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DEVELOPMENT OF HYBRID TOOLS TO SOLVE HIGHLY NON-CONVEX PROBLEMS

THESIS

TO OBTAIN THE DEGREE OF

DOCTOR EN CIENCIAS EN INGENIERÍA QUÍMICA

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DEDICATION

To nature, which wisely determines what to do, from whom we have much to learn and to whom we owe so much.

ACKNOWLEDGMENTS

I would like to thank all the people who have contributed in different ways in the realization of this work.

Limited by space and the haste of paperwork of the procedures, I hope I do not forget to mention or offend anyone. Once, a person very dear to me told me that important things in live take time and involve hard work to finish them. Variety of situations have proven that they were wise words and that it is certainly more difficult to maintain a position than achieved it. Enough to say thank you family for the support you gave me in the different stages of my formation.

You will never known how important is to me feel like a supported and lucky person for a group of such good friends. One of them is Rafael Maya, another one is Gladys Jiménez and of course Saúl Domínguez, thank you very much for your sincere friendship. Unfortunately, I cannot mention in this small space all the friends who, in one way or another, have contributed to this work.

Iris Sandoval, I really appreciate all the support you have given me during the time it took me to develop this work. Rather with your faithful company, with your words of encouragement in difficult times and the care you gave me when I felt bad. I will find a way to thank you for everything you have done for me and for decided to share your life with me. Sorry if I can not offer you more than this sincere thanks for everything.

I also acknowledge to the UMSNH and the financial support obtained from the CONACYT.

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FIGURES INDEX

NOMENCLATURE

ACM = Aspen Custom Modeler®

ANTIGONE = Algorithms for coNTinuous / Integer Global Optimization of Nonlinear Equations

BARON = Branch-And-Reduce Optimization Navigator

CF = Crossover Fraction

ChiTC = Chi-Squared Termination Criterion

COM = Component Object Module

COVID-19 = Coronavirus Disease 2019

DE = Differential Evolution

DOA = Deterministic Optimization Algorithm

DV = Decision Variables

F = Mutation Fraction

GA = Genetic Algorithms

GAMS = General Algebraic Modelling System®

GDX = GAMS® Data eXchange

GLOMIQO = Global Mixed-Integer Quadratic Optimizer

i = Target individuals

ICU = Intensive Care Unit

I-MODE = Improved Multi Objective Differential Evolution

IP = Integer Programming

LP = Linear Programing

LPC = Linking Program Code

MATLAB = Matrix Laboratory®

MILP = Mixed-Integer Linear Programming

MINLP = Mixed-Integer Non-Linear Programming

MNG = Maximum Number of Generations

MOA = Metaheuristic Optimization Algorithm

MOEA/D = Multi-Objective Evolutionary Algorithm based on Decomposition

MOO = Multi-Objective Optimization

MOP = Multi-Objective Problems

MS = Microsoft®

NLP = Non-Linear Programming

NSGA-II = Non-Dominated Sorting Genetic Algorithm-II

OF = Objective Functions

PS = Population Size

ROF = Reformulated Objective Function

RV = Response Variables

RVG = Random Values Generator

SARS-CoV-2 = Severe Acute Respiratory Syndrome Coronavirus 2

SOA = Stochastic Optimization Algorithm

SOF = Statistical Objective Function

SOO = Single-Objective Optimization

SQP = Sequential Quadratic Programming

SSTC = Steady State Termination Criterion

TL = Taboo List

TLS = Taboo List Size

TR = Taboo Radius

UPV = Uncertain Parameters Values

VBA = Visual Basic for Applications

WHO = World Health Organization

RESUMEN

DESARROLLO DE HERRAMIENTAS HÍBRIDAS PARA LA SOLUCIÓN DE PROBLEMAS ALTAMENTE NO CONVEXOS

Por

Luis Germán Hernández Pérez

Maestro en Ciencias en Ingeniería Química

Febrero del 2022

Dirigido por: Dr. José María Ponce Ortega

En el presente trabajo de investigación se propone el desarrollo de herramientas de optimización hibridas para la solución global de problemas que son altamente no convexos, los cuales se encuentran presentes en la industria química y de procesos. Se han reportado diferentes metodologías para la solución de problemas de esta naturaleza; sin embargo, estas metodologías sólo comprenden el empleo de herramientas metaheurísticas o simplificaciones en los modelos para utilizar optimización determinista. En este proyecto, se pretende proponer una metodología general de optimización global para resolver problemas de Ingeniería Química utilizando tanto la optimización metaheurística como la determinista, enfocándose en las ventajas de cada una de ellas y consiguiendo con ello la posibilidad de ofrecer alternativas viables para la solución de problemas altamente no convexos. Así mismo, se aplicará esta metodología para resolver problemas específicos en diferentes casos de estudio.

Palabras clave: *Herramientas híbridas de optimización global, Software de optimización determinista, Algoritmos de optimización metaheurística, Vinculación entre programas de simulación de procesos, Metodología general de optimización para considerar la incertidumbre.*

ABSTRACT

DEVELOPMENT OF HYBRID TOOLS TO SOLVE HIGHLY NON-CONVEX PROBLEMS

by

Luis Germán Hernández-Pérez

Master of Science of Chemical Engineering

February 2022

Directed by: PhD. José María Ponce-Ortega

In the present research work, the development of hybrid optimization tools is proposed for the global solution of highly non-convex problems, which are present in the chemical and process industry. Different methodologies have been reported for solving problems of this nature; however, these methodologies only include the use of metaheuristic tools or simplifications in the models to use deterministic optimization. In this project, it is intended to propose a general global optimization methodology to solve Chemical Engineering problems using both metaheuristic and deterministic optimization, focusing on the advantages of each of them and thereby achieving the possibility of offering viable alternatives for the solution of highly non-convex problems. Likewise, this methodology will be applied to solve specific problems in different case studies.

Keywords: *Hybrid global optimization tools, Deterministic optimization software, Metaheuristic optimization algorithms, Linking between process simulation programs, General optimization methodology to consider uncertainty.*

1. INTRODUCTION

The avoidance of the depletion of natural resources (Reilly, 2012) to maintain an ecological balance (Shiva, 2002) is essential to guarantee sustainability (Thiele, 2016). To address environmental problems (Dunlap and Jorgenson, 2012) to offer a sustainable development (Elliott, 2012) that allow meeting the current demands of the growing population (Ezeh et al., 2012), a series of alternatives have been proposed including the correct use of natural resources (Sachs and Warner, 2001) to minimize the effects caused by climate change (Chen et al., 2012).

1.1. GENERALITIES

Several researchers have reported alternative solutions to propose economically efficient processes and at the same time to mitigate the environmental impact through the study of biofuels supply chains (Bowling et al., 2011), optimal waste management (Santibañez-Aguilar et al., 2013), and water-food-energy grids (González-Bravo et al., 2018), among others. The search strategies used in the aforementioned researchers are based on deterministic optimization (Ponce-Ortega and Santibañez-Aguilar, 2019), whose approach usually corresponds to mixed-integer non-linear programming (MINLP) formulations (Costa and Oliveira, 2001) that are based on superstructures (Yeomans and Grossmann, 1999) through disjunctive programming formulations (Grossmann and Ruiz, 2012). Most of the research mentioned above was realized using deterministic optimization approaches, where the general algebraic modeling system (GAMS) software (Brooke et al., 1992) is frequently used.

Mathematical programming strategies have as a main limitation the availability to produce optimal solutions in non-convex problems (Coello-Coello et al., 2002), and frequently it is not possible to find an optimal solution (Devillers, 1996). To address this problem, the use of metaheuristic algorithms (Sharma and Rangaiah, 2016), nature-inspired cooperative strategies (González et al., 2010), and nature-inspired optimization algorithms (Yang, 2014) through external links with process simulators have 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).

Figure 1-1 shows the optimization and global search classification into three categories: enumerative, deterministic, and stochastic (Coello-Coello et al., 2002). Evolutionary computation is classified in evolution strategies, evolutionary programming, genetic algorithms, and genetic programing (Devillers, 1996).

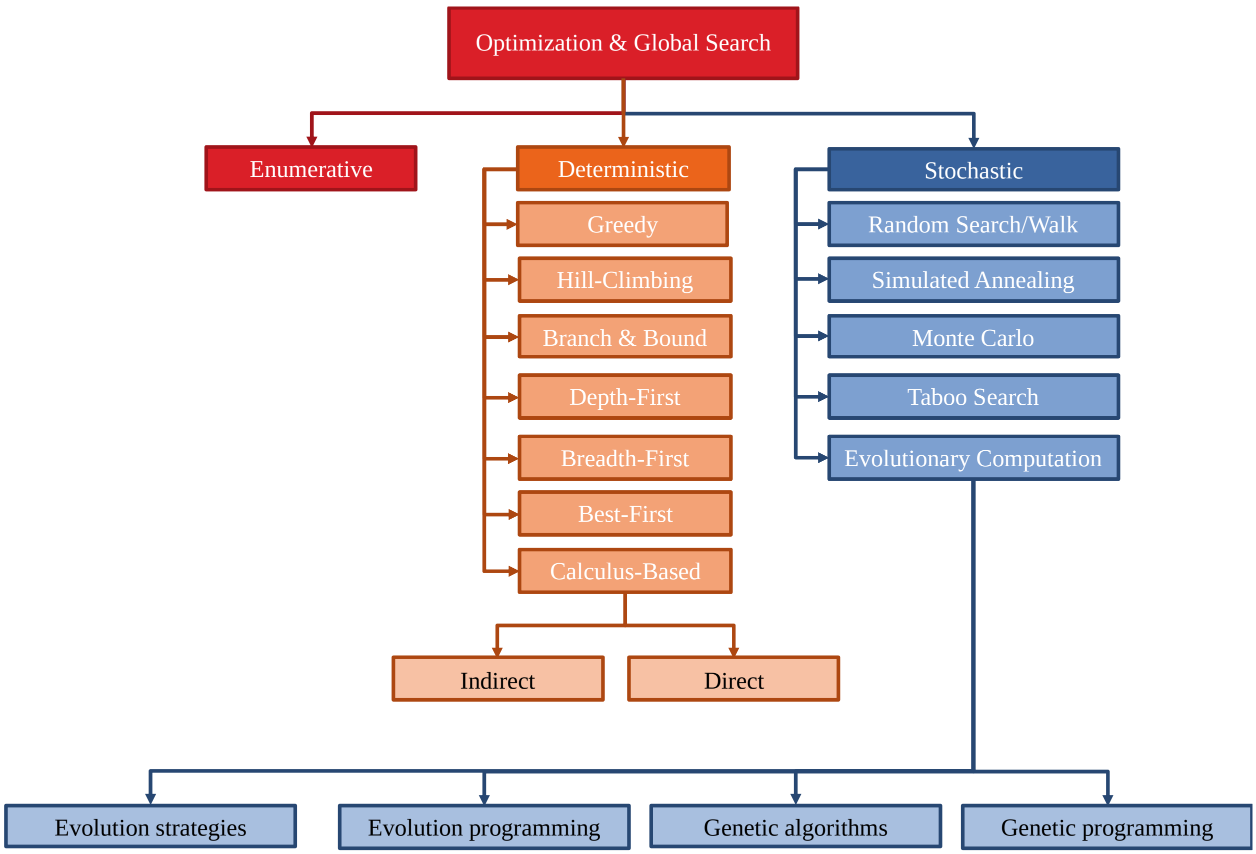

Figure 1-1: Optimization and global search classification.

This research presents a methodology for optimizing highly non-convex models using simultaneously deterministic and metaheuristic approaches, as well as the consideration of the uncertainty associated with the value of some parameters in the mathematical model. The optimization method uses modules programmed in visual basic for applications (VBA) from Microsoft® (MS) Excel to manipulate GAMS data exchange (GDX) files. The improved multi-objective differential evolution (I-MODE) algorithm (Sharma and Rangaiah, 2013) was selected as a metaheuristic optimization technique, which has been used in mathematical modeling simulation and optimization for process design (Sharma and Rangaiah, 2016).

1.2. JUSTIFICATION

Many real-world scientific and engineering multi-objective problems (MOP) are limited by their requirements associated with the problem domain, knowledge, and the search space, which can be exceptionally large. It should be noticed that deterministic methods are often ineffective when applied to high-dimensional problems. However, metaheuristic optimization tools have the great disadvantage that they do not work efficiently to solve problems involving a large number of degrees of freedom, a situation in which deterministic algorithms are very efficient. For this reason, a new optimization strategy that allows solving a complex optimization problem by using both deterministic and metaheuristic approaches is necessary.

1.3. HYPOTHESIS

A hybrid (deterministic and metaheuristic) optimization methodology will solve highly non-convex problems, where deterministic strategies are limited and in less computing time than using metaheuristic tools.

1.4. OBJECTIVES

1.4.1. GENERAL OBJECTIVE

Development of a general hybrid optimization method to take advantage of each of deterministic and metaheuristic approaches to solve highly non-convex problems, without the need for convexification strategies allowing structural configuration in process flowsheets.

1.4.2. SPECIFIC OBJECTIVES

a) Develop a general methodology to link metaheuristic algorithms with process simulators software (Aspen Plus® and Aspen HYSYS®).
b) Establish a method to solve structural configuration in flow diagrams of process simulators using metaheuristic techniques.
c) Propose a methodology that reconciles optimization approaches of deterministic search and metaheuristic techniques.
d) Consider uncertainty in a generalized hybrid methodology applying it to complex optimization problems indicating the advantages and disadvantages with respect to the other methods according to each case study.

e) Analyze the proposed general multiobjective optimization methods, to indicate the advantages and disadvantages with respect to the other methods according to each case study.

2. THEORETICAL FRAMEWORK

It should be noticed that deterministic methods are often ineffective when applied to high-dimensional problems because they are limited by their requirements associated with the problem domain, knowledge (heuristics), and the search space, which can be exceptionally large. Because many real-world scientific and engineering MOP exhibit one or more of the above-mentioned characteristics, stochastic searches have been developed as alternative approaches for solving these irregular problems (Coello-Coello et al., 2002).

2.1. MODELLING AND SIMULATION

A mathematical model of a chemical process is a simplified representation of the physicochemical behavior of the real process, which is used to predict values of output variables for given input variables and process design (including operating) variables. A model can be used for what-if studies and process troubleshooting and it has many applications for process optimization, process control and operator training. Models are often difficult to solve analytically, and so they are mostly solved numerically (**Figure 2-1**). Modeling refers to all the steps in developing and validating a model for the process, whereas simulation refers to the use of the developed model for studying the process behavior/response for one or more sets of input and design variables (Sharma and Rangaiah, 2016).

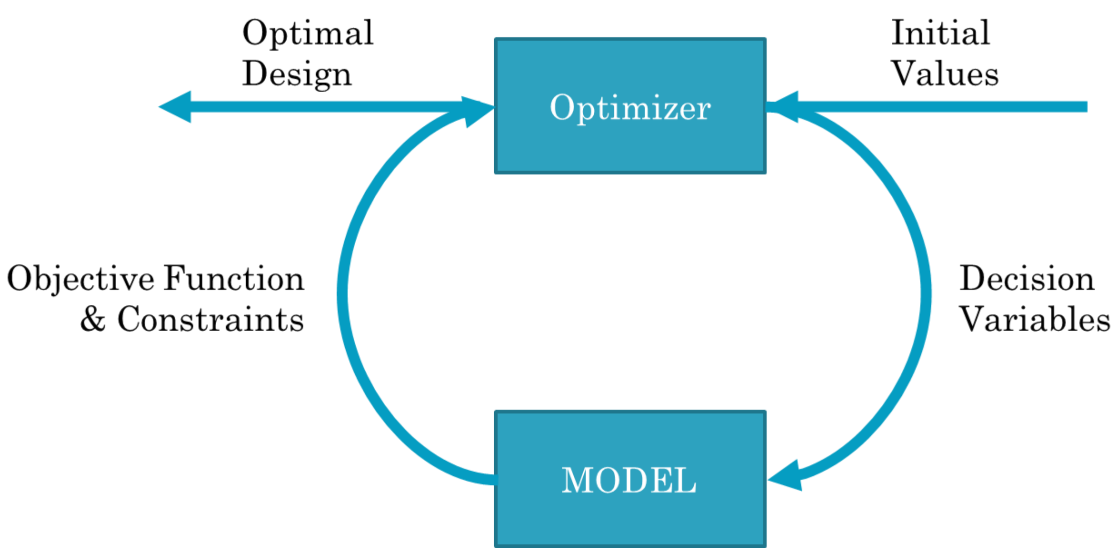

Figure 2-1: Representation of the numerical optimization framework.

In general, modeling and simulation are used to optimize the process operation and design. Optimization improves the performance of a process by changing the operating conditions such as temperature, pressure, and flow rate of process streams but without changing the size of any equipment or process flowsheet. Process retrofitting and revamping refer to the re-design of a plant for the specified objective(s) such as increased throughput, decreased energy consumption and revised product quality. This is achieved by changes in existing equipment and/or the addition of new equipment (leading to a new process configuration) besides changes in operating conditions (Ponce-Ortega and Hernández-Pérez, 2019).

Nowadays, several process simulators such as Aspen Plus® and Aspen HYSYS® are commercially available for simulating complete chemical processes, where common process units and a property database for numerous chemicals are available. However, models for less common and/or new process units are not readily available in the simulators, but they may be available in the literature or can be developed from first principles. A mathematical model for a new process unit can be implemented in Aspen Custom Modeler® (ACM), and then it can be exported to (included in) Aspen Plus® or Aspen HYSYS® for simulating processes having a new process unit besides common process units such as heat exchangers, compressors, reactors and columns.

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).

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 and 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 and 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 and Rangaiah, 2016), nature-inspired cooperative strategies (González et al., 2010), and nature-inspired optimization algorithms (Yang, 2014) through external links with process simulators have 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).

2.2. OPTIMIZATION STRATEGIES

Optimization has been successfully used to obtain optimal design and operating conditions of chemical processes. Single objective optimization (SOO) methods can be classified into two broad types; namely, deterministic (for example, Quasi-Newton and Sequential Quadratic Programming, SQP) and stochastic (for example, Genetic Algorithm, GA and Differential Evolution, DE). It is often desirable to consider several criteria for evaluating the performance of a process. Multi-objective optimization (MOO) methods (for example, ε-constraint, Non-Dominated Sorting Genetic Algorithm-II, NSGA-II, and Improved Multi-Objective Differential Evolution, I-MODE) can be used to explore the trade-off among conflicting objectives. Process simulators have some built-in optimization methods; for example, SQP is available in Aspen Plus®. Generally, SOO methods available in process simulators are not global optimization methods. Global optimization methods for SOO and MOO have been implemented in MS Excel®, MATLAB® (Matrix Laboratory), C++® and others. Hence, interfacing a process simulator with a global optimization program is required to improve the process design and operation (Sharma and Rangaiah, 2016).

2.2.1. DETERMINISTIC OPTIMIZATION ALGORITHMS

Some global optimization (Törn and Žilinskas, 1989) approaches based on mathematical programming (Horst and Tuy, 1990) have been implemented in the software GAMS (Brooke et al., 1992). Some of these solvers include the branch-and-reduce optimization navigator (BARON) (Ryoo and Sahinidis, 1996), LINDOGLOBAL (Lin and Schrage, 2009) ANTIGONE (Misener and Floudas, 2014) and GLOMIQO (Misener and Floudas, 2013). However, these resolvers are limited to handle only specific problems such as bilinear terms, concave functions, etc. (Wicaksono and Karimi, 2008).

2.2.2. METAHEURISTIC OPTIMIZATION ALGORITHMS

Nature-inspired algorithms (Gonzáles et al., 2010; Yang, 2014) have been proposed to solve structural configuration (Hernández-Pérez et al., 2020b) in process simulations (Ruiz-Femenía et al., 2019) of chemical engineering problems (Dragoi and Curteanu, 2016) using commercial software (Segovia-Hernández and Gómez-Castro, 2017) through external links (Ponce-Ortega and Hernández-Pérez, 2019). For example, metaheuristic techniques and evolutionary optimization (Holland, 1992) algorithms (**Figure 2-2**) like genetic algorithms (Gen and Lin, 2007) and simulated annealing (Kirkpatrick et al., 1983).

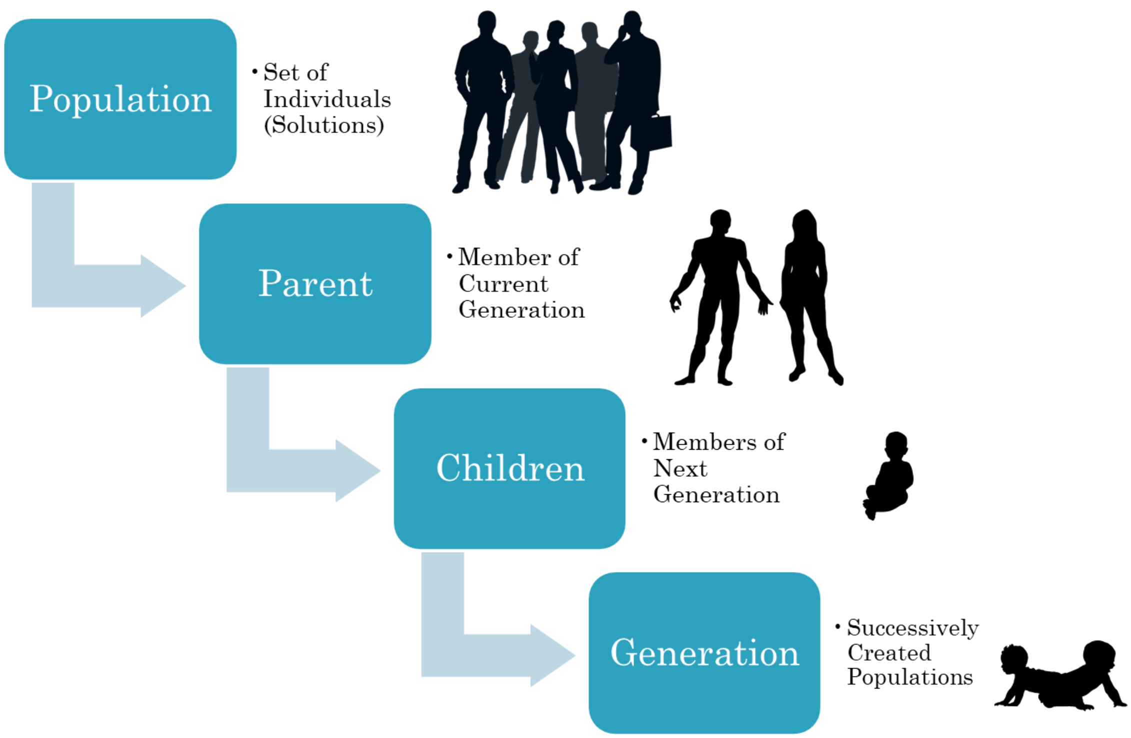

Figure 2-2: Evolutionary optimization algorithm components.

DE is an evolutionary algorithm that was developed to handle optimization problems. DE algorithm has been used for solving chemical engineering problems (Dragoi and 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 an 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.

The multi-objective optimization problem states an important degree of difficulty so that a suitable optimization strategy must be used. In this work, it has been used an improved multi-objective DE algorithm developed by Sharma and Rangaiah (2013), which works with a termination criterion using the non-dominated solutions obtained as the search progresses. The multi-objective optimization hybrid method is called I-MODE (Sharma and Rangaiah, 2013). The I-MODE works with three different termination criteria: chi-squared termination criterion (ChiTC), steady-state termination criterion (SSTC) and after the maximum number of generations (MNG).

The I-MODE algorithm (Sharma and Rangaiah, 2013) was selected as a metaheuristic optimization technique, which has been used in mathematical modeling simulation and optimization for process design (Sharma and Rangaiah, 2016). For example, Hernández-Pérez et al. (2019) used the I-MODE for the optimization of the microalgae-to-biodiesel production process and the structural and operating optimization of the methanol process (Hernández-Pérez et al., 2020a) incorporating the occupational health (Hernández-Pérez et al., 2021a).

The parameters that are specified in the I-MODE optimization algorithm are: population size (PS), MNG, taboo list size (TLS), taboo radius (TR), crossover fraction (CF) and mutation fraction (F). How the parameters of the evolutionary algorithm are determined is heuristic. Taboo radius, crossover fraction and mutation fraction are parameters of the I-MODE that are generally set at these values as default. While population size is the number of individuals that will be generated in the algorithm in each generation, this parameter provides a diversity of solutions, while the maximum number of generations indicates how many times the algorithm will be iterated, these two are directly related to computing time. Taboo list size is usually half the population size.

In the I-MODE (flowchart is presented in **Figure 2-3**), a population of PS individuals is randomly initialized inside the bounds on decision variables. Then, values of the objectives and constraints are calculated for each individual of the initial population. The TLS is half of the PS, and the TL is randomly filled with 50% individuals of the initial population, initial individuals are also identified as target individuals (i). A trial individual is generated for each i by mutation and crossover on three randomly selected individuals from initial/current/parent population. The elements of the mutant vector compete with those of the target vector, with a probability CF to generate a trial vector. Taboo check is implemented in the generation step of the trial vector of I-MODE, and the trial individual is generated repeatedly until it is away from each individual in the TL by a specified distance called TR. Euclidean distance between a trial individual and each individual in TL is calculated in the normalized decision variables space for accepting the trial individual. After that, objectives and constraints are calculated for the temporarily accepted trial individual. The trial individual is stored in the child population and added to TL. After generating the trial individuals for all the target individuals of the current population, non-dominated sorting of the combined populations and child populations followed by crowding distance calculation, if required, is performed to select the individuals for the next generation. The best PS individuals are used as the population in the subsequent generation.

Part of how the optimization algorithm operates in the training part of the next generation is to take the best solution obtained in the current generation and calculate the difference it has with the best solution of the previous generation. In the optimization of each configuration, a value of 0.0003 was specified for the VAR-limit (GD) and 0.1 for the VAR-limit (SD), which are also parameters of the I-MODE algorithm. Concerning evolutionary algorithms, this is one of the main disadvantages, there is no exact way to determine the best values of the algorithm parameters. However, there are many references useful to choose a good value (for example Sharma and Rangaiah (2013). In this work, there was implemented a sensitivity analysis to select these values, which consists in proposing a given number for each parameter (number of individuals, number of generations, etc.), then the result obtained after running the optimization is analyzed, afterward 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 and Rangaiah (2013).

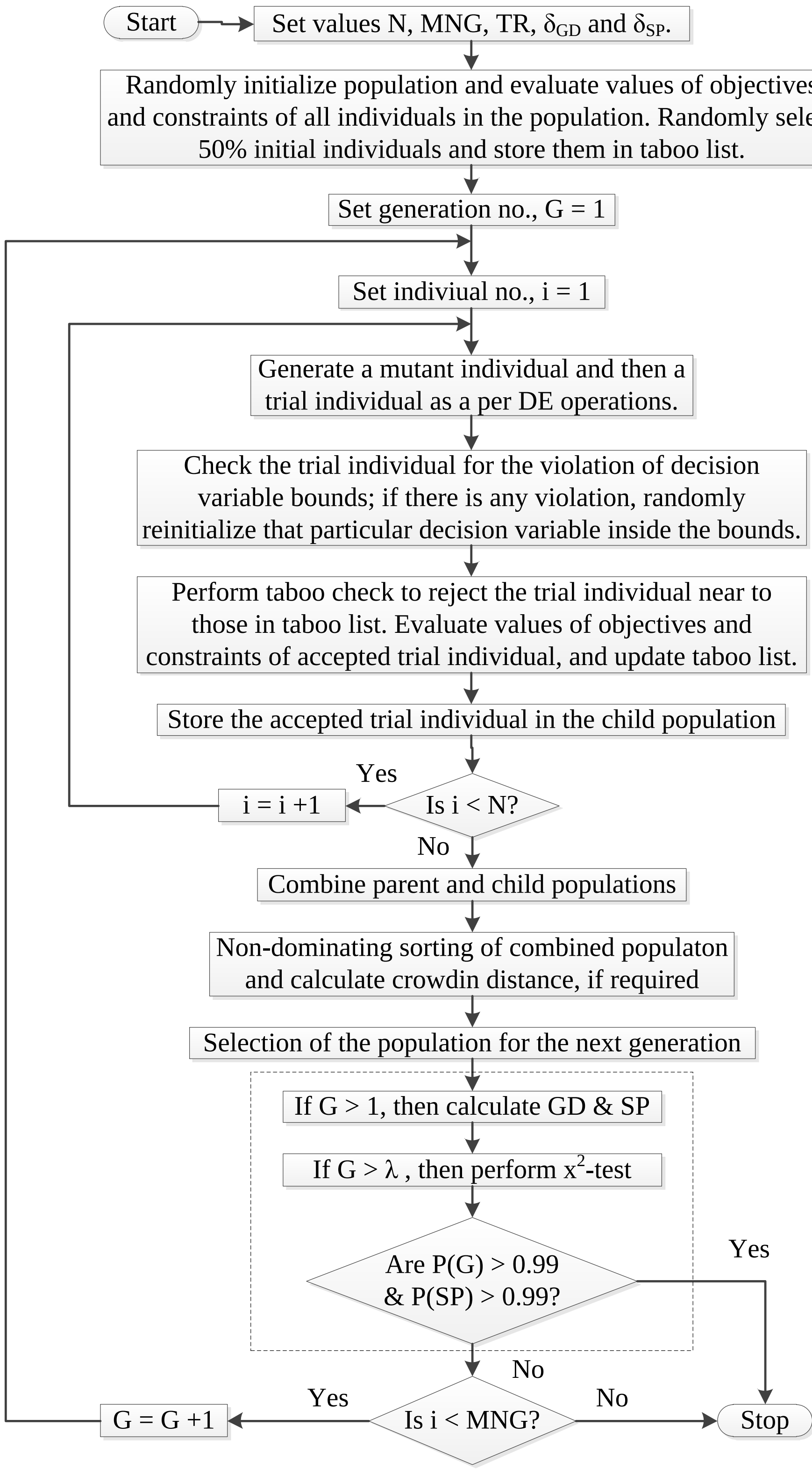

Figure 2-3: Flowchart of I-MODE algorithm.

It is important to note that metaheuristic strategies, such as hybrid evolutionary algorithms (including I-MODE), are simulation-based stochastic optimization methods that cannot guarantee solution optimality. However, metaheuristic techniques represent the best alternative to perform process optimization in highly non-convex problems and where deterministic optimization strategies may not converge or require initial values very close to the optimal ones. Furthermore, metaheuristic techniques are very useful to optimize closed box models, like the case of the model used in process simulators.

2.2.3. STOCHASTIC OPTIMIZATION ALGORITHMS

Optimization under uncertainty (Sahinidis 2004) refers to the branch of optimization where there are uncertainties involved in the data or the model, and it is popularly known as stochastic programming (Shapiro 2008) or stochastic optimization (Ermoliev and Wets 1988). Stochastic refers to randomness, and programming refers to mathematical programming techniques. The best-known mathematical programming techniques are linear programming (LP), non-linear programming (NLP), integer programming (IP), mixed-integer linear programming (MILP), and MINLP (Costa and Oliveira 2001). Probabilistic techniques like simulated annealing (SA) and GA are sometimes referred to as stochastic optimization techniques because of the probabilistic nature of the method. In general, however, stochastic programming and stochastic optimization involve optimal decision-making under uncertainties (Diwekar 2008). In this context and to avoid confusion, throughout this text the term stochastic will be used to refer to uncertainty and the metaheuristic term for evolutionary optimization (Holland 1992) algorithms (such as SA and GA).

2.3. LINKING PROGRAMS

It is necessary to write a linking sub routine for the programs to interact; this is achieved through COM Technology using VBA. This research presents a methodology for optimizing highly non-convex models using simultaneously deterministic and metaheuristic approaches, as well as the consideration of the uncertainty associated with the value of some parameters in the mathematical model. The optimization method uses modules programmed in VBA from MS Excel to manipulate GDX files.

3. METHODOLOGY

3.1. OPTIMIZATION OF PROCESS FLOWSHEETS THROUGH METAHEURISTIC TECHNIQUES

The methodological strategy that is followed consists in the construction of a process flow diagram for the simulation process, in this way, the operating conditions or design specifications can be manipulated to fulfill objective functions, as shown in **Figure 3-1**. In general, it consists in specifying the process flowsheet of each of the possible configurations, likewise, subsequently it is necessary to feed the simulations with the data requested by the simulation program until the degrees of freedom are exhausted. Once it has been verified that all simulations corresponding to the configurations have run successfully and without any error, it is necessary to specify the parameters related to the metaheuristic optimization algorithm and declare the objective functions. As the last step in this methodology, it is necessary to write a linking sub routine for the programs to interact, this is achieved through COM Technology using VBA as previously reported by Ponce-Ortega and Hernández-Pérez (2019).

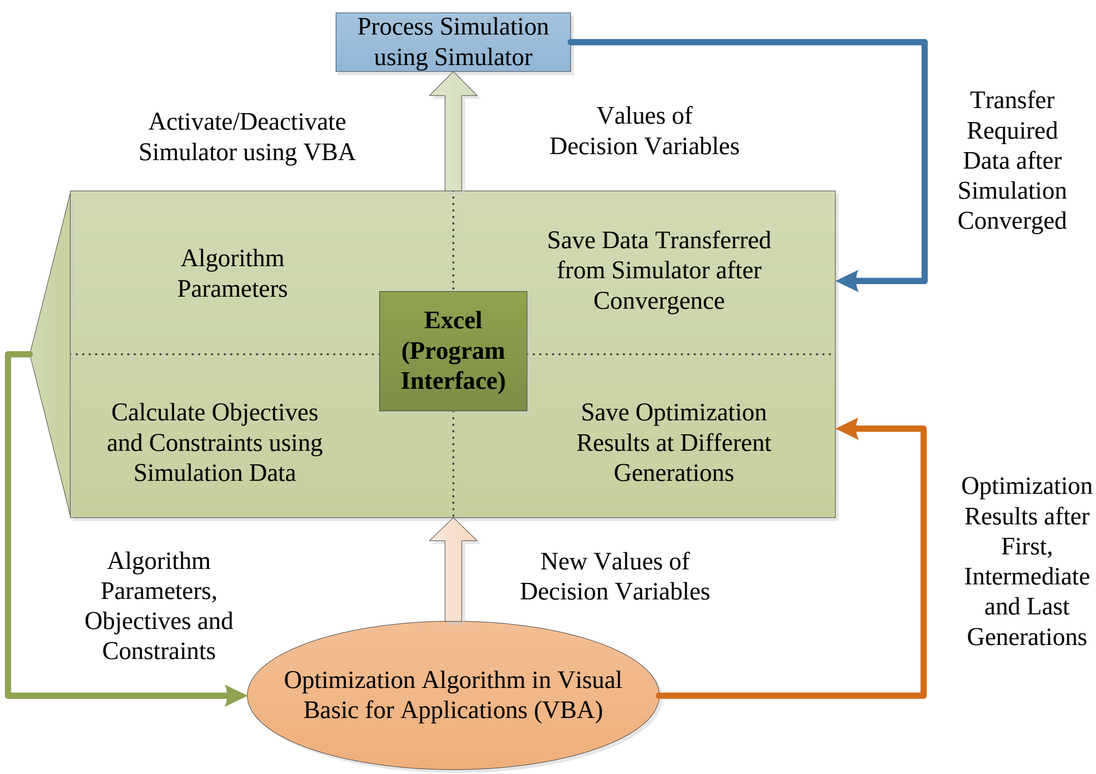

Figure 3-1: Interfacing between a process simulator and an optimization program.

3.1.1. OPTIMIZATION USING ASPEN PLUS®/HYSYS®SIMULATOR

The implementation of the global optimization approach involves a hybrid platform, which links Aspen Plus®/HYSYS® and MS Excel® through COM Technology (flowchart is presented in **Figure 3-2**). During the optimization process, the decision vector of design variables is sent from MS Excel® to Aspen Plus®/HYSYS®, in this process simulator rigorous calculations for the data that identify a design of the process are obtained (e.g., temperature and pressure in the reactors) via resolution of the mass and energy balances in each unit and accounting for the thermodynamic and design equations. These data are returned from Aspen Plus®/HYSYS® to MS Excel® for calculating both objective functions, the values obtained for the objective functions are evaluated and new vectors of design variables are generated according to the stochastic procedure of the used method.

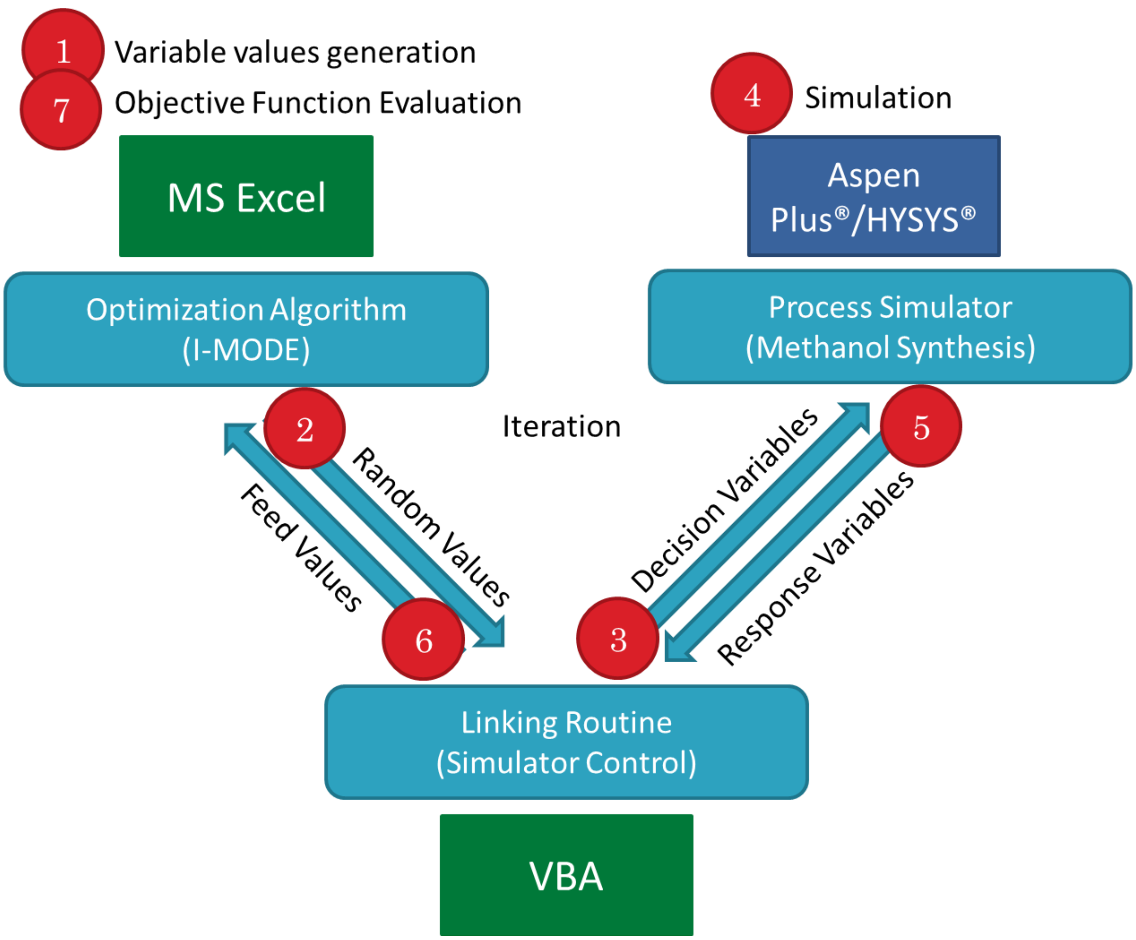

Figure 3-2: Methodological strategy for optimization of process flowsheets.

3.2. STRUCTURAL CONFIGURATION OF PROCESS FLOWSHEETS

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 combine process simulators with metaheuristic techniques for simultaneous optimization of process flowsheets with the corresponding operating conditions. A method through which it is possible to analyze simultaneously multiple configurations of the same process is proposed; 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 the next generations displacing the configurations with the worst objective function values. In a conventional way to search for an optimal solution, it is necessary to simulate each configuration with possible sets of values until a termination criterion is reached, which consumes considerable computational time. However, with the method proposed here, it is possible to find the best-operating values in the best configuration in the equivalent computation time to perform the search in a single case.

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 **Figure 3-3**). 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 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.

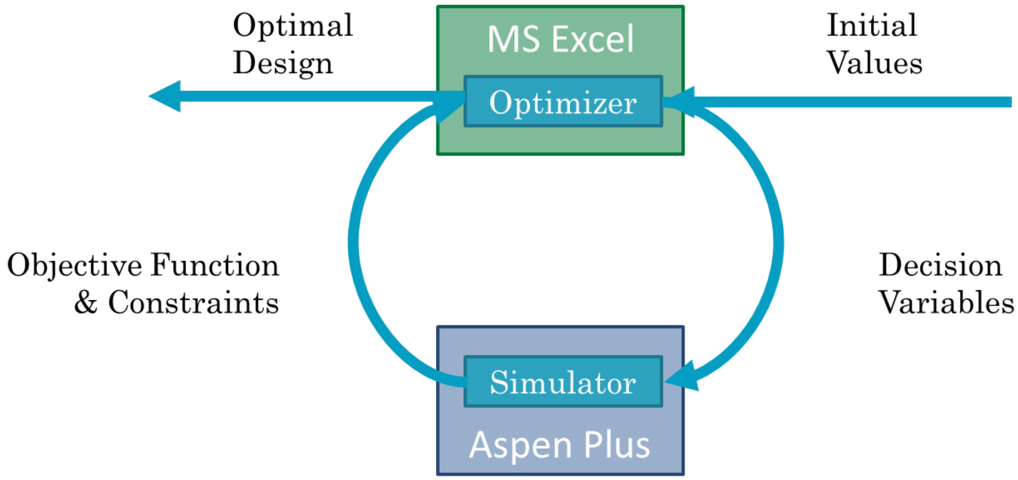

Figure 3-3: Conventional single-case optimization framework.

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 (**Figure 3-4**). 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.

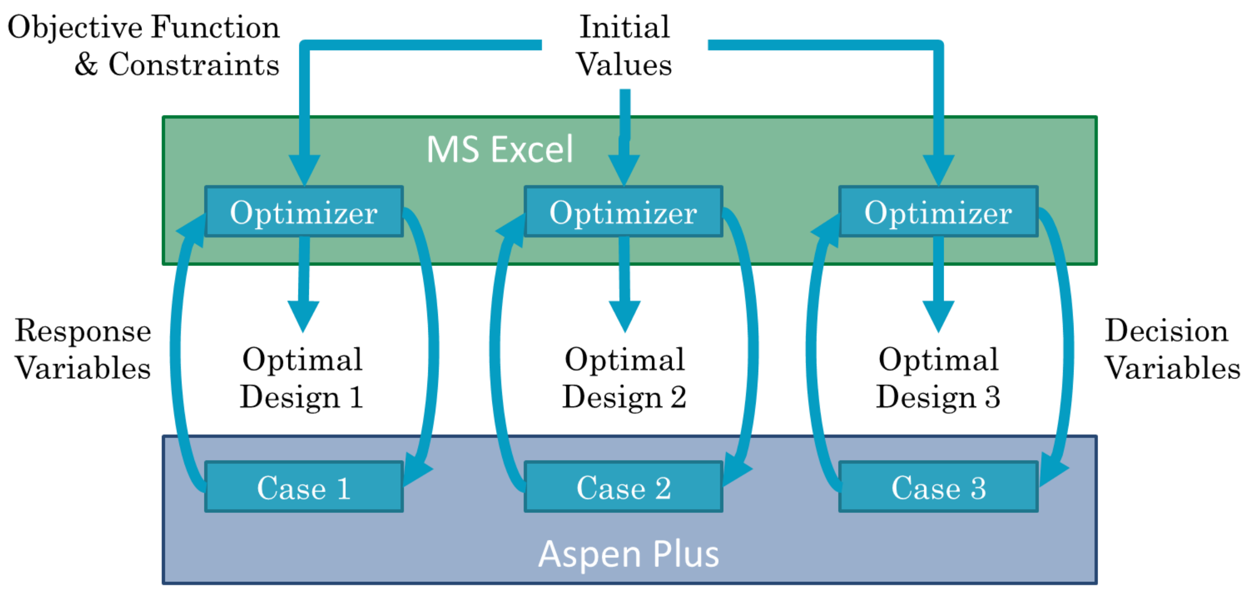

Figure 3-4: Optimization framework where multiple configurations are possible.

The simulation would fail in some operating conditions 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 (**Figure 3-5**). 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 (**Figure 3-6**). 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.).

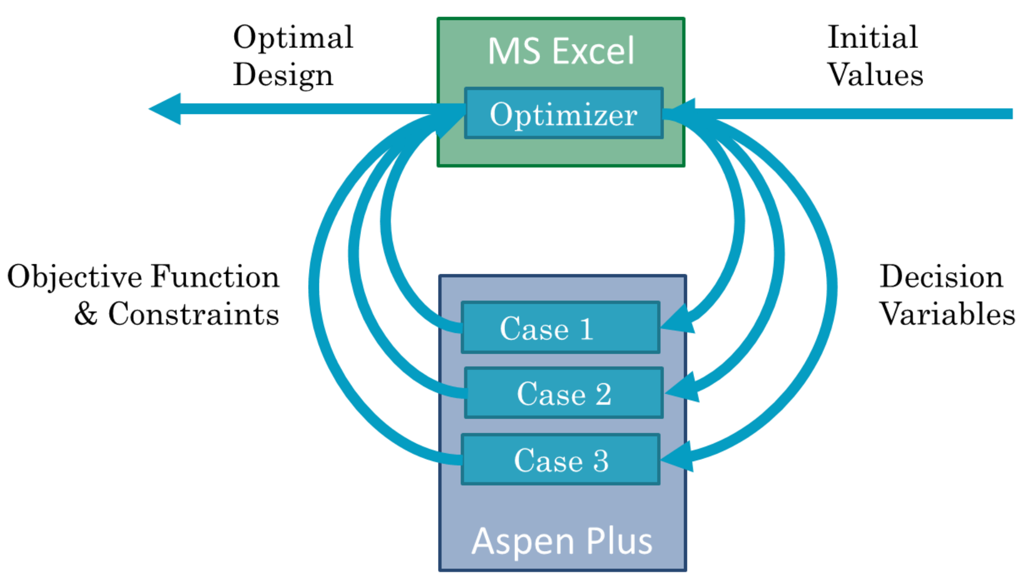

Figure 3-5: Multi-case optimization framework.

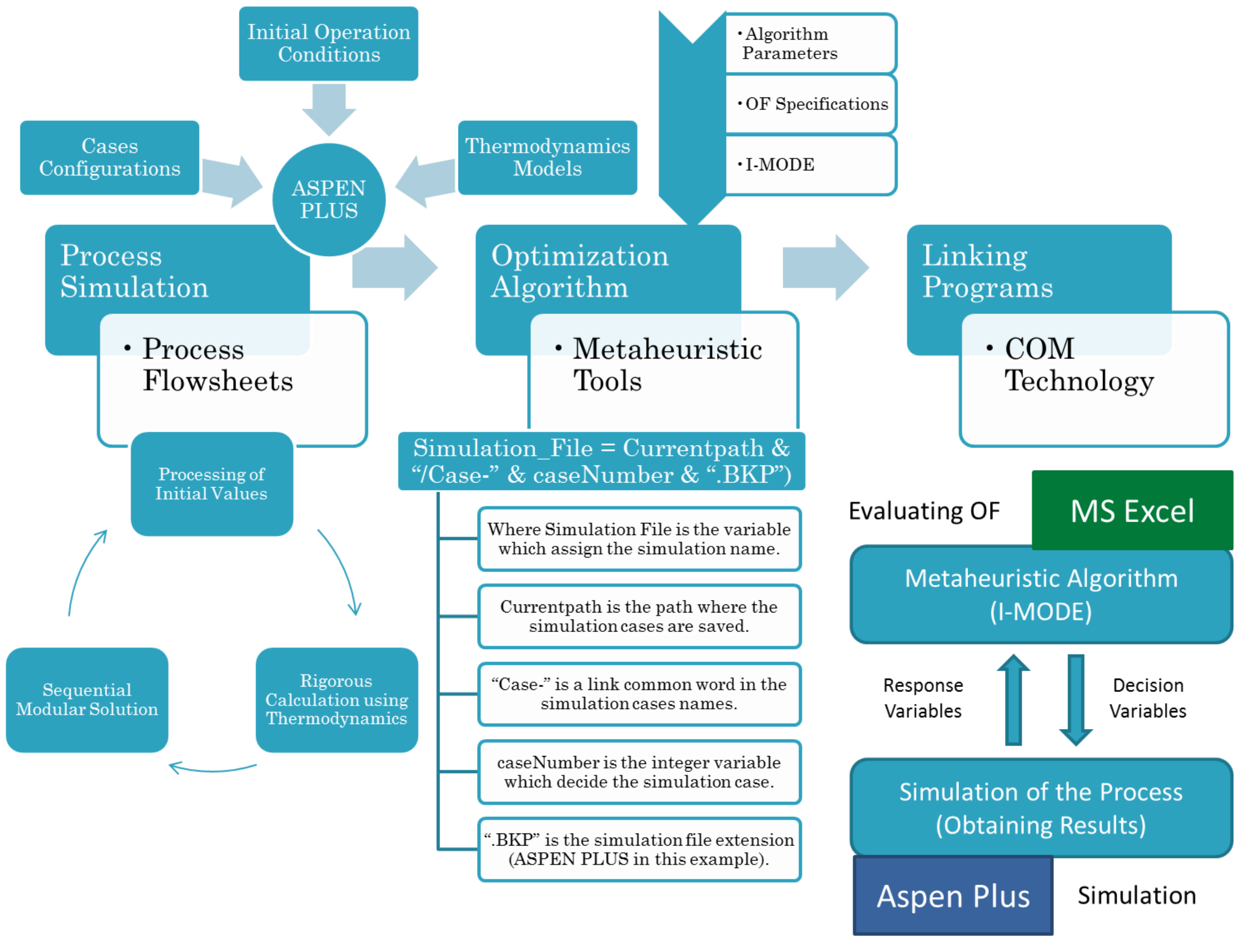

Figure 3-6: Methodological strategy for structural configuration of processflowsheets.

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 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 **Figure 3-6**, 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.

3.3. HYBRID MOO USING DETERMINISTIC AND METAHEURISTIC TECHNIQUES

A code was implemented to link the GAMS program with the I-MODE algorithm through VBA. To successfully link GAMS to MS Excel, the use of a GDX file is necessary. The method proposed in this paper allows to control the run instruction of GAMS since VBA code, and with this, a different combination of the decision variables (DV) values can be tasted in each GAMS optimization process and the objective function (OF) performance is evaluated through the response variable (RV) values in the metaheuristic algorithm. Approaches for linking GAMS with other programs are available in such software. For example, the McCarl GAMS User guide describes how to establish intercommunication between GAMS and other programs such as MS Excel. The McCarl Transport Model is included in the installation package of GAMS and the VBA code can be found in the GAMS installed directory.

The new numerical method proposed in this work is necessary because it allows solving complex optimization problems where the use of only one of the approaches (deterministic or metaheuristic) does not offer attractive solutions for the set of implications that make up the whole problem. The main advantage of this new method is that it can solve complex optimization problems that involve a mathematical model with a large number of variables and equations, and at the same time they are highly non-convex problems, on the other hand, the evolutionary algorithms used in metaheuristic optimization strategies do not guarantee finding the global optimum, which constitutes a disadvantage in this type of stochastic tools. The numerical robustness of this method depends on the own parameters of the metaheuristic optimization algorithm, because an adequate handling of the sets of variables and the number of generations, offer better solutions. Regarding the demand for computing time, as reported in the results section, it is between 14 and 25 minutes, which is competitive considering that a total of 1000 sets of proposed schedules were analyzed for each scenario. The main limitation of this method lies in the manipulation of the linking routines, since the analysis of a new case study involves the development of a custom code, however, once established, it allows the analysis of multiple configurations. In general, it must be used when there is a problem that cannot be solved using only conventional mathematical programming strategies, that is, when it is necessary to establish the value of some variables to avoid excessive complexity of the model and thereby find approximate solutions that depend on the initial values. Even though optimality cannot be verified in this method, the comparison with previously reported works allows evaluating its effectiveness to find better values than those obtained by applying a completely deterministic technique. Due to the search mechanism used by metaheuristic optimization tools, this strategy is capable of appropriately solving numerical problems regardless of the type of mathematical model, type of variables, number of equations or restrictions. Likewise, the effectiveness of the method is demonstrated in relation to other strategies in the results and discussion section.

This paper presents a new optimization approach to link GAMS with MS Excel through VBA; this way, the deterministic part of the problem will be solved in GAMS and the highly non-convex part will be solved by MS Excel through a metaheuristic algorithm which allows disaggregating the problem. For this purpose, the methodology implemented to solve this problem consists of the following steps. At first, it is necessary to develop a mathematical model in the GAMS environment. Second, to establish the optimization parameters to use the I-MODE algorithm. Finally, to write the code to link GAMS and the I-MODE algorithm through VBA.

In general, the proposed optimization approach is schematized in **Figure 3-7**. The methodology consists in solving a complex optimization problem using different searching strategies. Each of the searching strategies focuses on solving the part of the optimization problem in which it is most efficient to find optimal values. For this purpose, it is necessary to establish a link between a deterministic mathematical model of a specific process and the metaheuristic optimization algorithm. The link is established through a sub-routine code written in the same VBA language that contains the MS Excel metaheuristic optimization program. The VBA values are sent to the GAMS program and the RV are received after running the deterministic optimization program. After that, the metaheuristic optimization algorithm is going to evaluate the OF performance and propose new values of the DV in each iteration.

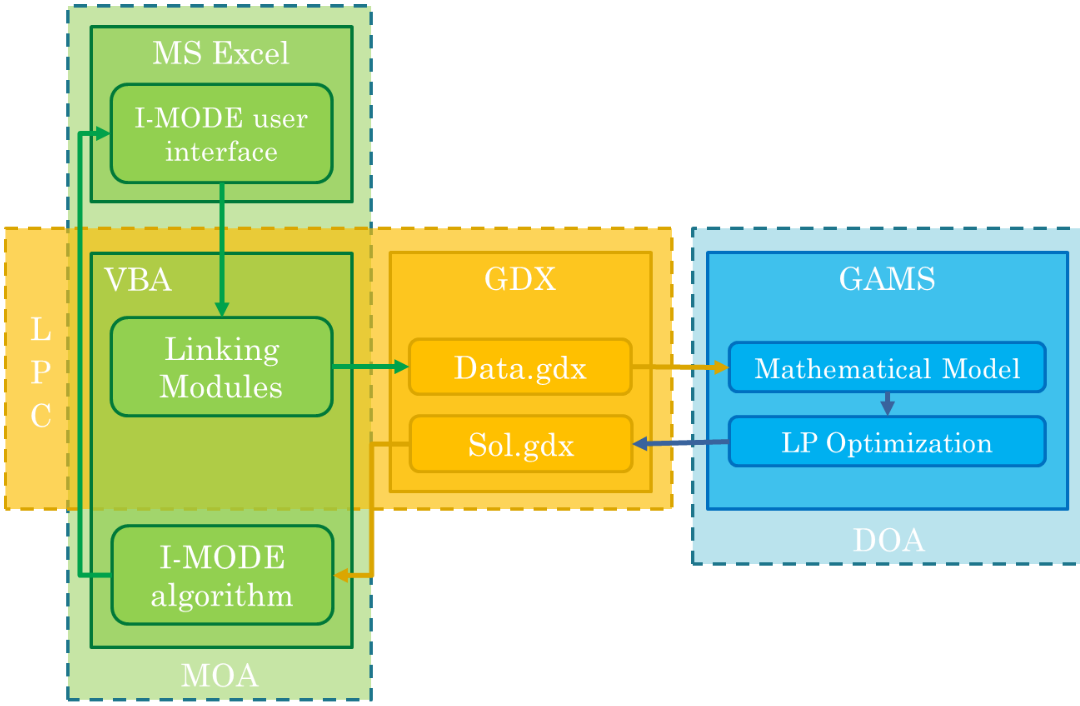

Figure 3-7: Programs communication for hybrid MOO.

In order to offer a better explanation of how the proposed methodology works, the terms used are standardized to describe it as follows: deterministic optimization algorithm (DOA), metaheuristic optimization algorithm (MOA) and linking programs code (LPC). From now on, DOA refers to the mathematical model that describes the process to be optimized and it is understood that it has been developed in the GAMS environment. MOA is the optimization tool that is based on Differential Evolution (DE) that allows solving the highly non-convex part of the problem, likewise, it is understood that this part of the solution strategy has been previously programmed in MS Excel. Finally, the LPC is the subroutine also developed in MS Excel, more specifically in VBA, which allows the intercommunication of GAMS and MS Excel for the exchange of data between DOA and MOA, respectively.

The following information describes the way of how the proposed optimization methodology works. The rationale for using a joint optimization methodology, both deterministic and metaheuristic, is that it seeks to solve a problem that consists of a part that can be solved in a commercial optimization program such as GAMS, whereas for the complex problem the use of metaheuristic optimization tools is necessary. Therefore, before starting with the steps of the methodology, it is necessary to verify that the problem has no solution by applying some strategy of convexification that allows its solution in a single deterministic optimization program.

- **Step one**: Construction of the DOA. A fundamental part of this methodology is the development of a mathematical model that describes the behavior of the process. This model is made up of a set of parameters, variables and equations that are used simultaneously for the optimization of an OF in a specific target of maximization or minimization. For the development of the DOA, it is necessary to know the process in depth. In this paper, the problem that is sought to be solved with this methodology is the flowback water management during HF operations.

- **Step two**: Specification of parameters in the MOA. Another very important step to be able to apply the methodology proposed in this work is to have a previously programmed MOA. The MOA used in this case is the I-MODE, and for this the specification of certain parameters specific to this algorithm is required. These necessary parameters obey, for the most part, those that correspond to any DE optimization algorithm. The parameters that are specified in the I-MODE optimization algorithm are: population size (PS), maximum number of generations (MNG), taboo list size (TLS), taboo radius (TR), crossover fraction (CF) and mutation fraction (F).

- **Step three**: Writing the LPC. The last of the steps of the methodology proposed here consists in writing the LPC. The code for linking programs is a subroutine that allows intercommunication between the programs that participate in the optimization process. This subroutine is based on the creation of GDX files for the export and import of data to the MOA. Later this part of the methodology will be described in detail.

By following the steps of the proposed optimization methodology shown in **Figure 3-8**, it is possible to solve a complex optimization problem using a hybrid optimization approach, deterministic and metaheuristic.

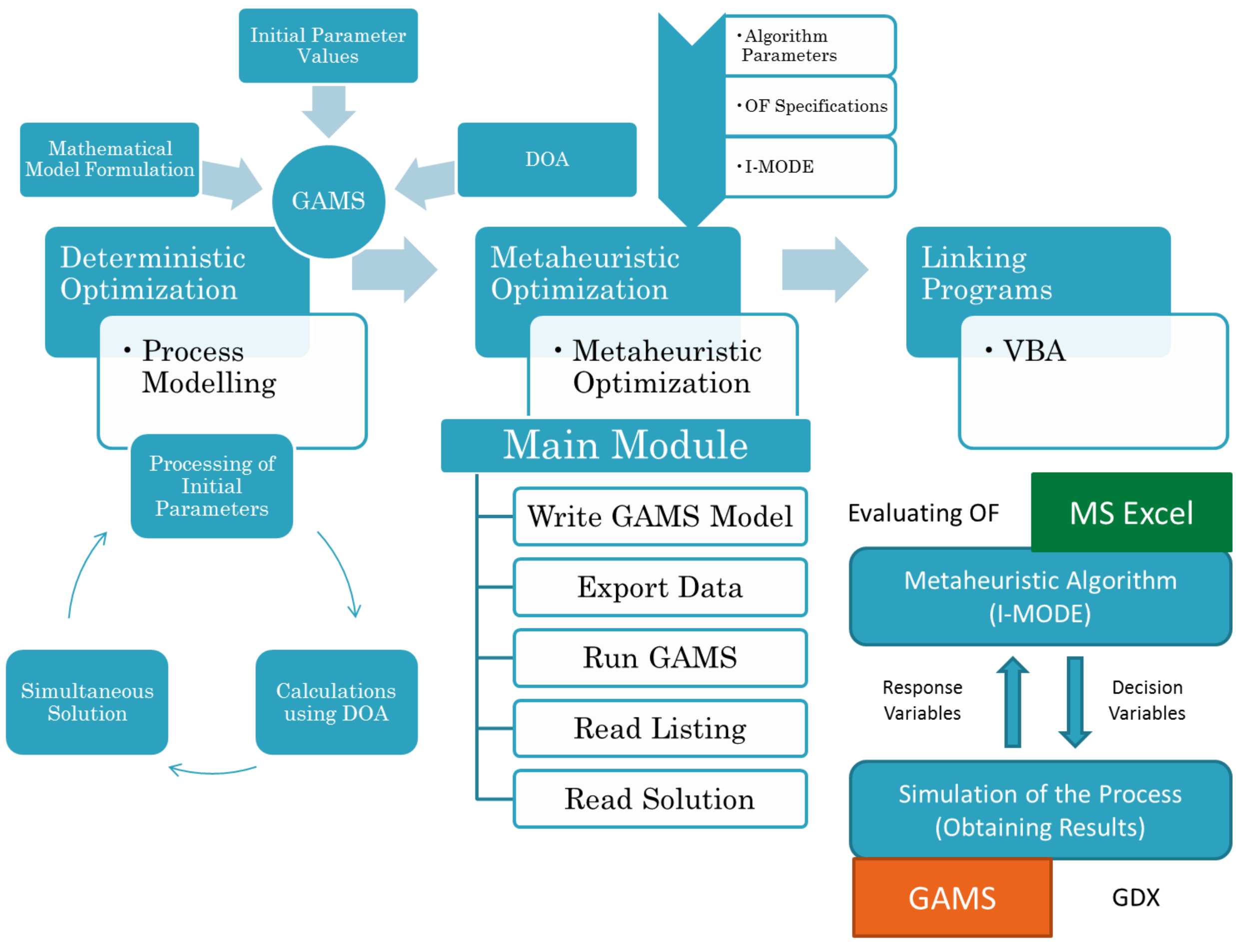

Figure 3-8: Methodological strategy for hybrid MOO.

3.4. USE OF STATISTIC FUNCTIONS TO CONSIDER UNCERTAINTY IN MOO METHODS

The methodological proposal of the optimization framework presented here consists of an algorithm by which values are generated randomly for certain parameters of the mathematical model or the function to be optimized. These parameter values are evaluated in conjunction with the values of the search variables and a value of the objective equation is obtained. Once the performance of each of these functions has been found with a certain set of search variable values and for each uncertain value, two new target equations are calculated using statistical metrics such as the mean and standard deviation.

A new approach to consider model uncertainty through metaheuristic optimization techniques is presented in this work. The methodological proposal consists of two fundamental parts, one stochastic and the other metaheuristic. Metaheuristic optimization algorithms are often referred to as stochastic due to the uncertainty with which they are inherently associated. However, when it is said that this is a stochastic optimization methodology using metaheuristic tools, it means that one part of the problem will be solved by proposing uncertain values while the other part will analyze said values of uncertain parameters with an evolutionary optimization algorithm. This way, the general optimization framework is made up of the stochastic optimization algorithm (SOA) and the metaheuristic optimization algorithm (MOA). Each of these algorithms will be described in detail in a later part of this text.

A code was implemented in visual basic for applications (VBA) to generate uncertain parameter values (UPV) at the same time that the MOA process is carried out. The MOA proposes random values of the decision variables (DV) and calculates the performance of the objective function (OF). This way, it is possible to evaluate the performance of multiple OFs by changing the UPV. After calculating the performance of all the individuals that conform to a generation, a statistical treatment of the data is made where a new OF is evaluated. The new OF that is evaluated consists of a statistical objective function (SOF). To obtain the SOF value, the calculation of a reformulated objective function (ROF) is necessary, which consists in the incorporation of different UPV in the original OF and after that using statistical indicators to choose the individual with the best performance. The statistical indicators used to select the best individuals of a generation are the mean and standard deviation.

The new proposed optimization strategy consists of the analysis of the performance of the specified OFs obtained with the DV values proposed by the metaheuristic algorithm with a set of UPV by a random values generator (RVG) code. This optimization strategy is implemented by a subroutine made up of multiple instructions in different code sections and developed in a VBA environment. The flowchart of the algorithm that describes this code is presented in **Figure 3-9**, where the algorithm sequence is described as follows:

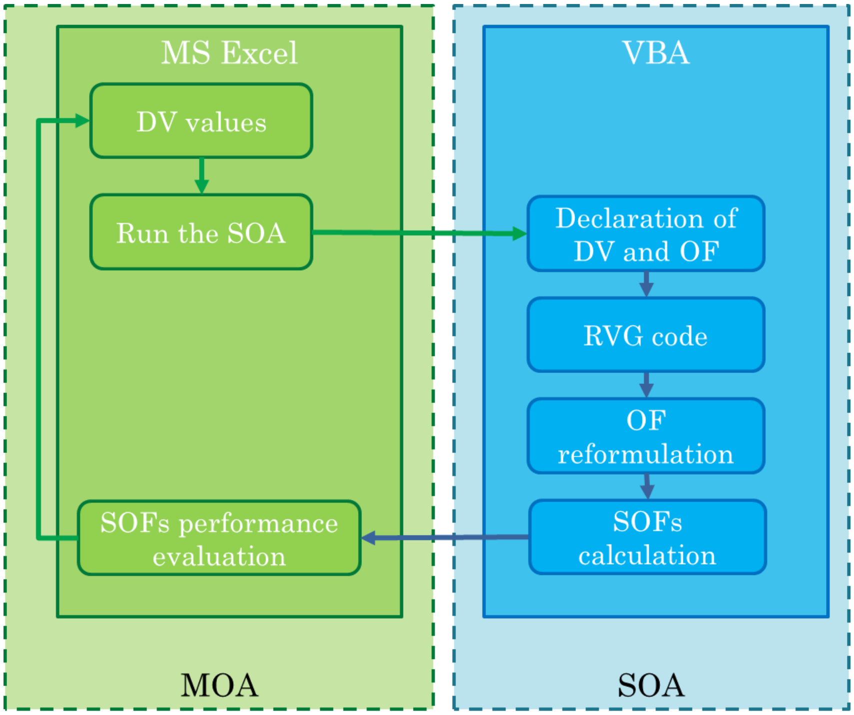

Figure 3-9: Methodological strategy for use of statistic functions to consider uncertainty in MOO methods.

1. **DV values by MOA:** Given the proper parameters of the selected optimization algorithm, I-MODE, such as population size (PS) and a maximum number of generations (MNG), it proposes DV values (chromosomes) that compose the possible solution set.
2. **Run the SOA for each set of DV and each iteration:** For each of these individuals, an SOA subroutine is run for the creation of UPV by the RVG code. This instruction is carried out in each individual or set of values of the DV and each generation or iteration of the MOA. In this subroutine, not only the UPV creation is carried out, but also the calculation of the OF is made and, by a reformulation, the SOFs are obtained.
3. **Return to MOA for SOFs performance evaluation:** The values of the SOFs calculated in the previous step, are sent again to the I-MODE algorithm to be evaluated in a multi-objective optimization framework. With this information, a new set of individuals will be generated according to the performance in the SOFs considering the MOA procedure.

It is especially important to clarify that the fundamental part of the contribution of this new methodology lies in the SOA. In this part of the general algorithm of the proposed methodology, the creation of UPV and the reformulation of the OF are carried out to send SOFs to the MOA and propose the new generation of individuals.

Another fundamental aspect that must be mentioned is that the analysis of a single-objective or mono-objective function problem is reformulated into a bi-objective function problem. This is because each OF involves the analysis of two statistical metrics, the mean and the standard deviation, each of which becomes a SOF that will be evaluated in the MOA. So, a bi-objective problem will be reformulated in four SOFs and the MOA will solve a multi-objective problem. To solve an optimization problem that is originally bi-objective, it is necessary to make changes to the SOA code, which involves declaring two OFs and twice SOFs.

3.5. MOO APPROACH BASED ON DETERMINISTIC AND METAHEURISTIC TECHNIQUES UNDER UNCERTAINTY

The development of a new multi-objective optimization methodology that allows the use of deterministic optimization and metaheuristics considering uncertainty is essential for optimal resource management in crisis scenarios such as what occurs during a pandemic.

In the present methodological proposal that is shown in this work, it is proposed to link the computer programs that allow the use of deterministic optimization in GAMS and metaheuristics through a DE algorithm programmed in MS Excel. The link between these programs is carried out through the action of a code or subroutine developed in the VBA environment. Likewise, it offers the user a simple and easily manageable interface developed in a program with which many users are familiar.

The review of the different optimization approaches that are carried out is to show that there are multiple types of problems and various alternatives to address them according to their nature. Likewise, to establish that even though efficient search procedures have been proposed in solving optimization problems with deterministic or metaheuristic approaches, but not both simultaneously, considering also the uncertainty associated with emergency scenarios. These types of problems are addressed because they are the ones that, due to their complexity, require a methodological strategy that involves the simultaneous use of different optimization algorithms, but it may well be used in other types of problems with associated uncertainty.

As mentioned previously, mathematical programming is a tool that consists of the representation of phenomena in models for their subsequent analysis and optimization. Optimization is a strategy to search for the best values that a decision variable can take with which the best possible performance of an objective function is achieved. However, the set of possibilities of configurations of a process (including those of transport) can become very exhaustive due to the large number of variables, equations, parameters, and restrictions that are involved in the mathematical model. For this, the implementation and solution of these mathematical models in a computational tool are essential.

Optimization strategy programming is possible from a root language such as C++ and Java. However, there are currently a variety of commercial programs with deterministic optimization tools, such as Lindo and Gurobi. MS Excel, which can also be used to contain a metaheuristic optimization program (Hernandez-Perez et al. 2020b). Thus, it can be used by itself for linking with the simulation program and optimizing the problem using parameters specified by the user.

In this paper, a linking program code (LPC) was implemented to link the GAMS program with MS Excel through VBA code. This strategy is done to send and receive data (like DV and objective functions values) from the deterministic optimization algorithm (DOA) that is carried out in GAMS, with the metaheuristic optimization algorithm (MOA) that is previously programmed in MS Excel. Likewise, a stochastic optimization algorithm (SOA) is proposed from which uncertain parameters values are created by the action of a random values generator (RVG) code, in this way the uncertainty is incorporated into the proposed optimization approach.

The methodological strategy proposed in this work consists of three fundamental parts, the MOA, the DOA and the SOA, each is described below:

- **Deterministic optimization algorithm**: The DOA is where the mathematical model is contained, which is successively solved in GAMS software from the values that the MOA generates. The DOA reads the values of the decision variables that the MOA generates through the LPC.
- **Stochastic optimization algorithm**: The SOA is part of the methodological proposal, developed in VBA environment, which is responsible for incorporating the uncertainty from the uncertain parameter values that create the RVG code. The SOA creates a

determined number of uncertain parameter values calling RVG code for each set of decision variable values. Therefore, several new functions must be analyzed in a statistical treatment and this way select the values of the objective functions that will be sent through the LPC to the MOA for its performance evaluation.

- **Metaheuristic optimization algorithm**: The MOA is the algorithm based on DE previously programmed in MS Excel. The MOA generates the sets of values (individuals) of the decision variable that may be the optimal solution. Likewise, it is in the MOA where the evaluation of the objective functions is carried out to select the sets of values with the best performance and propose new values for the next iteration (generation).

These optimization algorithms are independent and are commonly used separately, however, due to the complexity of the case study that is addressed in this work, a hybrid methodology is developed that allows the use of deterministic optimization simultaneously with the metaheuristic optimization tools, while incorporating uncertainty by a stochastic algorithm. Each of the algorithms that are part of the methodology are described in detail below.

In this work, a stochastic hybrid (deterministic and metaheuristic) multi-objective optimization algorithm is developed. Consideration of uncertainty is essential to analyze problems in which there is a high probability of change in the value of the parameters. There are several problems in which considering uncertainty offers a better picture of the general behavior of the analyzed phenomenon. Comparing the performance of different solution proposals in which the uncertainty associated with the change of parameter values within the model is considered allows a more realistic analysis of the problem to be addressed. This is because an alternative solution may well represent the best solution with fixed values of certain parameters, but the same proposal may have a lower performance if the value of these parameters changes randomly. In this way, the methodological proposal that considers the random manipulation of constants to consider the performance of a proposal calculated with the values of decision variables offers better resilient solutions to the random change of uncertain parameters. The general optimization approach is shown in **Figure 3-10**. The proposed methodology consists of the steps described below.

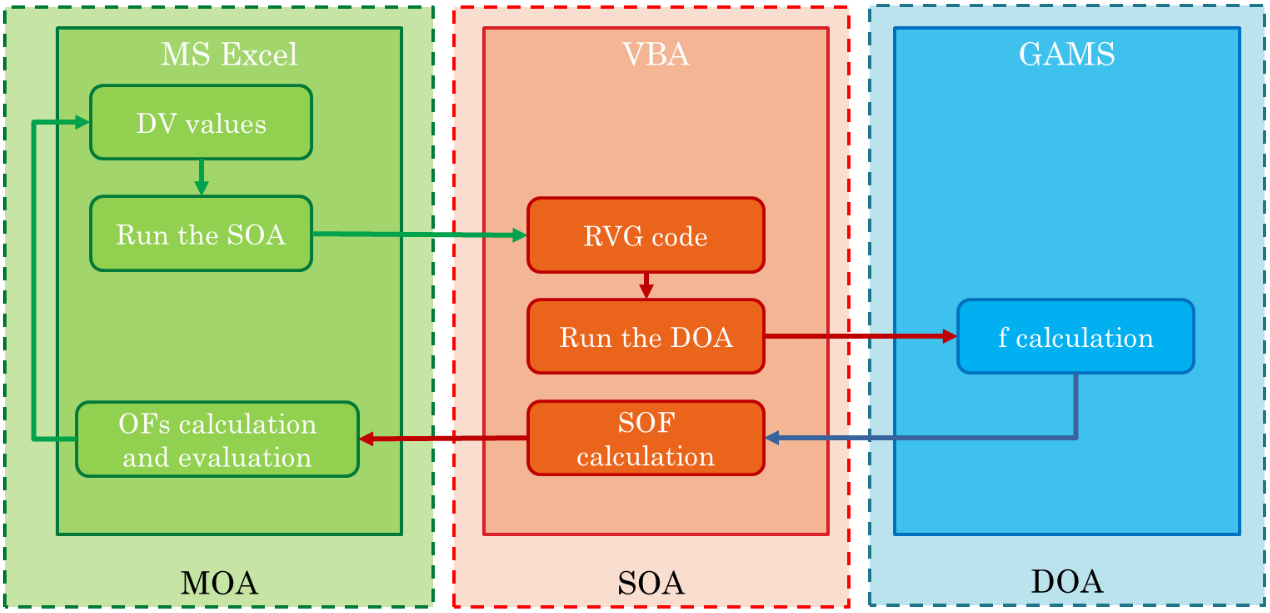

Figure 3-10: Methodological strategy for MOO approach based on deterministic and metaheuristic techniques under uncertainty.

1. **Decision variable values generation by MOA**: The MOA proposes sets of decision variable values that may be the optimal solution. The values proposed by the MOA are based on the user's specifications regarding the nature of the variable (continuous or integer) and their manipulation intervals. It is in the MOA where the number of sets of values of the decision variables (population size, PS) and the number of iterations (maximum number of generations, MNG) are declared. Likewise, in the MOA it is possible to declare inequality constraints and parameters for the operation of the metaheuristic algorithm.
2. **Uncertain parameter values creation by RVG**: For each set of decision variable values proposed by the MOA, the RVG assigns a specific number of uncertain parameter values. The number of uncertain parameter values is specified by the user in the SOA programming. After the execution of the RVG code, the SOA assigns the uncertain parameter values to variables of the MOA that together with the decision variable values are sent to the DOA.
3. **Sending decision variable values by LPC**: The values of the decision variables proposed by the MOA and the uncertain parameter values created by RVG are sent to the SOA by the action of the LPC. For this purpose, the LPC is composed of a set of subroutines or

macros developed in VBA that allow the exchange of data between the MOA and the DOA, that is, between the GAMS software and the MS Excel platform. The set of macros that allow the linking of programs can be complicated, therefore, if a more detailed explanation of the particular methodology for linking the MOA with the DOA is required, more detailed information about it can be found in Hernández-Pérez et al. (2020).

4. **Objective function values calculation by DOA**: In DOA, the single-objective optimization process is carried out. From the values of the decision variable proposed by the MOA and the uncertain parameter values created by the RVG of the SOA, the deterministic optimization process of a single-objective is carried out considering these variables as parameters in each iteration of DOA in GAMS. The calculation of the objective function in the DOA is made for each individual in the population and for each UPV.
5. **Importation of the objective function value by LPC**: After the calculation of the objective function value in the DOA, this value is sent back to the SOA by the LPC.
6. **Objective function statistical treatment in SOA**: Once the objective function values for each set of decision variables and uncertain parameter values are calculated and imported into the SOA. After that, a statistical treatment is carried out with the values of the objective functions. This statistical treatment consists of calculating the mean of the set of values of the objective functions. This new objective function is called the statistical objective function.
7. **Statistical objective function performance evaluation in MOA**: Finally, for each individual in the population in each iteration, performance evaluation of the statistical objective functions calculated by the SOA is made. For this purpose, the statistical objective function is considered as one of the objective functions in the MOA. In this part of the proposed methodology, the performance evaluation of the objective functions is made to propose the values of the new individuals according to the selected metaheuristic optimization procedure.

By following the steps mentioned above, it is possible to use deterministic optimization simultaneously with metaheuristic tools and consider uncertainty. This methodology can be applied in solving the problem of optimal resource management for health crisis scenarios such as those that occur during a pandemic.

4. RESULTS

To test the efficiency of the new proposed methodologies, five case studies were addressed as described below:

4.1. CASE STUDY 1: STRUCTURAL AND OPERATING OPTIMIZATION OF THE METHANOL PROCESS USING A METAHEURISTIC TECHNIQUE

This paper has presented a multi-objective optimization method for the methanol production process with simultaneous consideration of the economic and environmental aspects. The economic function is maximized while the environmental function is minimized. The solution strategy developed to solve the multi-objective problem involves a new approach to couple black-box models and computer-aided simulation with metaheuristic optimization approaches. A client-server interface was created using COM technology to control the simulator software repetitively for multiple sets of variables. A multi-objective optimization hybrid method (I-MODE) was used with a termination criterion using the non-dominated solutions obtained as the search progresses. The I-MODE algorithm determines graphics at steady stage termination criterion and after the maximum number of generations where different points (objective functions values at sets of decision variables values) are shown and decision-maker can choose the best option.

The proposed methodology was applied to a case study about a methanol production process. The change of the values on the search variables significantly impacts the performance of the objective functions, mainly in the entire annual emissions of CO_2, which were reduced (except in Case 4 where there was an increase of 2%) up to 17% in the obtained solutions (in Case 5 and in Case 7 there was not a change), whereas the total annual income presents an increase up to 45% (except in Case 6 and Case 7, where there is not a considerable change of the value for NP). Even in case 2a, in which the value of the NP was negative from the real values, there was a 7% improvement in said objective function which represents a smaller amount of losses. Likewise, the operating conditions found for this case represent a 12% reduction in the TAE. The results indicated that a slight manipulation of the operating conditions allows finding a better performance of the objective functions. Likewise, the use of metaheuristic tools allowed to make the selection of the best structural configuration when simultaneously comparing the performance of the two objective functions in the best operation values of the search variables.

An important aspect that can be concluded from this research is that the variables that are considered as well as the search intervals are decisive in the obtained results. In this work, it was decided to work with variables whose manipulation definitely has a considerable impact on the performance of the objective functions. Likewise, it was observed that specifying a very large number of MNG as well as of i, generated inflexible solutions that ended with stopping the algorithm. The parameters of the use of the evolutionary algorithm proved to be efficient in solving this particular case. The simultaneous analysis of the possible configurations previously raised in the process flow diagrams and simulated in the software, allows not only to find the best-operating conditions of each one, but also to choose among all of them which are the ones that have the best performance, as reported in this work (**Figure 4-1**).

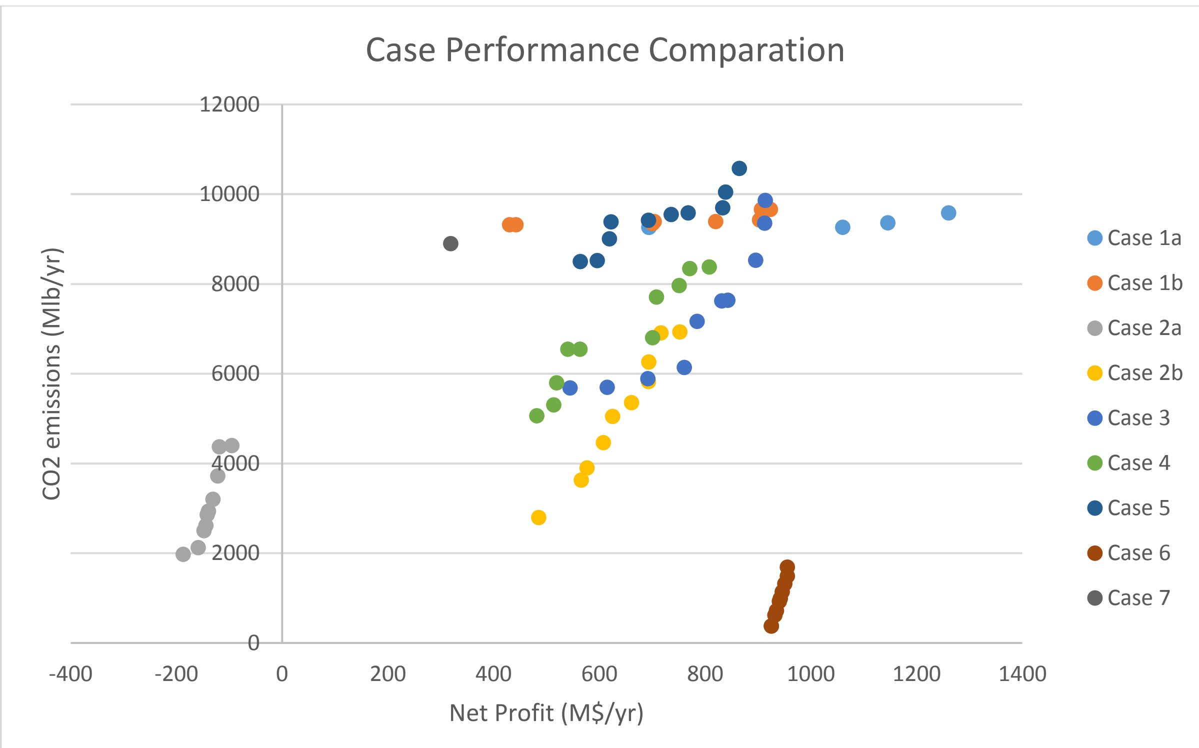

Figure 4-1: Case Performance Comparation.

For more information on the implementation of this methodology in the case study, consult the following sources: Hernández-Pérez et al. (2020a) and Hernández-Pérez et al. (2021a).

4.2. CASE STUDY 2: SIMULTANEOUS STRUCTURAL AND OPERATING OPTIMIZATION OF THE SOLAR-GRADE SILICON PROCESS

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 (Solar-Grade Silicon Process) 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 Case 2, whereas the Total Profit 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 (**Figure 4-2**).

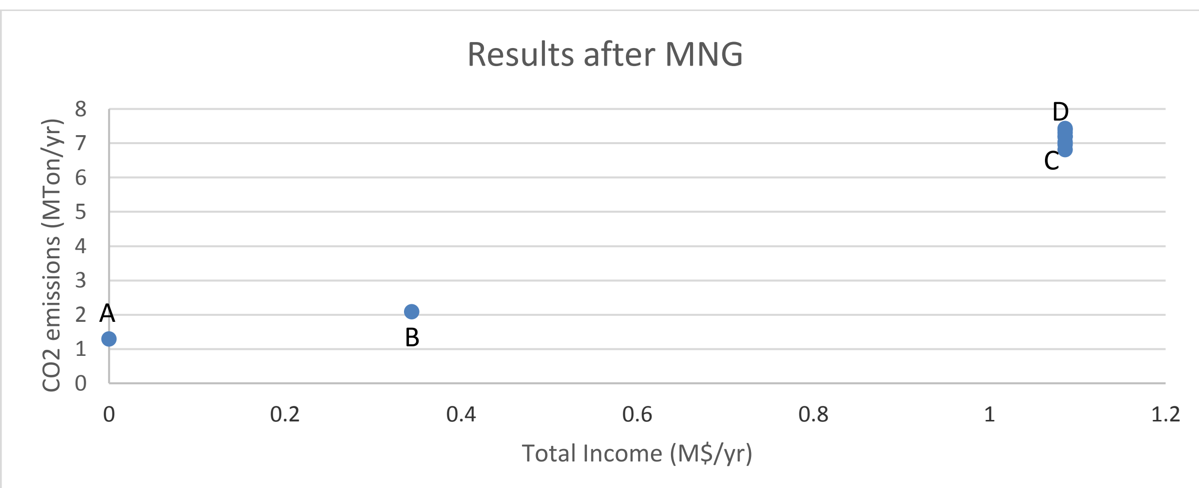

Figure 4-2: Results after maximum number of generations for Cases 1 to 3.

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.

For more information on the implementation of this methodology in the case study, consult the following source: Hernández-Pérez et al. (2020b).

4.3. CASE STUDY 3: HYBRID MOO FOR FLOWBACK WATER REUSING IN HYDRAULIC FRACTURING PROCESSES

This work has presented a new multi-objective optimization methodology using deterministic and metaheuristic techniques. The program to solve the deterministic problem was GAMS and the metaheuristic used technique is the I-MODE algorithm, coded in VBA. A linking code is developed through VBA to run the GAMS solver. The proposed methodology consists in manipulating some parameters in the GAMS problem and evaluating the OF performance in the I-MODE algorithm.

The proposed methodology was applied to wastewater management in HF processes. However, this methodology is general and it may be applied to the solution of other complex problems. It should be noticed that the analysis of a simple model would not be a candidate to use this methodology, since it precisely consists in solving complex problems. In general, the proposed methodology allows the solution of problems through the intercommunication of programs in which a part of it is solved using deterministic optimization and another metaheuristic optimization. The results that are offered are attractive for the economic and environmental objectives that were intended to be solved in the HF process to obtain shale gas and better concerning those found by setting the well scheduling (**Figure 4-3** and **Figure 4-4**). The use of real data in the mathematical model can offer a correct prediction of the resulting values that would be obtained in reality. This way, the proposed optimization strategy can be used to make decisions in a problem of flowback water management in the extraction of shale gas in an existing real-world situation.

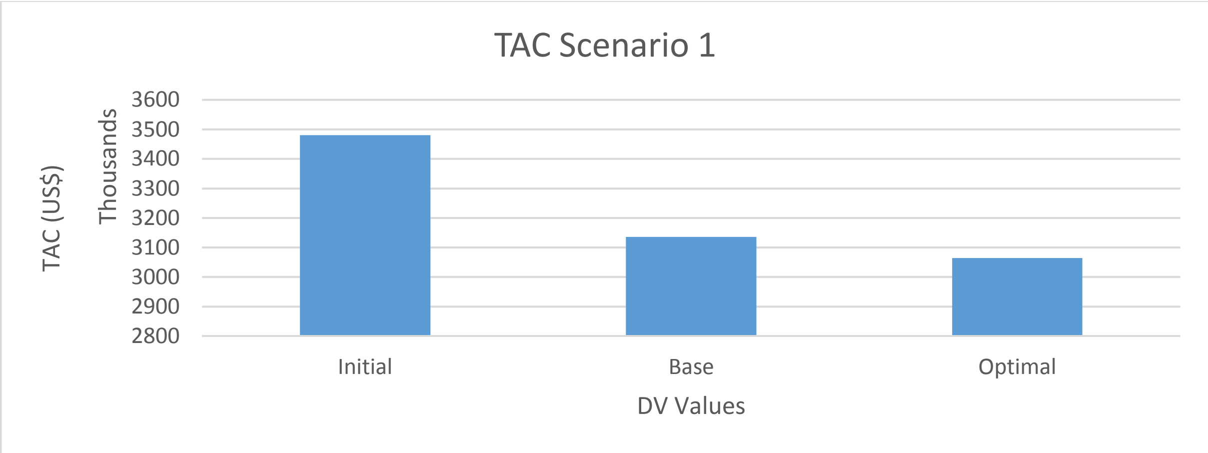

Figure 4-3: TAC performance comparison with each strategy in Scenario 1.

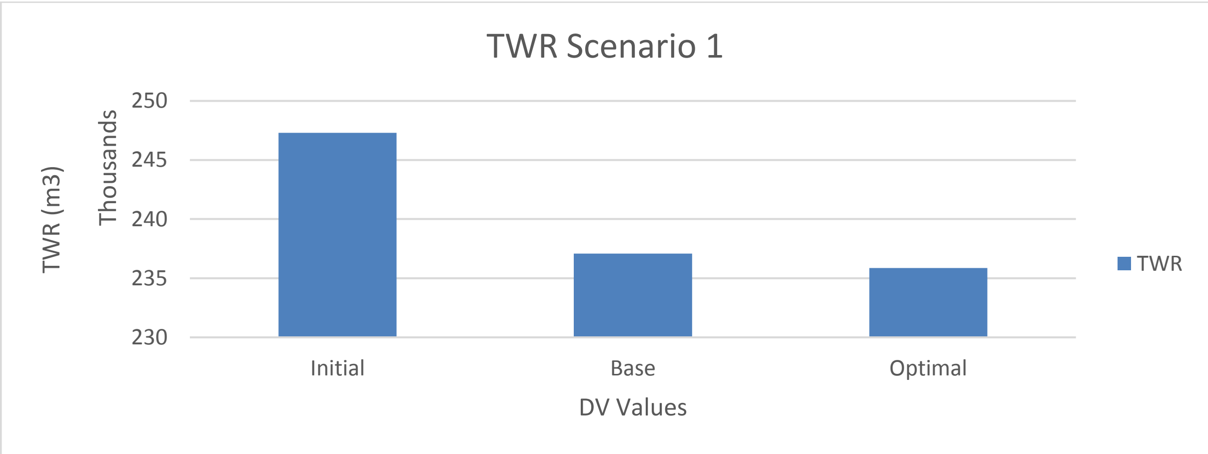

Figure 4-4: TWR performance comparison with each strategy in Scenario 1.

The use of the present methodology allowed the exploration of different scenarios in which the exclusive use of deterministic algorithms would have implied numerous infeasibilities and the use of convexification strategies would have been necessary.

For more information on the implementation of this methodology in the case study, consult the following source: Hernández-Pérez et al. (2020c).

4.4. CASE STUDY 4: USE OF STATISTIC FUNCTIONS TO CONSIDER UNCERTAINTY IN MOO METHODS

This work proposes a new methodological strategy to solve optimization problems in which it is necessary to consider uncertainty through the use of metaheuristic algorithms. To achieve the implementation of the proposed methodology, the manipulation of two essential parts is specified, the metaheuristic and the stochastic optimization algorithms.

About the MOA, it is important to highlight that it is a search algorithm based on metaheuristic optimization frequently used in the solution of problems were the conventional deterministic strategies are not efficient. The MOA can be any optimization algorithm based on evolutionary algorithms or DE that allows the solution of complex problems, non-linear models, and potentially highly non-convex problems. The selected MOA is the I-MODE, because it has proven to be efficient in various general optimization methodologies.

Regarding the SOA, this consists of the creation of random values for the UPVs in the RVG code. Likewise, the SOA implies the reformulation of the original OFs in ROFs by incorporating the UPV values in the mathematical model that defines the OFs. Subsequently, a statistical treatment of the ROFs is made and the SOFs that correspond to the mean and the standard deviation of the ROFs are calculated.

In solving the case studies, a numerical constant was manipulated in the objective equation for each of them, however, this methodology can consider the manipulation of more than one uncertain parameter per function. Likewise, the UPV was declared in the RVG to generate integer random values, however, they can also be manipulated so that continuous random values are generated.

The proposed methodology was applied to the solution of 3 case studies. This method was approached from two perspectives, in the SOPs only one objective function is considered, while in the BOPs the 2 objective functions (Osyczka test) are considered. For the case studies, complex equations, constraints, and manipulation intervals for DVs were considered (**Figure 4-5** and **Figure 4-6**).

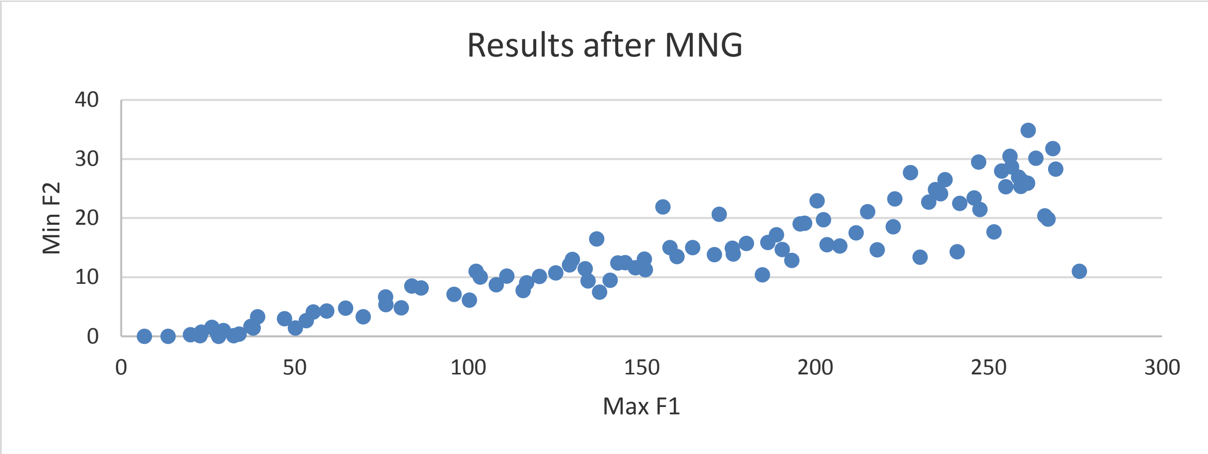

Figure 4-5: Results after MNG for Case Study 3 for OF1 and OF2.

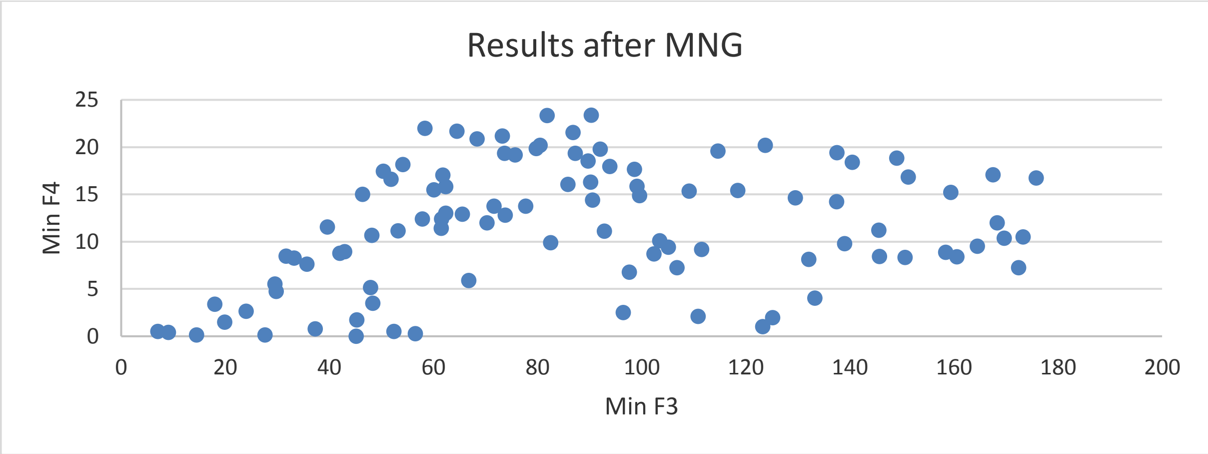

Figure 4-6: Results after MNG for Case Study 3 for OF3 and OF4.

In general, the optimization strategy can find the solution, through the use of metaheuristic techniques, of single-objective and bi-objective optimization problems, complex problems, non-linear models, and potentially highly non-convex problems where is necessary to consider uncertainty. Likewise, following the same indications in the pseudo-code presented, it is possible to analyze multiple OFs with more than two objectives (bi-objective problems).

The main advantage offered by the use of the new proposed methodology with respect to those previously reported, consists in the simultaneous consideration of the performance value of a population of reformulated objective functions in which random parameters are considered. This allows a comparison, through statistical analysis, of the performance of the objective functions if uncertainty is considered. Thus, the metaheuristic optimization algorithm selects the best alternative solution for a function or set of functions, subject to change due to the random behavior of some constant value in the mathematical expression.

An analysis of the behavior of the algorithm is as follows: if for each solution proposal we consider not the performance of the function or functions, but the value of the average and the standard deviation of a set of performance values of reformulated objective functions, this allows the algorithm to select the best proposals for the next generation that not only have good values of the decision variables, but are also resistant to random changes.

However, it is also important to highlight, in which cases it is not advisable to use this methodology. As can be seen from the graphs resulting from reaching the selected termination criterion of the metaheuristic optimization algorithm, twice as many values of objective functions are obtained from those originally proposed in the problem. Therefore, the use of the proposed method is not recommended for solving problems that have many objective functions. As can be seen from the case studies, it works well for single-objective and bi-objective problems.

The fundamental idea of proposing this type of multi-objective optimization strategies is to apply it in the solution of complex real-world problems that require the use of unconventional strategies for their solution. The methodology proposed in this work may well be used in the solution of more complex schemes to solve sustainability aspects, specifying objective functions of costs and social aspects.

For more information on the implementation of this methodology in the case study, consult the following source: Hernández-Pérez and Ponce-Ortega (2021b).

4.5. CASE STUDY 5: MOO APPROACH TO RESOURCE MANAGEMENT IN HEALTH CRISIS SCENARIOS UNDER UNCERTAINTY

This work has presented a new multi-objective stochastic optimization framework based on deterministic optimization and metaheuristic tools to solve complex problems considering uncertainty. Also, the user is offered a familiar and easy-to-use interface to quickly manipulate the values and make appropriate decisions in each possible scenario that the advance of the pandemic may form.

The methodology presented in this work consists of solving the problem using different algorithms: DOA, SOA and MOA. The MOA proposes values of the decision variables, the total capacity to attend patients with the current capacity plus the capacity due to the medical equipment acquired. The SOA creates random values of the uncertain parameters to bring the uncertainty to the model. Based on the values of the decision variables of the MOA and the uncertain parameter values of the SOA, the DOA solves the patient distribution from the origin hospitals on demand to the destination hospitals that can serve them, either with the medical equipment available or acquiring new.

To test the effectiveness of this method, the case study of the optimal distribution of resources in health crisis scenarios such as those that occur during a pandemic is addressed. The data used to make the analysis of the specific case study correspond to those of the current COVID-19 pandemic caused by SARS-CoV-2. It also considers a balance of patients who require hospitalization to update the distribution requirements. If this methodology is used, it is possible to establish the best patient distribution.

For the solution of the scenarios that are addressed in the case study, real data reported by the WHO of the COVID-19 pandemic were used. These data were collected on September 1, 2020; however, it is possible to update the numbers and run the optimization methodology presented here again. Likewise, it is possible to change the data of distances between locations, capacities and demands. As for the uncertainty, a different interval can be manipulated to create uncertain parameters.

Optimization functions obey the fulfillment of two simultaneous objectives, one social and the other economic. The social objective corresponds to minimizing the number of rejected patients, thereby increasing the chances of saving lives. While the economic objective corresponds to minimizing the total costs of both transportation and acquisition of medical equipment (hospital beds and ICUs). The results show the optimal configuration of the medical equipment acquired by analyzing medical resource 1 (hospital beds) and medical resource 2 (ICUs) as well as the adequate distribution of patients from hospitals on-demand to destination hospitals that can attend them considering the uncertainty associated with changes in demand (**Figure 4-7** and **Figure 4-8**).

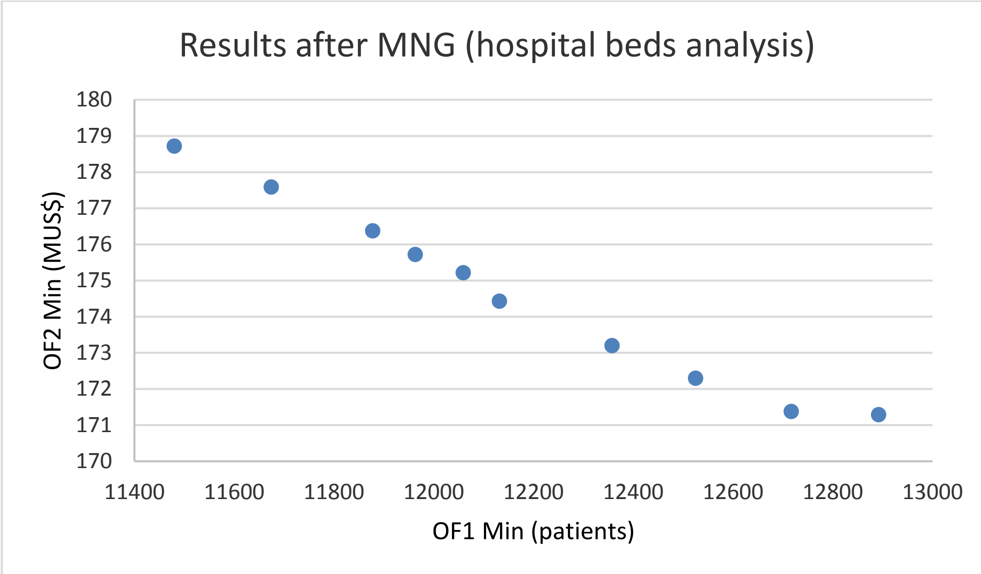

Figure 4-7: Results after MNG for medical resource 1 (hospital beds).

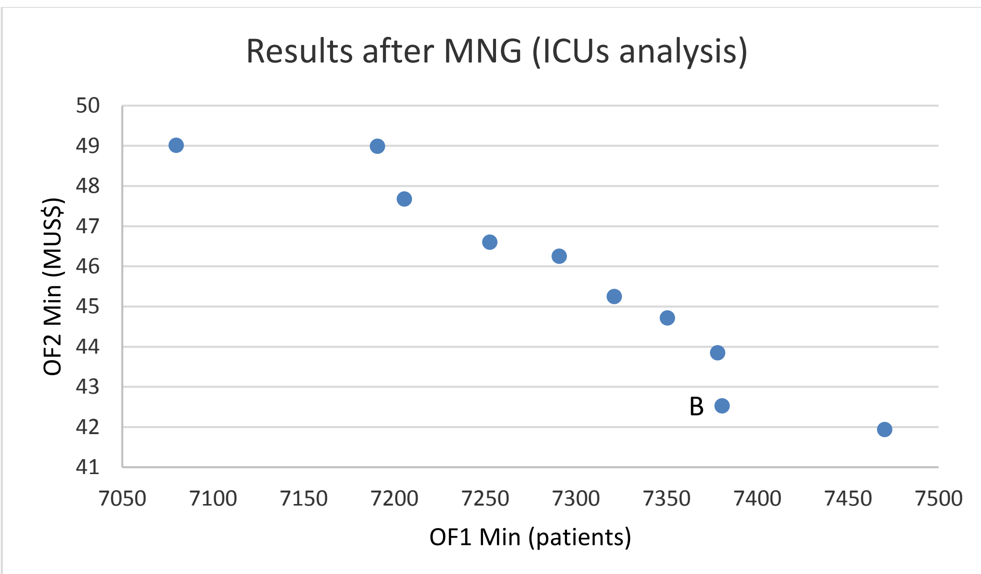

Figure 4-8: Results after MNG for medical resource 2 (ICUs).

The methodological proposal presented in this work is general and can be applied to solve other problems in which it is necessary to analyze different solution alternatives where there is uncertainty associated with parameters within the model. This methodology can be used in different deterministic models with other data and by specifying search variables different from those specified in the metaheuristic tool. This makes possible to analyze the sustainability of multiple processes looking for the most efficient solutions with social, economic, and even environmental objectives.

For more information on the implementation of this methodology in the case study, consult the following source: Hernández-Pérez and Ponce-Ortega (2021a).

CONCLUSIONS

- A client-server interface was created using COM technology in order to control the simulator software repetitively for multiple sets of variables. A multi-objective optimization hybrid method (I-MODE) was used with a termination criterion using the non-dominated solutions obtained as the search progresses. The I-MODE algorithm determines graphics at steady stage termination criterion and after the maximum number of generations where different points (objective functions values at sets of decision variables values) are shown and decision-maker can choose the best option.
- The main contribution of the present optimization approach is to combine process simulators with metaheuristic techniques for simultaneous optimization of process flowsheets with the corresponding operating conditions. A method through which it is possible to analyze simultaneously multiple configurations of the same process is proposed; 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 the next generations displacing the configurations with the worst objective function values. In a conventional way to search for an optimal solution, it is necessary to simulate each configuration with possible sets of values until a termination criterion is reached, which consumes considerable computational time. However, with the method proposed here, it is possible to find the best-operating values in the best configuration in the equivalent computation time to perform the search in a single case.
- This work has presented a new multi-objective optimization methodology using deterministic and metaheuristic techniques. The program to solve the deterministic problem was GAMS and the metaheuristic used technique is the I-MODE algorithm, coded in VBA. A linking code is developed through VBA to run the GAMS solver. The proposed methodology consists in manipulating some parameters in the GAMS problem and evaluating the OF performance in the I-MODE algorithm.
- This work proposes a new methodological strategy to solve optimization problems in which it is necessary to consider uncertainty through the use of metaheuristic algorithms. To achieve the implementation of the proposed methodology, the manipulation of two essential parts is specified, the metaheuristic and the stochastic optimization algorithms.

- This work has presented a new multi-objective stochastic optimization framework based on deterministic optimization and metaheuristic tools to solve complex problems considering uncertainty. Also, the user is offered a familiar and easy-to-use interface to quickly manipulate the values and make appropriate decisions in each possible scenario that the advance of the pandemic may form.

RECOMMENDATIONS AND FUTURE WORK

This work proposes a series of general methodologies to solve complex multiobjective optimization models of highly non-convex problems, therefore, using the strategies proposed here, multiple problems can be solved with a set of scenarios and possibilities in which due to the complexity of the model, conventional optimization strategies cannot be used. For future work, it is possible to develop a general multiobjective optimization strategy of a highly non-convex problem using deterministic optimization for the linear part of the model and metahuristics for the non-convex part, in this way an optimization by parts can be done; an interesting case study to address this type of methodologies is in the use of waste heat.

Another line of opportunity to develop the proposed methodologies is the use of an exploration of different possibilities for the number of variables to optimize, this requires complex programming to vary the number of variables that are considered in the metaheuristic optimization algorithm, a case of an interesting study to analyze these schemes is the consideration of uncertain resources (such as water) in the shale-gas extraction process by means of hydraulic fracturing.

A very complex problem where the proposed methodologies can be tested is in the case study of the water-energy-food nexus (WEF) where it is also very important to consider the uncertainty, in this type of problems it would be very novel to consider three objective functions simultaneously, which can be an economic, an environmental and a Social.

Likewise, a multiplatform optimization methodology can be developed that combines the different optimization schemes proposed here, that is, linking a process simulator with a deterministic optimization solver and a metahuristic optimization algorithm.

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