is the total number of simulations needed to obtain the results. The termination criterion corresponding to the MNG refers to a value specified by the user in the optimization program interface as a parameter and tells the algorithm to finish iterating. The graph shown in Fig. 8 is a Pareto chart where the points shown there are those obtained from the interaction of the two conflicting objective functions, each of those points is an optimum, however, it is up to the decision maker to choose which of them best matches both objectives. Values of the search variables correspond to each of the points shown in Fig. 8. The results of the search variables shown in Table 3 correspond to point C.

Table 3
Optimal values for decision variables.

Case	Value	Unit						Objective Functions	
		Reactor 1		Reactor 2		Reactor 3			
		Temp	Press	Temp	Press	Temp	Press	F1	F2
2	Actual	773	3.6	773	3.86	973	4	1.09	7.48
	Optimal	701.12	3.34	752.61	3.76	1394.23	3.60	1.09	6.81
	Percent	-9%	-7%	-3%	-3%	43%	-10%	0%	-9%

6.2. Optimal values for search variables

The I-MODE algorithm gives the Pareto graph according with the chosen termination criterion. In that graphic, it is possible to select by the decision maker a point which properly reconciles both objective functions. Also, it is possible to read the optimal value for every decision variable in the selected point. Temperature was expressed in Kelvin and pressure in Mega Pascals. TP is expressed in millions of US$ per year (MUS$/yr) and TE is expressed in millions of Tons per year (MTon/yr)

The optimal values of the selected decision variables after running the optimization of chosen scenario are shown in Table 3.

The best configuration according with this optimization methodology was the Case 2.The results in the Pareto chart corresponding to Case 2 are the points from C to D, that is, all intermediate points between the previous two are optimal solutions of the configuration represented in Case 2.

The reason why Case 2 was selected as the configuration with the best results was that the points corresponding to this equipment arrangement are the ones that best reconcile both objective functions with intermediate values for both. While in points A and B that correspond to the configurations of Case 3 and Case 1, respectively, show decreases in the economic objective function, this means that if they significantly reduce the environmental objective function (CO_2 emissions fall to 2.08 MTon/yr equal to 72%) but compromise likewise the profit of the process (net profit fall to 0.34 MUS$/yr equal to 69%) in point B. While point A exhibits a net gain of zero, so it is not analyzed in this study.

6.3. Optimal values for objective functions

As can be seen in the Pareto graphics after MNG, there are different optimal solutions for this problem. In Fig. 8, four important points can be identified (A, B, C and D). Point A has a gross TP but the minimum value for TE, this point corresponds to Case 3. In point B can be seen intermediate values for both objective functions, this point corresponds to Case 1. Point C shows the minimum increase in TP with a considerable increase in TE, this set of points until point D corresponds to optimal solutions obtained in Case 2.

Table 3 also shows the values for the objective functions at the optimal values found for search variables in the selected configuration case with the best performance (Case 2).For this purpose, point C was selected within the set of optimal values that take part in the solutions of that case because it represents intermediate values for both objective functions.

Finally, Table 3 shows the percentage of change for decision variables and objective functions. A positive percentage represents an increment of the values and in the same way a negative percentage represents a decrement in the values for search variables and for objective functions. As can be seen in this table, the solutions generated according to the stochastic procedure of this method does not represent a considerable improvement in the performance of the economic objective function (TP), however it presents a reduction in the environmental objective function (TE) of 0.67 MTon/yr, which is equivalent to reduce 9% the CO_2 emissions. The above is due to the objective of satisfying two contradictory objectives at the same time, so that the optimization algorithm will find solutions in which there is a desired value for a single objective function as well as some intermediate values of both.

6.4. Algorithm mechanism analysis

It should be noticed that the proposed methodology was displacing the cases with the worst performance, the metaheuristic optimization algorithm focused on simulating the most successful configurations. However, in this work a multi-objective optimization was incorporated, so the algorithm retained the configurations that had the best performance in the other objective function. This explains why in the last generation the configurations appear with a lower TP (maximization objective), but also with a lower TE (minimization objective).

The pareto graph shown in Fig. 8 offers one point for each unsuccessful configuration (Case 1 and Case 3 for points B and A, respectively), while for the most successful configuration (Case 2) it offers seven optimal points (of the which point C). The mechanism of the algorithm is described as follows. As the first step of the algorithm, random values of the search variables are proposed within the limits specified by the user, the values of these variables will be subsequently exported to the process simulator (Aspen Plus). The structural configuration of the process is represented in a simulator file that only differs by a number (from one to three in this study). As an integer variable corresponding to the process configuration (Case Number) that could change from one to three was declared, this value is also proposed randomly by the algorithm, so a structural configuration is being chosen at the same time as values of search variables. As it is an evolutionary algorithm, it will gradually reproduce the simulations of the configuration that offers better values for both objective functions, however, in the pareto the points corresponding to the less successful configurations will continue appearing because they have similar extreme values. Therefore, after a specified number of generations (considering MNG as the selected termination criteria), the algorithm will offer a graph with the points corresponding to the best values for the objective functions without the need to simulate the configurations that do not offer a good outcome. In this way, it saves the computing time that it would take to evaluate each configuration with random values and then compare them.

The optimal solutions are unevenly distributed due to the way the graph is elaborated. A more detailed description of how the optimization algorithm offers the points for the graphical reading can help to better understand this behavior. For each of these points, the minimum is one in one of the axes, that is, it is based on the minimization of one of the objective functions and with this, the values of the other axis are calculated, so that each of the points shown in the solution graph can be considered as optimal. However, the decision maker is the one who chooses a single point of the graph as the best solution which conciliates in the most convenient way the performance of both objective functions and that these are usually conflicting. In the same line, it may be that the solution graph presents a series of points grouped in a zone (such as the series of points between C and D), which means that it is in this part where a greater number of solutions have been found feasible. Indeed, the difference between points C to D does not represent a considerable change in the economic objective function, so the best option for the decision maker would be to choose point C, since it represents practically the same gain as point D but with less CO_2 emissions.

7. Conclusion

This work has presented a new multi-objective optimization methodology where it is possible to optimize the structural configuration of the process flow diagram simultaneously with the best operating conditions. This technique is possible through a code that uses the case number of the configuration as an integer variable, in this way, it is proposed randomly the solution of a particular configuration with values of the search variables and through generations move less successful configurations and search variable values are proposed only for the most successful flowsheets. Using this multi-objective optimization methodology through metaheuristic techniques, it is possible to considerably reduce the computation time by just simulating the best configurations.

A case study for the optimal production of silicon grade silane is presented. Three different process configurations were simultaneously optimized. The results obtained in the case study (SGSP) are attractive for both objective functions, and the computation time is almost the third part of the case of optimizing each configuration separately. In the addressed case study, the entire annual emissions of CO_2 were reduced between 9% in the Case 2, whereas the TP presents a constant value, that is, by changing only the operating conditions of the reactor of said configuration, it is possible to reduce CO_2 emissions and at the same time maintain the same economic gains.

The main contribution of this work is not only the algorithm used, but also the strategy of simultaneous optimization of various possible configurations to displace the least successful ones in the performance of the objective function. In such a way that the objective of this methodology is not to be faster than other metaheuristic tools, but rather to be faster than using the same algorithm when solving each configuration separately.

Finally, the proposed approach can address different processes because it is general. The case studies to which this methodology can be implemented are in those in which multiple configurations can be chosen. Likewise, it is necessary that the search variables can be shared in the process flow diagrams to be chosen.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2020.106946.

CRediT authorship contribution statement

Luis G. Hernández-Pérez: Conceptualization, Investigation, Methodology, Writing - original draft. **César Ramírez-Márquez:** Conceptualization, Investigation, Writing - original draft. **Juan G. Segovia-Hernández:** Conceptualization, Funding acquisition, Writing - review & editing. **José M. Ponce-Ortega:** Conceptualization, Funding acquisition, Writing - review & editing.

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