I&EC research
Industrial & Engineering Chemistry Research

Article

Cite This: Ind. Eng. Chem. Res. 2019, 58, 18684−18702

pubs.acs.org/IECR

110th Anniversary: On the Departure from Heuristics and Simplified Models toward Globally Optimal Design of Process Equipment

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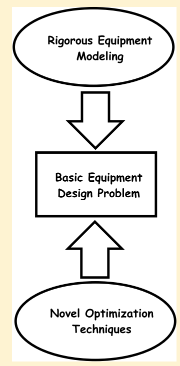
ABSTRACT: Despite the large advances in computational tools attained by the Process Systems Engineering community, industry for the most part still performs basic design of process equipment using trial-and-verification procedures guided by heuristic rules. In this opinion article, we present a discussion on how to depart from the use of these heuristics-based procedures, most step-by-step, sometimes computer-aided. We believe that there are direction changes, some incipient and some in full development already, toward the use of optimization tools for the task. The academic literature is dominated by mixed-integer nonlinear models, solved using different techniques (mostly stochastic or mathematical programming-based). These procedures have practical limitations that have hindered the migration of practitioners away from current heuristics and simplified model-based tools. We discuss these drawbacks and propose solutions. We first show how the use of commercially available discrete values of the design geometrical variables followed by reformulation can render linear models, solved using mixed-integer linear programming, sometimes integer linear programming. We also show how reformulation or judicious discretization of continuous variables can lead to a large reduction in the number of nonlinearities, such that they can be solved using commercial and noncommercial global solvers with larger efficiency and robustness. Next, we present the use of set trimming to aid global optimization of equipment designs, as means of reducing the search space. Then, we present the technique of smart enumeration, which can be used instead of MINLP models and eventually after set-trimming. We also discuss changes in modeling and propose to move away from simple models, where we argue for abandoning physical properties as well as transport-like coefficients that are based on averages, to use properties and transport coefficients calculated locally inside and along the equipment. Then, we discuss the impact of the above proposals on flowsheet synthesis and retrofit problems. As these advances show higher memory and speed needs, we discuss how parallel computing (using the cloud, small computer clusters, or supercomputers) can address the aforementioned challenges.



1. INTRODUCTION

Even though the last decades have seen an explosion of simulation and optimization tools in the area of Process Systems Engineering (PSE),[1−5] it has had limited impact in the practical procedures for basic design of equipment (heat exchangers, condensers, reboilers, distillation columns, absorption, adsorption columns, etc.) in the chemical process industry. The use of heuristics-based and rules of thumb-based step-by-step procedures continues to be dominant in engineering practice. In addition, the existing design-optimization approaches are based on simplified models, averaged properties and parameters, and are rarely replaced by optimal design procedures that consider geometrically local physical properties, even though there are good simulation methods. Finally, flowsheet optimization uses even more simplified models that ignore most of the equipment geometry. Thus, heuristics and rules of thumb need to be abandoned, models need to be improved, and solution procedures need to overcome speed and memory problems.

We start making the wording more precise: basic process equipment design consists of generating a set of geometrical data of the apparatus, so that a detailed designer can translate these data into a construction blueprint. For example:

- For shell and tube heat exchangers, the basic data consist of selecting the number of shells, shell diameter and length, number of shell and tube passes, tube diameter, number of tubes, number of baffles, baffle cut, etc.[6,7] Other exchangers, such as plate exchangers, double-pipe hairpin heat exchangers, etc. have similar data.
- For trays distillation columns, aside from the number of trays and the feed tray location, the basic design involves the selection of the column diameter, type of tray, tray spacing, number of tray passes, etc.[8]
- For packed distillation columns, the basic design consists of the selection of the diameter, height, packing type and size, number of liquid redistributors, etc.[8]
- For reactors, the basic design includes reactor type (e.g., tank reactor × tubular reactor), diameter, length, number of tubes, etc.[9]
- For vapor−liquid equilibrium (VLE) and vapor−liquid−liquid equilibrium (VLLE) separation equipment, the data consists of diameter, height (or length), inlet and

Received: May 15, 2019
Revised: August 14, 2019
Accepted: August 20, 2019
Published: August 20, 2019

outlet nozzles position, demister type, size, and position, etc.[8,10]

One of the key reasons to have this level of geometric dimensioning at the basic engineering calculations is to get a better assessment of costs, before moving to the detailed engineering phase where blueprints are generated, thus avoiding quick and inaccurate simplified models. Other reasons for increasing the level of detail in the phase of basic engineering are the need to anticipate good control, the need to anticipate efficiently the CO_2 emissions and other pollutants discharge/treatment, etc. Indeed, for FEL 1 (Front-End Loading Appraisal and Selection Phase), referred to as Alternatives Evaluation and Preliminary Process Design, there is a need of accurate costing so that the phase of selection, which includes preliminary design, is successful. For FEL 2, which is known as Front End Engineering Design Study (FEED), equipment is to be designed to satisfy safety and reliability, equipment data-sheet as well as P&ID, utility balances, etc., and it is known to have an uncertainty between −20% and +40% of the cost estimate. All this information feeds FEL 3, the Detailed Process Design Package also known as Schedule A or Basic Engineering Design (BED). The list of items of FEL 2 is augmented by adding drawings, buildings, relief systems, HAZOP studies; the uncertainty of the cost estimate is limited between −15% and +25%. Industrial practice in design and retrofit makes frequent use of manufacturer produced estimates of equipment cost, usually in an iterative manner, even at the FEL 1 level.[11] Most of the time, it is at this level alternative flowsheets are explored, by analogy of previous designs performed by experienced designers nowadays with the aid of simulation and some optimization tools. It is therefore imperative that the industrial community is fed by increasingly accurate tools that can best screen structural alternatives.

The philosophy of trial and verification is the established mainstream paradigm in educational books and in many specialized texts.[6−8] The main idea is that designers (who many times need to be experienced) propose equipment geometries and other operational parameters (trial step) and then feasibility is tested (verification step). When the verification step fails, the designer makes judicious changes that can vary from designer to designer, until feasibility/viability is achieved. The procedure rarely encourages improvements based on new trials after the design is verified as viable, or some sort of optimization. Traditional procedures rely on designer experience, but the downsizing of engineering staff associated with the retirement of the baby-boomer generation yields a shortage of specialized personnel at engineering companies.[12] While some advances took place in using optimality as design criteria within the PSE community, the mainstream educational system and the established practices in industry seem to have a huge inertia to adapt and to adopt a new basic design philosophy.

As it will be outlined throughout this article, there is a need to depart from trial-and-verification procedures toward model-based, optimization-driven procedures (stochastic or mathematical programming-based), an activity that has already started.

At this point in time, we feel it is important to also clarify the nomenclature used. We call those sets of equalities and inequalities based on equations containing algebraic or transcendental functions and also differential equations that define a region in hyperspace a mixed integer nonlinear model (MINLM). Any point that is inside this region is called a candidate point, that can be feasible or not. When a function of these candidate points is maximized or minimized, most of the time a unique point emerges as optimal. To obtain this point, various classes of procedures exist: (a) stochastic (simulated annealing, genetic algorithms, particle swarm optimization, etc.), (b) mathematical programming-based (NLP, MILP, ILP, MINLP, disjunctive programming, MPCC, MPEC), and (c) enumerative-based, where the objective function corresponding to given integer combinations of binary variables are evaluated, either exhaustively or using some stopping criterion. Many branch and bound procedures are said to be an "implicit enumeration", which is different from the enumeration we refer to in (c), which is for that matter, "explicit". Many times, a MINLM, is referred to as a "MINLP model", a nomenclature that we believe is incorrect; this is because the mathematical model that describes the behavior of the system and the algorithm to solve the corresponding optimization problem are different concepts. It is up to the PSE community in the future to use this distinction that we propose. In our analysis we focus on the last two optimization approaches (b and c) because the first (a) cannot guarantee global optimality. It requires procedure parameters to be tuned with ad-hoc procedures that have not proven to be amenable to automation or generalization to other problems and even to other case studies. To ameliorate some computational problems presented by MINLP as well as MPCC/MPEC tools or disjunctive programming approaches, we discuss a rigorous reformulation of these models without making approximations, rendering MINLMs with smaller number of nonlinearities, or even mixed integer linear models (MILMs).

Despite the existing advances just mentioned, an important limitation of PSE tools that hinders a more pervasive and more efficient utilization for basic process design in practice is the nature of the mathematical models employed. Indeed, basic design approaches presented in the optimization literature use what we called uniform properties models, where physical properties are based on averages of input/output values, and where the derived transport coefficients are based on said averages. One example is in the area of heat exchanger (shell and tube, plate, air cooler, etc.), for which heat transfer coefficients are based on physical averages of the properties, when it is known that they can vary inside the equipment, especially when phase change or large variation of temperatures take place. In the literature, many times some models are referred to as "lumped" models when variables that vary in space are assumed spatially uniform and are used instead of the full distributed representation. In our case, we make the distinction between uniformity of properties (like the same density, viscosity, heat capacity, etc.) used for all calculations along the equipment or not uniformity, but we do not preclude variations of the state variables (temperature, pressure, etc.) throughout it. In this article, we explore the idea of using models based on distributed values of properties linked to varying state variables (temperature, pressure, etc.).

The current practice of engineering involves the analysis of process flowsheets exploring the interconnections among the different equipment, mostly using simulators. Simulators allow the use of simple (heat exchanger models based on user-inputted overall heat transfer coefficient, Fenske-Underwood columns, etc.) or more sophisticated models (mesh or rate-based equations for distillation columns, HTRI models for

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

exchangers, etc.) to describe equipment behavior.[13] Some simulators offer limited optimization of the flowsheet, but the optimization does not include structural aspects. In other words, structural optimization of the flowsheet, as well as optimal design of its embedded equipment (simultaneous or not) have not significantly reached engineering practice using simulators. The reasons are varied, and we explore some of them briefly in this article.

Finally, despite the reformulations we propose, there are computational issues that will need addressing in the future. These are speed and memory problems, which we propose to solve using parallel computing.

This paper presents a discussion about how the obstacles for the application of optimization approaches to solve design problem in practice can be eliminated through the application of reformulations, more accurate models, and parallel processing to ameliorate computational issues associated with obtaining globally optimal solutions. We first discuss the nature of heuristics-based procedures (section 2). Next, we discuss the use of nonlinear models and optimization methods for equipment design, including their reformulations and associated computational issues (sections 3, 4, and 5). Later, we discuss set-trimming and enumeration as means to solve design optimization problems (section 6) and explore the utilization of models based on variable properties (section 7). We also analyze parallel computing as means to address emerging time and size problems (section 8). Finally, we discuss the application of the proposed ideas to entire process flowsheets (section 9).

2. HEURISTIC-BASED TRIAL AND VERIFICATION PROCEDURES

Trial-and-verification procedures for the design of process equipment propose one particular solution, many times guided by some preliminary estimates and/or the experience of the designer and follow with a set of steps based on heuristics and rule of thumb choices until the complete geometry is obtained. This result is then tested to see if it achieves the process equipment required goals. We call this "verification", that is, if the geometry is viable in this sense, then the procedure usually stops. These procedures do not focus on cost minimization. When the verification step does not render a viable design, they require the intervention of knowledgeable personnel to make new good choices and start over from the beginning or from some intermediate step. When the verification step identifies a viable solution, it is not known at that point whether this solution can be improved in terms of its cost (investment plus operational), that is, there are no optimality tests. Most practitioners acknowledge that a better design can exist, but they stop at that point nonetheless, or assume that an improvement would be marginal or that there is no more time available to fulfill the task.

Some attempts may be made that stem from common sense exhibited by experienced designers to reduce costs (like increasing its length, and reducing its shell diameter), but without any formal application. The above notwithstanding, some commercial software have routines that try to emulate the heuristic search for a design solution automatically, but their results present limitations. For example, Caputo et al.,[14] who developed a genetic algorithm for heat exchanger design, compared their results very favorably to HTRI, who have a very good rating software that employs distributed models and up-to-date correlations, but the presumably optimal or acknowledged suboptimal design solutions are obtained using simple search algorithms. Finally, modern computational procedures have allowed the utilization of more accurate tools for verification (i.e., CFD and others), but not for design optimization.

In the case of heat exchangers, heuristic procedures based on trial and verification are presented in most design books[8] and heat transfer technology books.[6,7] They are typically based on the following set of steps:

(1) Make basic specifications for the shell-and-tube heat exchanger according to the nature of the process task: fluid allocation (tube-side and shell-side), shell and head types, and heat exchanger configuration (e.g., number of tube and shell passes).
(2) Pick values for options of tube diameter, tube length, baffle spacing, etc.
(3) Evaluate the area using an estimate of the overall heat transfer coefficient (U^{est}):

$$A^{est} = \frac{\hat{Q}}{U^{est}\Delta\hat{T}_{lm}F} \quad (1)$$

where $\hat{Q}$ and $\Delta\hat{T}_{lm}$ are the heat load and the logarithmic mean temperature difference, given according to the thermal task, and F is the correction factor of the logarithmic mean temperature difference.
(4) Pick a number of tubes and a corresponding compatible shell diameter in a tube count table, such that the area matches near to the estimated area A^{est}.
(5) Calculate the overall heat transfer coefficient through the evaluation of the heat transfer coefficients for the tube-side and the shell-side, use recommended values of fouling factors and evaluate the tube-side and shell-side pressure drops resulting from the geometric choices.
(6) Compute the heat exchanger area based on the chosen geometry and compare it to the required area calculated through eq 1 using the evaluated overall heat transfer coefficient from the previous step.
(7) If the overdesign is within an acceptable range and the pressure drops are below the maximum allowable values, then the design is usually finished.
(8) If step 7 is not true, adjustments to geometrical variables are made based on the analysis of the current trial, with an aim to fix the problems observed and return to step 5.

Another example is the case of distillation columns, more specifically, sieve tray columns. While the number of trays is established by shortcuts (Fenske-Underwood) or using MESH equations to verify functionality, the trays themselves are another example of a sequential application of rules of thumb/heuristics aided by empirical correlations.[8] One example of cross-flow tray design is the following:

(1) Select tray spacing.
(2) Use Fair diagram to obtain the flooding velocity (u_f as a function of the parameter $F_{lv} = \frac{\hat{L}}{\hat{V}}\sqrt{\frac{\hat{\rho}_L}{\hat{\rho}_V}}$, where $\hat{L}$ and $\hat{V}$ are the liquid and vapor flow rates in the tray, respectively; and $\hat{\rho}_L$ and $\hat{\rho}_V$ are the corresponding densities.
(3) Design for 85% flooding by picking a lower vapor velocity; that is, $u_n = 0.8\ u_f$.
(4) Obtain the net area required (A_n) as follows: $A_n = \frac{\hat{V}}{u_n}$.

DOI: 10.1021/acs.iecr.9b02611
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(5) Assume a total downcomer area to be 12% of the total area, and obtain the column cross sectional area: $A = A_n/0.88$.
(6) Make a trial plate layout based on net area (A), diameter (D), net active area (A_n), downcomer area as assumed above ($A_D = 0.12A$), and net hole area assumed as 10% of the active area ($A_h = 0.1A_n$). Pick a weir height (h_w). This is related to the efficiency: larger weir height increases efficiency but also increases pressure drop. Choose hole diameter (d_h) and hole pitch (triangle or squared).
(7) Obtain weir liquid crest, that is $h_{ow} = 750\left[\frac{\hat{L}}{\hat{\rho}_L h_w}\right]^{2/3}$
(8) Calculate the minimum vapor velocity for weeping:

$$u_{h,\min} = \left[\frac{K_2 - 0.9(25.4 - d_h)}{\hat{\rho}_V^{1/2}}\right]$$

where K_2 is obtained from a graph as a function of ($h_w + h_{ow}$).
(9) Check the weeping condition $u_{h,\min} = \hat{V}A_h > u_{h,\min}$.
(10) Calculate plate pressure drop (dry hole + liquid height + residual pressure drops).
(11) Check downcomer back-up.

The above procedure relies on some correlations and starts with some assumptions: the area of the downcomer is 12% of the total, the area of holes is 10% of the active area and the velocity is 80−90% of the flooding velocity. With these assumptions, a diameter is obtained. The rest of the steps consist of picking a hole diameter and checking for weeping, pressure drop, and downcomer flooding/drying conditions. If any of those conditions do not pass, the recipe calls for adjustments in geometry until the tray is verified as viable. It gets even more complicated if one diameter is to be chosen among many trays of a column section (usually rectifying and stripping). There are several other step-by-step procedures presented in the literature, and there are different sources for the different correlations.[15]

Little is said by proponents of these procedures regarding how the recursive interventions in the successive design alternatives should be handled toward a final solution when a new trial is needed, nor are there clear recommendations to drive the design to most economical solutions. This is handled by somebody with expertise. A similar approach for the case of designing vertical and horizontal separation vessels, distillation packed columns design, reactors, etc. can be found in the literature.[8,16]

Many times, the final design is not close to one that can be obtained by optimization of MINLMs, either using MINLP or other techniques. Rather significant deviations may take place. For example, Caputo et al.[14] found significant differences in shell and tube exchangers designed using genetic algorithms to those obtained by traditional methods.

The limitations of the traditional design approaches present an opportunity for optimization tools to contribute with better solutions. In particular, stochastic methods do not guarantee optimality, while mathematical optimization renders local optima, if not global. Despite the number of papers published that try to fill this gap, important limitations hinder the utilization of such approaches for practical problems, as discussed in the next section.

To summarize, most heuristic-based trial-and-verification procedures do not incentivize iterative procedures aimed at obtaining an optimal solution in some sense. In other words, they provide step-by-step heuristics and require expertise to obtain a feasible answer, not an optimal one, a solution that they only sometimes seek to improve. Sometimes, when inserting formal objective functions (cost), the answer may depart significantly from heuristics-based results because the latter are not optimization driven.

3. USE OF MATHEMATICAL OPTIMIZATION TOOLS

Three main approaches are employed to obtain optimal design solutions: stochastic methods, mathematical programming, and enumerative-based procedures, many of them not capable of guaranteeing global optimality. In the next paragraphs, we present the main features of each class of algorithms, with examples of their application for the solution of equipment design problems. Later, we present an analysis about possible reasons that could explain why optimization tools present limited application in real problems.

The use of stochastic methods (meta-heuristic methods) is based on strategies to propose new and improved solutions until there is confidence that improvement may not come (i.e., abandon generating new solutions when no improvement is seen after some number of iterations). Typically, the structure of meta-heuristic algorithms is based on the emulation of a natural phenomenon (GA, PSO, etc.). There is a large number of papers in the literature that employed stochastic optimization methods for the design of shell-and-tube heat exchangers, using different algorithms, such as, simulated annealing,[17] genetic algorithms,[18] particle swarm optimization,[19] and artificial bee colony,[20] among others. Stochastic methods were also employed for the design of distillation systems and tray geometry by Ramanathan et al.,[21] Lahiri,[22] and Matsumoto et al.[23]

Mathematical programming involves algorithms based on optimality conditions and faces the inconvenience of nonconvex formulations. Moreover, for example, shell-and-tube heat exchanger design solution procedures evolved from older nonlinear models[24] to mixed integer nonlinear models.[25−27] MINLP was also applied to the design of other thermal equipment, such as furnaces[28] and air coolers.[29] Examples of the application of MINLP algorithms for the design of distillation columns (optimal number of trays and feed tray location) can be found in Luyben and Floudas,[30] Yeomans and Grossmann,[31] Lang and Biegler,[32] and Ballerstein et al.[33] The use of generalized disjunctive programming was attempted by Barttfeld et al. using decomposition.[34] Interestingly, the design of internals have not been solved using MINLP. Instead, performance goals (such as 80−85% of flooding limits), but not economic objectives associated with these devices, are sought after.

Enumerative-based procedures involve the recursive selection of different solution candidates in the search of the optimal solution (differently from stochastic methods and mathematical programming, these algorithms do not mimic a natural phenomenon and are not based on formal optimality conditions). Some of these methods employ graphical techniques, and when a purely heuristic rule is used to guide the search, the global optimum may be missed. Examples of an enumerative-based search for the design of heat exchangers are found in Ravagnani et al.[35] and Kara and Güraras.[36]

DOI: 10.1021/acs.iecr.9b02611
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A more detailed analysis of the literature about the utilization of optimization techniques indicates several aspects that limit the utilization of the aforementioned tools as well as the quality of the models for practical applications:

(a) Stochastic methods are highly dependent on an adequate selection of search engine control parameters, which may demand a tedious step of tuning, many times only suitable for the case study. Additionally, these methods do not guarantee optimality, neither local nor global, and a different solution can be obtained at each optimization run. The need to spend time to tune the algorithm before its application and the possibility of obtaining different solutions in different runs are aspects of the stochastic methods that become important obstacles for their adoption by practitioners.

(b) MINLP procedures are associated with convergence problems and multiple local optima with different values of objective function. Aside from local optimality, the most relevant problem is the lack of robustness, that is, the inability to find a solution with some or no initial values.[37,38] This last is an important barrier for the acceptance of this kind of tool by a broader audience, as there is no method other than repeated random trials, to propose successful initial values. While academics may find ways around this issue, practitioners become increasingly impatient as frustration grows, because they prefer software that does not require building expertise to obtain answers. Proposals of how to overcome this problem are discussed in sections 4 and 5.

(c) Enumerative algorithms are usually based on heuristic rules to guide the trajectory toward the solution. Additionally, the number of design variables explored is usually limited. Therefore, when purely heuristic rules are used, there is no guarantee of optimality that the most economical solution was found and limited notion, if any, how close one might be to the true global optimum. An analysis of an enumerative-based search algorithm to attain the global optimum with a reasonable computing time is presented in section 6.

(d) Mathematical models employed in the design optimization of process equipment are based on simplifications that are not fully valid for several real problems. For example, the literature about design optimization of shell-and-tube heat exchangers usually employs the LMTD method to describe the mathematical model of the equipment. This model is based on an analytical solution, for which the heat transfer coefficients have a uniform value along the heat transfer area and the heat capacity flow rates of the streams are constant; however, these hypotheses are not accurate in several situations. This problem is particularly important for services with phase change (vaporization or condensation), where the conditions along the flow can change considerably. The discussion of how to address this problem is presented in a later section.

To summarize, the existing optimization approaches for the design of chemical process equipment present several limitations such as initialization/convergence of algorithms, parameter tuning, and lack of realistic models. These issues hinder their utilization to be used by practitioners. Some ideas about how to overcome these obstacles are presented in the rest of the paper.

4. LINEAR VERSIONS OF MIXED-INTEGER-NONLINEAR MODELS

An approach to eliminate the problems associated with nonlinear models is to reformulate them to linear equations. This transformation exploits the discrete nature of the design variables. We now present the techniques that we have been introducing recently to promote this approach.

4.1. Use of Discrete Variables. Departing from the tendency to consider naturally discrete variables as continuous, hoping to later round the result to the nearest discrete value, our proposal is to restart the use of sets of discrete values for geometric variables directly. Thus, a discrete variable x_i with ***sximax*** available discrete options can be described as follows:

$$x_i = \sum_{sxi=1}^{sximax} \hat{px}_{i,sxi} y_{i,sxi} \tag{2}$$

$$\sum_{sxi=1}^{sdimax} y_{i,sxi} = 1 \tag{3}$$

where $y_{i,sxi}$ are binary variables and $\hat{px}_{i,sxi}$ is the corresponding numerical value of option sxi. eq 3 states that only one option can be chosen by eq 2.

For example, heat exchanger tubes come in discrete options ($^3/_4$, 1, 1$^1/_4$, 1$^1/_2$, 2 in.) and different discrete options for length (e.g., 12, 14, 16, 20 ft). The same can be said for shell diameters and other geometric variables that have been standardized. Thus, the diameter (dti) is expressed in terms of discrete options as follows:

$$dti = \sum_{sd=1}^{sdmax} \hat{pdti}_{sd} yd_{sd} \tag{4}$$

where yd_{sd} is a binary variable and $\hat{pdti}_{sd}$ is the corresponding discrete value. The expression also requires to be accompanied by

$$\sum_{sd=1}^{sdmax} yd_{sd} = 1 \tag{5}$$

4.2. Reformulation. Having the design variables in a discrete space allows reformulation to a linear form without losing model accuracy, that is, without approximations of any sort (like truncated Taylor expansions). The following ideas were advanced by Grossmann et al.[39] and later by Chen and Grossmann.[40]

Consider, for example, the calculation of the heat transfer coefficient for the tube-side flow using the Dittus−Boelter correlation (problem parameters are represented with a symbol ^):[41]

$$ht = \frac{0.023 Ret^{0.8} \hat{Prt}^{n} \hat{kt}}{dti} \tag{6}$$

where ht is the convective heat transfer coefficient, Ret is the Reynolds number, $\hat{Prt}$ is the Prandlt number, and $\hat{kt}$ is the thermal conductivity of the stream.

For one tube-side pass, the Reynolds number in relation to the mass flow rate is

$$Ret = \frac{dti\, v\, \hat{\rho t}}{\hat{\mu t}} = \frac{4\hat{mt}}{Ntt\, \pi\, \hat{\mu t}\, dti} \tag{7}$$

where v is the flow velocity, $\hat{\rho t}$ is the stream density, $\hat{mt}$ is the mass flow rate, Ntt is the total number of tubes, and $\hat{\mu t}$ is the stream viscosity.

Thus, substituting eqs 4 and 7 into eq 6, one obtains:

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

$$ht = \frac{0.023\left(\frac{4\hat{mt}}{\left[\sum_{sNtt=1}^{sNttmax} p\hat{N}tt_{sNtt} yNtt_{sNtt}\right]\pi\hat{\mu}\sum_{sd=1}^{sdmax} p\hat{dti}_{sd} yd_{sd}}\right)^{0.8} \hat{Prt}^{n}\hat{kt}}{\sum_{sd=1}^{sdmax} p\hat{dti}_{sd} yd_{sd}} \quad (8)$$

where $p\hat{N}tt_{sNtt}$ corresponds to the integer values of the total number of tubes and $yNtt_{sNtt}$ is the corresponding binary variable.

We also realize that the product of summations elevated at a certain exponent, even negative, can be rewritten in form that contains products of integers, as follows:

$$\left[\sum_i \hat{pd}_i yp_i\right]^{n1}\left[\sum_j \hat{qd}_j yq_j\right]^{n2} ... \left[\sum_k \hat{zd}_k yz_k\right]^{nm} = p^{n1} q^{n2} ... z^{nm} = \sum_{i,j,...k} \hat{pd}_i^{\,n1} \hat{qd}_j^{\,n2} ... \hat{zd}_k^{\,nm} yp_i\, yq_j ... yz_k \quad (9)$$

Thus, eq 8 can be rewritten as follows:

$$ht = 0.023\hat{Prt}^{n}\hat{kt}\left[\frac{4\hat{mt}}{\pi\hat{\mu}}\right]^{0.8}\sum_{sd=1}^{sdmax}\sum_{sNtt=1}^{sNttmax}\frac{yNtt_{sNtt} yd_{sd}}{p\hat{dti}_{sd}^{\,1.8}\, p\hat{N}tt_{sNtt}^{\,0.8}} \quad (10)$$

This expression is nonlinear in the binary variables and a resultant formulation of an optimization problem would be associated with the same drawbacks described above for the typical MINLP approaches for equipment design.

4.3. Conversion to a Linear Form. Now, it is possible to convert the model to a linear form, as follows.

The constraint in eq 10 (that is nonlinear due to the product of binaries) can be substituted by the following set of linear constraints:[42]

$$ht = 0.023\hat{Prt}^{n}\hat{kt}\left[\frac{4\hat{mt}}{\pi\hat{\mu}}\right]^{0.8}\sum_{sd=1}^{sdmax}\sum_{sNtt=1}^{sNttmax}\frac{wNttd_{sNtt,sd}}{p\hat{dti}_{sd}^{\,1.8}\, p\hat{N}tt_{sNtt}^{\,0.8}} \quad (11)$$

$$wNttd_{sNtt,sd} \le yNtt_{sNtt} \quad (12)$$

$$wNttd_{sNtt,sd} \le yd_{sd} \quad (13)$$

$$wNttd_{sNtt,sd} \ge yNtt_{sNtt} + yd_{sd} - 1 \quad (14)$$

where $wNttd_{sNtt,sd}$ is a continuous non-negative variable. A generalized expression for this equation, valid for any number of tube passes, including the relations associated with the tube count for a given shell diameter and its insertion in the overall heat transfer coefficient can be found in Gonçalves et al.[43]

The reformulations proposed are such that no approximations, such as linearizations by truncating Taylor series or other simplifications, are made. In other words, the reformulated model is such that every solution of one model is feasible in the other, that is, no loss of rigor takes place. Therefore, when the reformulated models are linear, all problems associated with local minima and initial values of MINLP formulations are eliminated.

This approach was applied successfully to different types of heat exchangers, such as air coolers[44] and double pipe heat exchangers.[45] However, this approach is not limited to thermal equipment, but it is a general formulation scheme that can be also employed to address the design of different types of equipment, such as separation vessels, distillation columns, etc.

Sometimes, the resulting reformulated model contains continuous variables participating in nonlinear terms that are not amenable to be discretized. In these cases, the resultant problem is not a linear one, but the reduced number of nonlinearities allows an easier application of a MINLP algorithm to solve it. This takes place in the example of the optimization design of an air cooler. While Souza et al.[44] managed to reformulate the problem for fixed air flow rate into an ILP problem, Carvalho et al.[46] discussed the case of variable air flow rate. In this case, the MINLM includes a well-known mechanical energy balance that is represented by the intersection of the system pressure drop curve and the fan head curve, which determines the corresponding flow rate for each fan selection and each tube bundle geometry. After the terms containing the discrete geometric variables are reformulated, the head vs volumetric flow rate equation remains nonlinear. In addition, as a consequence of considering a variable flow rate, several expressions used to calculate the overall heat transfer coefficient (Reynolds number, Nusselt number, air side heat transfer coefficients and consequently the overall heat transfer coefficient), become nonlinear, namely:

$$Rec = \frac{Dte\, vc\, \rho c}{\mu c} \quad (15)$$

$$Nuc = 0.38 Rec^{0.6} Prc^{1/3}\left(\frac{Aot}{Ar}\right)^{-0.15} \quad (16)$$

$$hc = \frac{Nuc\, kc}{Dte} \quad (17)$$

$$U = \frac{1}{\left(\frac{1}{hh} + \hat{R}fh\right)\left(\frac{Aot}{\pi Dti}\right) + \left[\frac{Aot \ln\left(\frac{Dte}{Dti}\right)}{2\pi\hat{k}t}\right] + \frac{1}{\eta t\, hc} + \frac{\hat{R}fc}{\eta t}} \quad (18)$$

where Dte is the outer tube diameter, Nuc, Rec, and Prc are the Nusselt, Reynolds, and Prandlt numbers for the cold stream (air), respectively; vc is the air flow velocity, Aot is the finned surface area, Ar is the tube area without the presence of fins (bare surface), nt is the finned surface efficiency, $\hat{R}fh$ and $\hat{R}fc$ are the fouling factors of the hot and cold streams, and hh and hc are the convective heat transfer coefficients of the hot and cold streams, respectively.

We also find the same situation in the case of heat exchangers when fouling is modeled. Traditionally, the design of heat exchangers addresses the fouling problem using fixed values of fouling resistances. However, the literature presents fouling models that can be embedded in the design equations, thus allowing the problem of fouling mitigation to be inserted into the optimal design problem. Sometimes, it is possible to include the fouling model and still generate a linear problem.[47] However, in more complex systems, these models may bring to the problem continuous variables involved in nonlinear terms that cannot be eliminated (e.g., fouling layer thickness), which demands MINLP optimization algorithms.

4.4. Discretizing Continuous Variables. One can always discretize continuous variables. This idea was proposed formally as a methodology and used successfully by the group of Prof. Manousiouthakis, employing his infinite dimensional state-space (IDEAS), which uses discrete points

DOI: 10.1021/acs.iecr.9b02611
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of the continuous space.[48] The approximation renders large mixed integer linear models (MILMs). We also note that prior to IDEAS, Grossmann et al.[39] and later Chen and Grossmann[40] used this concept. The underlying assumption that allows claiming optimality is that between one discrete point for one variable and the adjacent, while all the other variables remain continuous, the objective function is smooth with a continuous first derivative and monotone, a condition that is not difficult to hold for nonlinear models (no integers), but can present problems when binaries are present, especially those binaries that are connected to structural changes. We believe this helps in the solution of large problems, but we cast no opinion on the significance of the extent of the improvement.

4.5. Illustrative Example. Aiming at illustrating the benefits to use the proposed optimization approach in relation to the traditional design solution, an example is reported below in which a considerable cost reduction was obtained in the design of air coolers using a linear formulation, compared with a conventional design reported in a textbook.[6]

Souza et al.[44] addressed the design optimization problem of air coolers. An integer linear programming formulation employing the techniques described above was developed and applied to the thermal task described in Table 1.[6]

Table 1. Air Cooler Design Problem

	tube side		air side	
fluid	hydrocarbon		air	
mass flow rate (kg/s)	31.5			
inlet temperature (°C)	121.15		35.05	
outlet temperature (°C)	65.65		65.65	
fouling factor (m^2 K/W)	0.00017611		0	
allowable pressure drop (Pa)	105 000			
flow velocity bounds (m/s)	1	3		
Reynolds bounds	10 000		1 800	10^5

Table 2 shows the comparison of the solution obtained using the optimization formulation and the solution reported in the textbook, where it is possible to observe that the optimization identified a design alternative with a total annualized cost about 20% lower than the solution reported by Serth.[6] This cost reduction was attained through a better trade-off between capital and operating costs.

Table 2. Air Cooler Design Solutions

variable	Serth[6]	optimal results
capital cost ($/year)	16,317	23,553
maintenance cost ($/year)	1,092	1,499
operational cost ($/year)	19,422	4,759
total cost ($/year)	36,830	29,811

As it was discussed above, Serth[6] aimed at providing a feasible solution, without any additional effort to find an optimal solution associated with lower costs. This example illustrates the economic driving force that justifies the utilization of optimization tools for the solution of equipment design problems.

To summarize, using the discrete nature of some design variables to reformulate MINLMs to a linear form eliminates the drawbacks associated with MINLP approaches. Even when nonlinearities cannot be eliminated, the resultant model becomes simpler to be solved. Finally, the option to discretize continuous variables (guaranteeing that one can capture optimal points) is viable as means to reduce model complexity and eventually eliminating nonlinearities. The advantage of the utilization of optimization tools to solve equipment design problems is illustrated through an air cooler design example, where integer linear programming attains a considerable cost reduction compared with a traditional design solution reported in a textbook.[6]

5. COMPUTATIONAL ISSUES

Two issues are to be discussed, namely computational time and memory. Regarding the former, the organization of the search space described above involves one set of binary variables for each original design discrete variable. Further investigations indicated that a reorganization of the search space could reduce the computational time to reach the global optimum.[44,49] Indeed, instead of representing each discrete variable for a corresponding set of binaries, one can employ a single set of binary variables, where each binary corresponds to a combination of discrete values that represents a solution candidate. Therefore, the search space is represented by a table, where each row contains a set of discrete values associated with a solution candidate. Each row corresponds to a multi-index containing the identification of discrete values of the different variables of that individual solution candidate. The corresponding binary trees are different, and their performance is also, consequently, different.

This idea was explored by Gonçalves et al.[49] for the heat exchanger linear model based on the Kern method. Conceptually, it is as follows: Consider the discrete representation outlined above in eqs 2 and 3. Instead of using the different binaries for separate discrete variables, one can create a new set of binaries $yrow_{srow}$ such that

$$x_i = \sum_{srow} \hat{Prowx}_{i,srow} yrow_{srow} \tag{19}$$

$$\sum_{srow} yrow_{srow} = 1 \tag{20}$$

where $\hat{Prowx}_{i,srow}$ is the ith parameter of a set $\{\hat{Prowx}_{1,srow}, ..., \hat{Prowx}_{n,srow}\}$.

This approach brought a large reduction in computational time (98.10% to 99.33%) for the case of shell-and-tube heat exchangers[49] as it is discussed in detail, later in this section.

Regarding memory, the problem reformulations proposed here and in the previous section result in a significant increase of the dimension of the problem that can be an obstacle in certain situations (see next section). However, as discussed earlier, the transformations render a considerably smaller number of nonlinearities, which eliminate or reduce convergence drawbacks and the possibility of poor local optimum. We now discuss both linear and nonlinear reformulated models.

5.1. Linear Reformulated Problems. The availability of efficient solvers to handle linear problems and the possibility to reorganize the search space as discussed above avoid large computational times. However, computational obstacles have appeared in relation to memory limitations to run some kind of problems using less powerful computers.

We now illustrate the advantages and drawbacks: Gonçalves et al.[44,49] investigated the case of shell-and-tube heat

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

exchangers in a turbulent regime using the Kern model for the shell-side and the Dittus−Boelter correlation for the tube-side heat transfer coefficients, respectively. There are seven original design variables, with a number of options each, as follows: tube diameter (5 options), tube length (7 options), number of baffles (20 options), number of tube passes (4 options), pitch ratio (3 options), shell diameter (10 options), and tube layout (2 options). A sample of 10 different examples was solved using three different approaches: the original nonlinear formulation (MINLP); the mixed-integer linear programming formulation (MILP); and the integer linear programming formulation (ILP), using GAMS/CPLEX for the linear cases and SBB and DICOPT for the nonlinear ones. Tables 3, 4, and 5 describe the values of the objective function, the elapsed time, and the dimension of each option, respectively. The computational tests were conducted using a processor Intel Core i7 3.40 GHz with 12.0 GB RAM memory.

Table 3. Performance Comparison: Heat Transfer Area (m^2)—Kern Model[a]

example	ILP	MILP	MINLP DICOPT	MINLP SBB
1	677	677	NC	NC
2	319	319	319	319
3	199	199	NC	NC
4	872	872	872	872
5	144	144	NC	NC
6	332	332	355	341
7	207	207	225	207
8	914	914	914	914
9	287	287	287	287
10	327	327	NC	NC

[a]Note: NC = nonconvergence.

Table 4. Performance Comparison: Elapsed Time (s)—Kern Model[a]

example	ILP	MILP	MINLP DICOPT	MINLP SBB
1	12	1772	NC	NC
2	11	1606	8.8	1.3
3	11	211	NC	NC
4	12	153	87	0.4
5	12	931	NC	NC
6	11	2824	5061	1.8
7	12	2529	1.5	0.9
8	12	171	19	0.7
9	12	2058	9.3	0.9
10	12	2329	NC	NC

[a]Note: NC = nonconvergence.

Table 5. Performance Comparison: Problem Dimension—Kern Model

dimension	ILP	MILP	MINLP
total no. of variables	168 000	115 991	81
no. of discrete variables	168 000	51	51
no. of constraints	458 906	767 517	49

Table 3 shows examples for which the nonlinear alternatives do not converge or are trapped in a local optimum. Nonconvergence problems have occurred in 40% of the problems. Local optima were found in 33% of the converged runs using the DICOPT solver and 17% of the converged runs using the SBB solver. Table 4 indicates that the MILP usually involves the highest elapsed time and the ILP can bring a large reduction of the computational effort with reductions range from 98.10% to 99.33% in relation to the MILP alternative. The DICOPT solver may also consume a larger computational time sometimes and the SBB solver is the fastest algorithm (but it failed to converge in almost half of the sample). Table 5 shows the problem dimension of each alternative formulation investigated. Despite the relatively large dimension of the linear problems, they were solved easily in different desktop and laptop computers.

Gonçalves et al.[50] developed a linear formulation for the design optimization of shell-and-tube heat exchangers using the Bell−Delaware method for the shell-side and a set of different correlations for the tube-side heat transfer coefficient, both models with several disjunctions and able to represent laminar and turbulent regimes. Table 6 describes the dimensions of the resultant MILP problem (this formulation used a single set of binaries as discussed before, but there appears additional continuous variables due to the disjunctions) and Table 7 presents the elapsed time associated with the sample of the 10 examples using the same computer of the previous tests.

Table 6. Problem Dimension: Bell−Delaware Model

dimension	MILP
total number of variables	2 856 012
no. of discrete variables	168 012
no. of constraints	9 068 366

Table 7. Elapsed Time (s): Bell−Delaware Model

example	elapsed time
1	232
2	271
3	134
4	146
5	136
6	251
7	164
8	211
9	341
10	118

Because of the considerable increase of the dimensions of the problem, some computers tested were not able to run these problems due to memory limitations (e.g., a laptop with processor Intel core i3M370 2.40 GHz with 4.00 GB of RAM memory failed). Despite the computational times using the computer employed in the tests were not so high as can be observed in Table 7 (thus indicating that it is feasible to use the proposed approach in practice), the continuous development of more complex models suggests that this problem will be more frequent in the future. Section 8 discusses some computational alternatives to handle these obstacles.

5.2. Nonlinear Reformulated Problems. Reformulated, but still nonlinear models can be successfully solved using global optimizers, for example, Baron,[51,52] Antigone,[53] and

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

Rysia.[54] However, sometimes, the nonreformulated versions are not successfully solved by the aforementioned solvers.

To summarize, a reorganization of the search space associated with the reformulation techniques usually brings large reductions of the computational time necessary to solve different examples of design problems in its linear form. However, the reformulation techniques presented above can bring computational limitations associated with memory requirements. Reformulations that render nonlinear models with less nonconvex equations still represent challenges that need to be addressed. A later section discusses means to parallelize computations.

6. ALTERNATIVES APPROACHES FOR GLOBAL OPTIMIZATION

The reformulated MINLP formulations using discrete representations of geometric variables often produce MILP or even ILP models that are solvable using known techniques, making them also good models to be inserted in the design optimization of entire flowsheets.

However, as discussed in the previous sections, the complexity of the mathematical structure of the model may not allow a full reformulation of the design problem in a linear form and global optimization tools can be applied to handle the remaining nonconvexities, but sometimes unsuccessfully.

Aiming at circumventing the obstacles associated with mathematical programming when more complex mathematical structures are found, algorithmic alternatives to the utilization of conventional optimization tools, much to the dismay of many PSE mathematical programming enthusiasts (or their horror sometimes) are the application of set-trimming and enumeration-based search approaches. It is important to point out that, differently from meta-heuristic algorithms and enumeration search algorithms uniquely based on heuristic rules, the search schemes explored below guarantee the identification of the global optimum, many times without the need to use a MINLP or MILP. Another important difference is that typical meta-heuristic algorithms address a codification of the problem and do not explore the particularities of the problem. In contrast, our alternatives presented below accelerate the search based on the knowledge of the physical features of the system investigated.

6.1. Set-Trimming. A feasible solution for a design problem must obey a set of constraints. Some of these constraints correspond to nonlinear relations that represent the behavior of the equipment and their application for a given solution candidate may imply the utilization of a numerical algorithm (possibly through a computationally time-consuming step). However, other constraints are mathematically simple and can be applied for the entire search space directly, therefore cutting a large portion of the solution candidates prior to the search of individual alternatives. We call this procedure as set trimming.

For example, shell-and-tube heat exchangers must be built according to a length-to-diameter ratio between 3 and 15.[55] Therefore, during the design optimization of this kind of heat exchangers, all solutions outside these bounds can be eliminated immediately, without any time-consuming numerical algorithm for their evaluation. Any other geometrical constraint can also be used for set trimming, for example, baffle spacing limits. Some constraints may demand an additional computational effort, but can also be employed, such as the pressure drop bounds or the required area constraint.

While set trimming refers to the reduction of the set of candidate solutions to a set of feasible solutions by means of using different inequality constraints, the technique of cutting planes generates new constraints aimed at cutting some otherwise feasible integer points from the initial domain. Domain reduction is also a technique that adds constraints. There is little relation between these techniques and set trimming because set trimming relies on reducing the set of candidates by using logic propositions thus reducing the search space size. Cutting planes add constraints that hopefully will eliminate portions of the search space later during the execution of the optimization algorithm. Finally, domain reduction also adds constraints so that there is a lower and an upper bounds of variables, thus becoming a bound contraction tool. In set trimming, the size of the candidate set is reduced without introducing new constraints. Aside from cutting planes and other domain reduction techniques in which new constraints are added to the problem to aid/simplify/accelerate the search, we also point out that in the case of continuous variables, one can rely on interval analysis and other techniques[56] to reduce the distance between lower and upper bounds of each variable. Our set trimming technique is not related to any of these preprocessing techniques for continuous variables; it only applies to candidates that are described by sets of discrete variables. Moreover, the use of set trimming does not preclude the use of domain reduction techniques using the aforementioned interval analysis and other techniques, if and when MINLP/MILP techniques are used to identify the optimum after the set trimming is finished. We elaborate on this difference in future work.

The application of set-trimming for some problems can involve the successive application of all problem constraints, yielding a sequence of shrinking lists of solution candidates until the end of the processing, when only the feasible solution candidates remain and the optimal value can be identified through the application of a sorting procedure in relation to the objective function to this final set. For problems with more complex mathematical structures, set-trimming can be a preprocessing step applied prior to a smart enumerative procedure or even the use of MINLP/MILP approaches if so desired.

6.2. Smart Enumeration. A first direct and naïve attempt to solve the design problem is to test all of the possible combinations of the design variables (a "naïve enumeration"). However, despite the huge development of the computational power in the last decades, this approach has been considered not efficient in practice. The number of options to be investigated and/or the computational time for evaluating each solution candidate may be too high. Therefore, it is necessary to implement techniques that can accelerate the search, demanding only the exploration of a small fraction of the search space, which allows the identification of the solution of the design problem in a time compatible with the engineering practice. We call these enumeration search-based algorithms as "smart enumeration" and present below different procedures that can be inserted into to an enumeration search scheme aiming at accelerating the identification of the global solution.

Problem Structure. The enumeration algorithms we analyze here are suitable for problems where each solution candidate is composed of a set of continuous and discrete variables, and the number of degrees of freedom is equivalent to the number of discrete variables. Therefore, due to the structure of the problem constraints, the selection of each set of values for the

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

discrete design variables allows the determination of the values of the continuous ones through follow-up calculations. The discrete variables represent typically the dimensioning of the mechanical components available in commercial and/or integer values (e.g., set of commercially available tube diameters, number of baffles, etc.).

Therefore, the search space in this case may be represented by a combination of the different values of the discrete variables. Usually, the determination of the values of the continuous variables from the discrete ones demands the solution of the equipment mathematical model, thus the availability of efficient simulation algorithms may be an important aspect for the implementation of the enumeration-based algorithms.

Incumbent. An incumbent corresponds to the best feasible solution candidate already visited during the search. The update of the objective function of the incumbent may allow the elimination of solution candidates with higher values of the objective function. For example, a possible objective function in the optimization of shell-and-tube heat exchangers is the minimization of the total annualized cost. Therefore, if an incumbent is found with a given value of the objective function, equivalent solution candidates with lower baffle spacing can be eliminated from the search immediately, because they will be associated with the same capital cost but with a higher operational cost than the incumbent.

Set Trimming. Set trimming procedures can also be applied during the enumeration, through the utilization of the information on the solution candidates that were already visited to eliminate other similar solutions that were not yet evaluated, but presents similar structures to those already discarded. For example, in the design of shell-and-tube heat exchangers, if a solution candidate presents a higher pressure drop in the tube-side or in the shell-side than the corresponding maximum allowable pressure drop, then other alternatives equivalent to this one, but with a longer tube length, can also be eliminated without demanding an additional computational effort to explore them (the pressure drop of these alternatives will be higher than the solution candidate explored and, therefore, they will be infeasible too). Similarly, equivalent solution candidates, but with a higher number of tube passes and/or lower baffle spacing can be eliminated too in relation to the pressure drop bounds on the tube-side or the shell-side, respectively, for the same reason.

Ordering of the Search Space. The utilization of the incumbent associated with the ordering of the search space can be employed to provide alternative stopping criteria that can also accelerate the search. This procedure can be effective if the evaluation of the objective function of the solution candidates does not imply large computational efforts and can be applied to the entire search space previously of the search start. The typical stopping criterion of an enumeration search scheme is the absence of any unvisited solution candidate. However, if the search space can be previously ordered according to the value of the objective function (or at least a part of the objective function that could be easily evaluated) and the search starts from the smallest value to the highest one (for a minimization problem), the search can be stopped if the incumbent presents an objective function lower or equal than the current solution candidate.

For example, if the optimization of the design of shell-and-tube heat exchangers is based on the minimization of the heat transfer area for a given set of allowable pressure drops, the search space can be organized in a way where the solution candidates are in a crescent order of the heat transfer area and the search will stop if the current candidate presents a heat transfer area equal or higher than the incumbent area (i.e., all of the unvisited remainder solution candidates present higher values of the objective function and do not need to be visited).

The acceleration of the smart enumeration in relation of the naïve enumeration can be illustrated by the results obtained by Carvalho et al.[46] for the design optimization of air coolers including the fan selection. The full analysis of each solution candidate demands the solution of two numerical problems: a hydraulic problem, represented by the determination of the air flow rate through a mechanical energy balance; and a thermal problem, represented by the determination of the number of transfer units for checking the feasibility of the main thermal constraint. Therefore, the speed up of the smart enumeration aims to reduce the number of numerical problems that must be solved.

Table 8 contains a short description of the cooling task design solved by Carvalho et al.,[46] based on the data of Serth[6] and Souza et al.[44]

Table 8. Problem Data

	tube side	air side
fluid	hydrocarbon	air
mass flow rate (kg/s)	31.5	-
inlet temp. (°C)	121.15	35.05
outlet temp. (°C)	65.65	-
fouling factor (m^2 K/W)	1.7611×10^{-4}	0
allowable pressure drop (Pa)	105,000	-

Each design candidate is composed of a set of values for nine discrete design variables: (1) Finned tube commercial alternatives of diameter, fin diameter, number of fins per meter, and fin thickness; (2) tube length; (3) tube pitch ratio (ratio between the tube pitch and the outer tube diameter); (4) number of bays; (5) number of bundles per bay; (6) number of tubes per row; (7) heat exchanger configuration (combination of the number of rows and the number of tube passes); (8) number of fans per bay; (9) fan model (each associated to a specific fan diameter and fan curve). In the problem investigated, this set of variables corresponds to 302 400 solution candidates.

This design problem was solved using a naïve enumeration algorithm and two versions of the smart enumeration. The first algorithm (Smart Enumeration 1) employs a series of set trimming procedures before the search to reduce the number of solutions and the second algorithm (Smart Enumeration 2) also includes an incumbent and the organization of the search space in relation to the capital and maintenance costs (the analysis of the operational costs is not included in this previous organization of the search space, because it demands the numerical solution of the mechanical energy balance).

Table 9 displays computational time and the number of numerical problems solved during the search of the solution candidates for each algorithm alternative. The computational times correspond to codes implemented in Matlab R2018a and running in a computer with an Intel Core i7 3.6 GHz processor, with an 8 GB RAM memory. It is important to observe that all of the algorithms are able to obtain the global optimum of the design problem.

DOI: 10.1021/acs.iecr.9b02611
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Table 9. Performance of the Different Algorithms

variable	Naïve Enumeration	Smart Enumeration 1	Smart Enumeration 2
computational time (s)	7 390	206	141
no. of hydraulic problems solved	302 400	8 714	8 380
no. of thermal problems solved	302 400	1 885	1 391

The Smart Enumeration 1 reduced the computational time by 93.8% when compared to the Naïve Enumeration. The Smart Enumeration 2 brought an additional reduction of 31.5% in relation to the Smart Enumeration 2. These data indicate that the steps related to the smart enumeration can bring a considerable acceleration of the search for the identification of the global optimum.

In summary, set trimming and enumerative search algorithms are alternative procedures able to identify the global optimum that can be more effective than mathematical programming when very complex models are employed to describe the behavior of the equipment.

7. MINLM USING GEOMETRICALLY DISTRIBUTED PROPERTIES

One of the challenges ahead is to move away from simplified models based on uniform parameters and analytical solutions (e.g., LMTD method) and address the optimization problem using discrete portions of the equipment where properties are calculated locally. This issue becomes especially important for phase change services where the nature of the streams present a large variation along the flow path (e.g., in a total condenser, the inlet stream is saturated vapor and the outlet stream is saturated liquid). Instead of only using the end temperatures, the model contains equations related to the set of temperatures distributed along the flow path.

A fundamental issue about the design problem is the need to find a reliable solution for a given process task. A failure to reach a desired service duty due to a poor design can imply severe economic penalties (sometimes much higher than the equipment cost itself). Therefore, engineering companies and chemical process industries seek to acquire the most modern software to be used in the design of new equipment. As a consequence, intense research efforts have been focused on the development of mathematical models with increased accuracy.

However, many papers addressed design optimization problems using classical models employing analytical solutions based on simplifying assumptions, for example, uniform transport coefficients, linear driving forces, etc. Even considering that these models provide good results for a large set of engineering problems, there are important situations for which these model predictions present considerable limitations, which hinder their utilization for practical purposes. We elaborate further in section 7.2.

This scenario suggests one of the challenges ahead: how to move away from simplified models based on analytical solutions and address the optimization design problem using rigorous modeling. We have already found instances where better modeling avoids undersizing,[57] as presented later.

We discuss this issue next, focusing on the problem of the optimal design of thermal equipment.

7.1. Heat Exchanger Modeling.

The main equation employed in heat exchanger design is based on a logarithmic mean temperature difference (LMTD). For a counter-current heat exchanger, it yields

$$\hat{Q} = UA\Delta\hat{T}_{lm} \tag{21}$$

This equation is obtained through an analytical integration applied along the heat exchanger and is based on some hypothesis, for example, uniform overall heat transfer coefficient and constant heat capacities. The simplifications associated with the LMTD design equation may bring considerable errors in several situations such as streams with large variations of their physical properties with temperature and streams with phase change.

The convective heat transfer coefficients depend on the physical properties of the material streams, typically for nonphase change streams: density, heat capacity, dynamic viscosity, and thermal conductivity. Large variations in these properties, especially viscosity, render large variations in the heat transfer coefficients. For example, the viscosity of an engine oil has a 56-fold increase from 400 to 300 K.[58]

Condensers and vaporizers present streams that suffer phase change along the heat exchange process. Therefore, the convective coefficients may present considerable variations along the heat transfer surface. For example, a hot stream tube-side condenser may present different two-phase flow regimes: vapor, annular, wavy, stratified, slug, plug, bubbly, and liquid. Each flow regime is associated with different vapor fractions and flow patterns. Therefore, the value of the convective heat transfer coefficient varies along the heat transfer surface. Additionally, if the phase change stream is a (nonazeotropic) mixture, the vaporization/condensation is associated with a temperature variation, involving sensible and latent heat transfer. In these situations, the constant heat capacity hypothesis cannot be adopted.

Aiming at avoiding the accuracy problems described above, the optimization formulations must initiate their development returning to the original conservation equations. For a heat exchanger with no phase change streams, the set of differential equations is

$$\frac{dT_h}{dA} = \frac{U(T_h - T_c)}{m_h Cp_h} \tag{22}$$

$$\frac{dT_c}{dA} = \frac{U(T_h - T_c)}{m_c Cp_c} \tag{23}$$

where the subscripts h and c indicate the hot and cold streams.

Since typical mathematical programming formulations present an algebraic structure, the insertion of the heat exchanger modeling equations described above in optimal design problems involves the application of an adequate discretization technique, such as finite differences, finite volume, finite element, etc. In the resultant equations, the heat transfer coefficients can be calculated at each point of the grid employing correlations that describe the variation of the physical properties with the temperature. Particularly, these correlations usually imply (but not always) a nonlinear model.

The following subsections illustrate different solution approaches to address the problem described above suggested by our research group and some future problems and associated ideas to handle them. These different problems encompass the design optimization of a double pipe heat exchanger, the design optimization of an air cooler, and the

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

optimization of shell-and-tube heat exchangers with a nonuniform spatial distribution of the fouling rate.

7.2. Optimal Design of Double Pipe Heat Exchangers.

Double pipe heat exchangers are composed of two concentric tubes where one of the streams flows through the inner tube and the other stream flows in the annular region. Basically, each individual unit has a counter-current configuration and higher heat loads can be attained using several units together.

As discussed above, the rigorous modeling of heat exchangers would involve a nonlinear model. However, the one-dimensional counter-current nature of double pipe heat exchangers allows an alternative approach to provide a linear optimization problem.

Instead of applying the usual discretization procedure of the conservation equations in relation to the spatial variable, as it is typically employed in transport phenomena problems, we suggest to employ the temperature as an independent variable. Therefore, the grid of the resultant discretization is composed of an oriented set of temperatures, as illustrated in Figure 1 for the hot stream. It must be observed that since the temperatures are known at each point of the grid, all the physical properties are also already known.

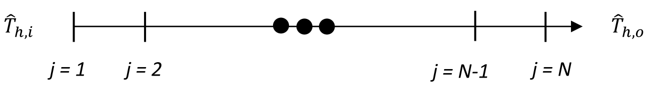

Figure 1. Temperature discretization grid.

The interpretation of the temperature field as the independent variable corresponds to the following representation of the energy balances (equivalent to a reorganization of eqs 22 and 23), where eq 25 relates the hot and cold stream temperatures.

$$\frac{dA}{dT_h} = \frac{\hat{m}_h \hat{C}p_h}{U(T_h - T_c)} \tag{24}$$

$$\frac{dT_c}{dT_h} = \frac{\hat{m}_h \hat{C}p_h}{\hat{m}_c \hat{C}p_c} \tag{25}$$

The discretization of eq 24 can be conducted through the approximation of the derivative by a second order central finite difference. The resultant algebraic model is (for the double pipe heat exchanger, $dA = \pi\ dte\ dz$):

$$\frac{z_{j+1} - z_{j-1}}{2\hat{\Delta T}} = \frac{-\hat{m}_h \hat{C}p_{h,j}}{U_j(\hat{T}_{h,j} - \hat{T}_{c,j})\,\pi\, dte} \tag{26}$$

where $\hat{\Delta T}$ is the increment of the temperature grid.

The discrete nature of the tube diameter yields

$$dte = \sum_{sd} p\hat{dte}_{sd} yd_{sd} \tag{27}$$

$$\sum_{sd} yd_{sd} = 1 \tag{28}$$

The expression of the overall heat transfer coefficient using adequate correlations for evaluation of the heat transfer coefficients can be inserted into eq 26, but it is important to observe that all the variables present in the correlations are related to geometrical design variables that can only assume discrete values. Therefore, the application of the techniques described in section 3 to transform the resultant mathematical expression in a linear model yields the following linear set of constraints:[57]

$$\frac{z_{j+1} - z_{j-1}}{2\hat{\Delta T}} = \frac{-\hat{m}_h \hat{C}p_{h,j}}{(\hat{T}_{h,j} - \hat{T}_{c,j})\pi} \sum_{sd} \sum_{sD} \hat{X}_{j,sd,sD} wD_{sd,sD} \tag{29}$$

$$wD_{sd,sD} \le yd_{sd} \tag{30}$$

$$wD_{sd,sD} \le yD_{sD} \tag{31}$$

$$wD_{sd,sD} \le yD_{sd} + yD_{sD} - 1 \tag{32}$$

where $\hat{X}_{j,sd,sD}$ is a parameter that depends on the physical properties and the discrete values of the design variables.

This optimization formulation was applied to the design problem described in Table 10.[57] The search space considers 5 options of tube length, 9 options of inner and outer tube diameters, and 20 options of number of units (aligned in series).

Table 10. Stream Data for the Optimization Problem

stream	flow rate (kg/s)	inlet temperature (K)	outlet temperature (K)
engine oil	1.3	310	295
cooling water	1.3	280	286

The solution of the resultant mixed-integer linear programming problem yields the optimal heat exchanger described in Table 11 (scenario 1). This table also displays other alternative scenarios: scenario 2 corresponds to the optimization considering constant physical properties evaluated at the average temperature; scenario 3 is obtained through the optimization with the overall heat transfer coefficient calculated as an average of its values at the inlet and outlet temperatures; and scenario 4 solves the optimization problem with viscosity calculated at the lowest temperature (conservative approach).

Table 11. Optimal Solutions Obtained for the Different Scenarios

scenario	total heat exchanger area (m^2)
1	30.28
2	28.26
3	24.22
4	40.37

The comparison of the different scenarios in Table 11 indicates that the simplifying assumptions employed in scenarios 2 and 3 yielded solutions with heat transfer areas lower than that of scenario 1. However, considering that scenario 1 employs a more rigorous model and the solution of the optimization is global (the model is a MILP), we can affirm that the solutions in scenarios 2 and 3 would fail in operation, because the heat exchanger areas calculated are too small. In an opposite way, the conservative approach provides a heat exchanger solution with an area more than 30% higher than the global optimum obtained in scenario 1.

7.3. Air Cooler Design Optimization.

Air coolers are an alternative for cooling services without depending on a cooling water supply. These heat exchangers are composed of one or

DOI: 10.1021/acs.iecr.9b02611
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more bundles of finned tubes, where the process stream flows through the tubes and the air flows in the outside. The air flow is promoted by the presence of one or more fans.

The tube bundle is organized in a set of tube rows with annular fins, where the air flows upward, as illustrated in Figure 2 (front view of the tube bundle). Here, for the sake of simplicity, we focus our discussions on air coolers with a single tube pass and multiple rows, but the main conclusions can be extended to other configurations too.

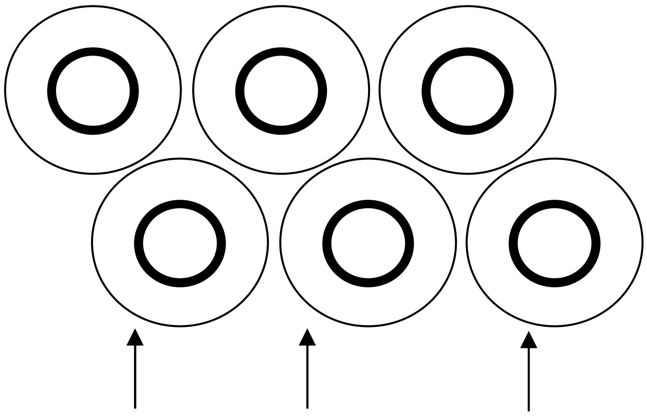

Figure 2. Tube rows in an air cooler.

The energy balance must be applied to each row, identified here by the index r:

$$\frac{dT_{h,r}}{dz} = \frac{U_r \pi\, dte\, Ntr(T_{h,r} - \bar{T}_{c,r})}{(m_h/Nr)Cp_{h,r}} \quad (33)$$

where Ntr is the number of tubes per row, Nr is the number of rows, and $\bar{T}_{c,r}$ is the average temperature of the inlet and outlet air flow in the row:

$$\bar{T}_{c,r} = \frac{T_{c,r} + T_{c,r-1}}{2} \quad (34)$$

Considering a control volume for row r, the energy balance for the air flow is given by

$$U_r \pi\, dte\, Ntr(T_{h,r} - \bar{T}_{c,r}) = Gc\, W\, Cp_{c,r}(Tc_r - Tc_{r-1}) \quad (35)$$

where Gc is the air mass flux and W is the bundle width.

The analysis of this model indicates a more complex problem to be addressed. The service task is defined by the outlet temperature of the air cooler, but this temperature is the result of a mixture at the header of the outlet temperature for each tube row. Therefore, the temperature field cannot be previously established, then the linear approach of the previous subsection cannot be applied to this type of thermal equipment.

The application of a discretization procedure for eqs 33−35 yields

$$\frac{T_{h,r,j+1} - T_{h,r,j-1}}{2\hat{\Delta z}} = \frac{U_{r,j} \pi\, dte\, Ntr\, Nr(T_{h,r,j} - \bar{T}_{c,r,j})}{\hat{m}_h Cp_{h,r,j}} \quad (36)$$

$$U_{r,j} \pi\, dte(T_{h,r,j} - \bar{T}_{c,r,j}) = Gc\, Ltp\, Cp_{c,r,j}(T_{c,r,j} - T_{c,r-1,j}) \quad (37)$$

$$\bar{T}_{c,r,j} = \frac{T_{c,r,j} + T_{c,r-1,j}}{2} \quad (38)$$

Two aspects here show an increase of the problem complexity in relation to the previous approach. The model is nonlinear due to the variation of the overall heat transfer coefficient along the tube length and the temperature field is bidimensional.

While new challenges emerge, LMTD and its correction factor F are not needed anymore. As usual, more accurate results are expected and problems such as obtaining infeasible equipment when using uniform properties-based methods are avoided.

7.4. Shell-and-Tube Heat Exchanger with Non-uniform Spatial Distribution Fouling Rate. Fouling is the undesired accumulation of deposits over the thermal surface of heat exchangers. The traditional approach to include the additional thermal resistance due to the deposits is to employ a fouling factor. This parameter is available in the literature, typically tabulated as a fixed value for different streams. The inaccuracy of this design parameter has been criticized.[59]

However, the fouling rate depends on variables related to the design, mainly the velocity and temperature. Therefore, different alternatives of heat exchangers for the same thermal task may be related to different values of fouling rates. Our research group has presented proposals for the inclusion of the fouling behavior in the optimization of the heat exchanger design. This problem was addressed considering the variation of the asymptotic fouling resistance with the velocity.[47] A more complex fouling model considering a "no fouling" condition[60] was also explored in the design optimization.[61] Both approaches employed the mathematical techniques described in section 3 that allowed the representation of the optimization as linear problems. Other approaches to include fouling models in the design can be found in Butterworth,[62] and Polley et al.,[63,64] but these are not based on mathematical programming.

Despite the efforts reported in the previous paragraph for the inclusion of the modeling of the fouling behavior in the design, by our research group and others, all of these design approaches employed lumped representations of the fouling resistance, that is, a single value of fouling resistance applied to the whole heat transfer surface. However, the variation of the temperature along the heat exchanger surface implies a nonuniform distribution of the fouling resistance. For example, Ishiyama et al.[65] presented simulations using a fouling threshold model, where one end of the heat exchanger becomes clean and the other subject to intense fouling, due to the difference of the thermal condition at each point.

Therefore, due to the nonuniformity of the fouling resistance distribution, the overall heat transfer coefficient will also be nonuniform, which demands a more rigorous mathematical modeling, based on the conservation equations.

More recent papers involving fouling monitoring migrated from lumped fouling models to distributed models, where the fouling resistance is calculated at each point along the heat exchangers.[66−69] However, despite the advances of these tools, they were not employed for the optimal design of heat exchangers yet.

The development of a complete model for the design of heat exchangers, considering a spatially distributed and time varying fouling rate, presents several obstacles. We illustrate now these issues using a cooler model, as described by Souza and Costa.[70] To save space, only the cooling water stream equations are

DOI: 10.1021/acs.iecr.9b02611
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presented for multiple-pass shell-and-tube heat exchangers, where fouling is resultant from salt precipitation of calcium carbonate. Additionally, the boundary conditions equations were also omitted.

The version of eq 23 for the proposed problem considering multiple tube passes with cooling water in the tube-side is

$$\frac{dT_{c,n}}{dz} = (-1)^{n+1}\frac{Ntt\, dte\, \pi}{\hat{m}_c Cp_c Npt} U_n(T_h - T_{c,n}),\quad n \in \{1, \cdots, Npt\} \tag{39}$$

where n is the index of the tube-side pass and Npt is the number of passes in the tube-side

After the discretization and the insertion of the dynamic behavior of the fouling, it yields

$$-T_{c,n,j-1,\tau} + \left(\frac{Ntt\, dte\, \pi}{\hat{m}_c Cp_{c,n,j,\tau} Npt}\right) 2\hat{\Delta z} U_{n,j,\tau} T_{c,n,j,\tau} + T_{c,n,j+1} - \left(\frac{Ntt\, dte\, \pi}{\hat{m}_c Cp_{c,n,j,\tau} Npt}\right) 2\hat{\Delta z} U_{n,j,\tau} T_{h,n,j,\tau} = 0 \quad \text{for } n \in \{1, 3, 5, 7, ...\}: \tag{40}$$

$$-T_{c,n,j-1,\tau} - \left(\frac{Ntt\, dte\, \pi}{\hat{m}_c Cp_{c,n,j,\tau} Npt}\right) 2\hat{\Delta z} U_{n,j,\tau} T_{c,n,j,\tau} + T_{c,n,j+1,\tau} + \left(\frac{Ntt\, dte\, \pi}{\hat{m}_c Cp_{c,n,j,\tau} Npt}\right) 2\hat{\Delta z} U_{n,j,\tau} T_{h,n,j,\tau} = 0 \quad \text{for } n \in \{2, 4, 6, 8, ...\}: \tag{41}$$

where τ is the index that identifies different time instants.

These equations must be associated with the fouling rate model,[71] represented below after its time discretization:

$$Rfc_{n,j,\tau+1} - Rfc_{n,j,\tau} = \frac{\varphi_{d,n,j,\tau} - \varphi_{r,n,j,\tau}}{\rho_f k_f} \tag{42}$$

where ρ_f and k_f are the density and thermal conductivity of the deposit, and ϕ_d and ϕ_r are formation and removal rates of the deposit, respectively.

Another aspect that must be considered in the model is the effect of the deposit thickness. Therefore, the overall heat transfer coefficient is

$$U_{n,j,\tau} = \frac{1}{\frac{dte}{dti - 2\delta_f}\frac{1}{h_{i,f,n,j,\tau}} + \frac{dte \ln\left(\frac{dti}{dti - 2\delta_f}\right)}{2k_f} + \frac{dte \ln\left(\frac{dte}{dti}\right)}{2k_{\text{tube}}} + \frac{1}{h_{e,n,j,\tau}}} \tag{43}$$

where the relation between the fouling resistance and corresponding fouling thickness (δ) is

$$Rfc_{n,j,\tau} = \frac{dte}{2k_{f,n,j,\tau}} \ln\left(\frac{dti}{dte - 2\delta_{f,n,j,\tau}}\right) + \frac{dte}{(dti - 2\delta_{f,n,j,\tau})}\frac{1}{h_{i,f,n,j,\tau}} - \frac{dte}{dti}\frac{1}{h_{i,n,j,\tau}} \tag{44}$$

The analysis of the resultant model represented by eqs 39−44 indicates the drawbacks for its inclusion in a mathematical programming formulation. Two aspects can be stressed:

(1) The modification of the temperatures during the operational horizon and the more complex structure of shell-and-tube heat exchangers do not allow the adoption of the approach described in subsection 7.2 to attain a linear model. Therefore, even with the application of the techniques involving discrete geometric variables, the problem will keep its nonlinear nature.

(2) There will be a considerable increase of the mathematical problem dimension, for example, the temperature field will have to be described for each tube-side pass, for each position along the tube length, and for each time instant during the time horizon.

To summarize, the models employed in the optimization design must evolve from analytical solutions based on simplifying assumptions to more realistic alternatives based on the discretization of the space where conservation equations are used. A numerical example where the solution of the design task of a heat exchanger using a conventional LMTD method is infeasible when tested against a more complex model highlights the notion that approximate models may not provide viable answers, necessarily.

8. PARALLEL COMPUTATION

The PSE community has been traditionally keen on reporting and giving high importance to the computational time for the solution of optimization problems. An emerging additional problem is the size of the models, as they are starting not to fit in regular computers.

Computational time has been used to compare effectiveness of different methodologies, sometimes almost exclusively, regardless sometimes of the ability to obtain or not globally optimal solutions, or the fact that the mixed integer nonlinear models are different. One needs to take this quest (sometimes a competition) for computational speed with a grain of salt. In other words, one needs to worry about speed only when it is warranted.

It is clear that computational speed is of outmost relevance when the information is needed for operational reasons, such as in control, when the aphorism "the faster, the better" applies. However, when the task is design of equipment or flowsheet synthesis, there is an upper limit of tolerance for the computational time that depends on a few important factors. For example, when the design-optimizations is a stand-alone and one-shot at the answer type, any time is good depending on the patience of the designer, as long as it is reasonable, like hours, a few days, a week, or any larger limit when patience wears thin. Usually, such time is tied to time allocated contractually. The other aspect is that many times, during such time the computer used is partially or not available. Where the computational time is of concern is when the design tool is used in a "what if" mode, in which different scenarios of external conditions (changing throughput, inlet conditions, design targets, etc.) are tested. For these types of situations, tolerance to upper bound time limits are significantly smaller, but in this case, there is a lower limit for the quest. Any application that runs below a few seconds is equally competitive for this "what-if" work, whether it runs in microseconds or those few seconds.

DOI: 10.1021/acs.iecr.9b02611
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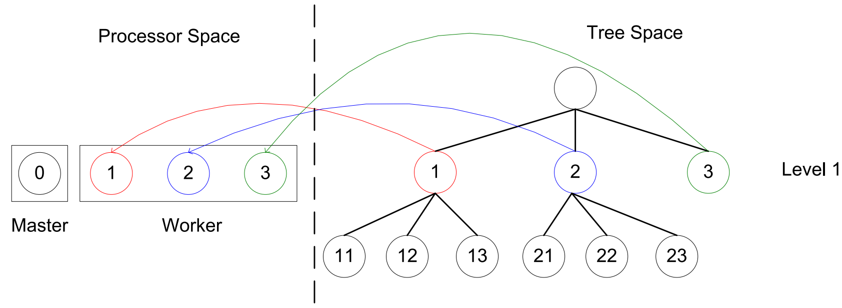

Figure 3. Mapping of nodes to processors.

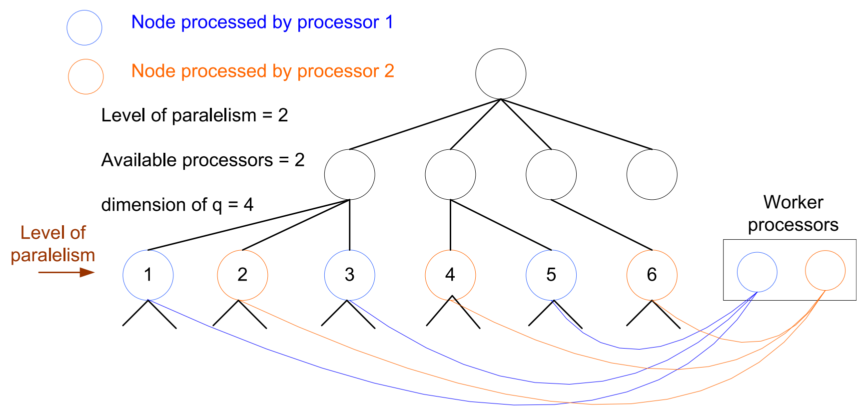

Figure 4. Assignment of nodes to the available worker processors.

In the case of memory, the problems are related to the large number of equations and/or the large number of variables, or discrete options associated with binary variables and related to geometrical options as well as other decision variables. We already experienced these issues in various attempts. For example, the linear model to design heat exchangers using the Bell–Delaware method,[50] faces the need to reduce the number of geometric options if one wants to run it in a less powerful memory-equipped laptop. We also experienced the same problem for a linear model for double-pipe hairpin-based linear model (upcoming paper). These problems will do nothing but explode in the future if distributed models start to be used (see section 7), and if such equipment models are embedded in larger flowsheet synthesis models.

The answer is to migrate to the cloud or supercomputer clusters and run in parallel, a technique that the computer science community started many years ago. While there is sophistication in a number of options to run in parallel, we refer here to two options:

- Pure parallelism: Divide the search space in various disjoint parts and solve it using as many processors as disjunct parts.
- Smart parallel processing: In this case, the search space is also divided into several disjoint parts running in separate processors, but now exchanging information.

The first option is easily implemented and only requires discussing how to partition the search space into subsets that will require similar computational effort. The second option requires said partitioning efforts and determining how the information will be shared.

Consider the following simple MINLP generic problem:

$$\left.\begin{array}{l} \min \sum_{\forall i} c_i q_i + f(x) \\ \text{s.t.} \\ \sigma_k(q, x) \le 0 \quad \forall\, k \in I_s \\ q_i \in \{0, 1\} \quad \forall\, i \end{array}\right\} \tag{45}$$

where $\sigma_k(q,x)$ and $f(x)$ are, for simplicity and without loss of generality, convex, and all the cost coefficients c_i are positive.

Consider the case of a search space encompassing 25 binary variables and 600 processors. The number of combinatorial options is 2^{25} combinations, close to 33 million. One way is to pick 9 variables and create 2^9 = 512 combinations and solve each problem with these combinations in each 512 processors. At the end, the best answer is obtained from comparing the 512 results. This option is illustrated for three processors in Figure 3, where the master node distributes the tree searches among the three processors (processors 1, 2, and 3 are given the task to explore the subtrees corresponding to nodes 1, 2, and 3) and reads the results of exploring each corresponding tree by each processor to determine the optimum. Figure 4 shows allocations made for the case of less processors than the number of nodes in the selected level (two processors and six nodes).

Among the different properties of the enumeration tree, there is one that is of concern here, that is, the tree is unbalanced with respect to the number of nodes. Indeed, the number of nodes on the left side of the tree is larger than those on the right side. This leads to the need of node balancing. This consists of a judicious allocation to make all the processors get to explore a tree that has similar number of nodes. The other option to assign nodes to the worker processors is to keep the list in the master node and the master

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

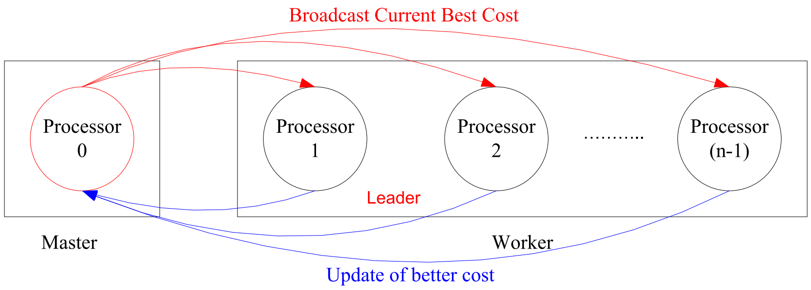

Figure 5. Parallel programming with dynamic broadcasting.

will assign a node each time a worker reports that it is idle. This strategy is known as Dynamic Load Balancing.

Simple exploring of all nodes is therefore straightforward, once balancing is achieved. However, each subtree in each processor can be solved using branch-and-bound procedures. We stop discussing further all the alternative options and their intricacies of this allocation to concentrate on the mechanisms of exchanging information.

Hitherto, we discussed node allocation, through initial exploration and possibly by dynamic allocation. We now consider the possibility that each processor can broadcast information that can be useful to other nodes.

To achieve information exchange, the master processor always listens for the better cost found by the worker processors (Figure 5). Whenever the master receives any better cost from any of the processor worker, the incumbent is updated and it broadcasts this value to all others (dynamic broadcasting). This current best cost is used by the processor-workers as a stop criterion.

Other efforts to resolve the above issues of time and/or memory have been proposed suggesting the use of agents,[72] without guaranteeing global optimality.

To summarize, the computational time and memory challenges associated with the optimization design problems can be addressed using parallel computing, in which the computational effort can be distributed to several different processors that can work independently or, in a higher efficient architecture, exchange information about the incumbent.

9. DESIGN/RETROFIT OF ENTIRE PROCESS FLOWSHEETS

The current paradigm in PSE regarding process design and/or retrofit is one in which one first uses approximate models to determine structure and then one eventually performs basic equipment design. As early as 1971, there were proposals of automatic flowsheet generation,[73] but for several decades, and only until recently, the simultaneous flowsheet synthesis with basic equipment design was not explored. We believe that the PSE community needs to advance seeking to incorporate more detailed equipment models into the whole optimization. Therefore, better designs/retrofits can be accomplished.

For example, consider heat exchanger network design/retrofit: With a few exceptions, all existing methods optimize using a-priori selected values of heat transfer coefficients. We believe that even structural changes can come from using different values of these parameters. The only chance to address it is to include the detailed exchanger design into the modeling. Consider stages or stages/substages models as well as other superstructure models, even using nonisothermal mixing. In these and other superstructures, the area of each exchanger between hot stream i and cold stream j is

$$A_{i,j} = \frac{Q_{i,j}}{\hat{U}_{i,j}\Delta T_{lm,i,j}F_{i,j}} \tag{46}$$

where $\hat{U}_{i,j}$ is considered a parameter. Solutions of the HEN synthesis problem will vary substantially if this parameter is modified. To improve on this, the equations for the superstructure can be combined with the equations for a heat exchanger model.[74] This means that the geometric variables for each potential exchanger and the equations to obtain $U_{i,j}$, now a variable, have to be introduced in the model. In such a case, the following two equations have to be used.

$$A_{i,j} = Nt_{i,j}\pi\, dt_{i,j}L_{i,j} \tag{47}$$

$$A_{i,j} \geq \frac{Q_{i,j}}{U_{i,j}\Delta T_{lm,i,j}F_{i,j}} \tag{48}$$

This thought is extended to the whole process design. The challenges are as follows:

Viable Models: The major obstacle is convergence when initial values are used in solvers, and if the solver is not global, the solution is usually a local optimum, because most problems are nonconvex. Even when initial values are provided, solvers may not make progress toward an optimal point (local or global). The major reason for the failures to converge even with initial values is the presence of complex nonconvexity, sometimes involving transcendental functions. When rational functions are used, problems can be reformulated as quadratic (nonconvex), at the expense of a large number of variables (see Manousiothakis and Sourlas[75]). To ameliorate the aforementioned model problems, we note that the introduction of discrete variables and the subsequent reformulation reduce the number of nonconvex equations to a few and that could be an advantage.

Model size: some large models do not fit in regular computers and, as it was mentioned above, can be run using parallel schemes.

To summarize, we believe that the problem of process flowsheet synthesis/retrofit will benefit from expanding it to accommodate more realistic models of the individual equipment. The accuracy of solutions improves with such inclusion, and most important, the optimal structure can vary. The computational challenges can be addressed using the parallel computing techniques discussed above.

■ CONCLUSIONS

PSE has attained remarkable advances in the last decades, providing a myriad of computational tools to solve chemical

DOI: 10.1021/acs.iecr.9b02611
Ind. Eng. Chem. Res. 2019, 58, 18684−18702

engineering problems. For example, process simulators are widely employed to provide solutions in chemical process industries. However, despite the advances obtained in problem formulation and solution algorithms, the design problems are still solved in practice using the same trial-and-verification approach. Possible reasons that hinder the direct utilization of PSE tools to solve real design problems were discussed in this paper: lack of robustness and simplified physical modeling. We are trying to address the former issue using reformulation techniques to generate linear optimization problems and, when this approach is not sufficient, we suggest the utilization of global optimization solvers or set trimming and enumeration techniques. We are also investigating solutions for the latter issue of simplified models, based on the adoption of discretized models for the formulation of the design problem, therefore overcoming the lack of accuracy of analytical solutions in certain situations (e.g., condensers and vaporizers). Parallel computation is in our view becoming an increasingly needed tool and we offer some thoughts. To conclude, the impact on flowsheet synthesis was discussed. We omitted discussing conceptual design approaches throughout the article. Our opinion is that with the ability of MINLP and stochastic methods to address more complex MINLM models effectively, the latter are preferred. It also contributes that the reality of the practitioners in industry is that they have no time to develop the required expertise to implement conceptual design, but it is easy to adopt computer optimization models they do not need to understand in detail. All this said, it has to be said that conceptual approaches are excellent tools for understanding systems and should be taught in undergraduate education. This would be similar to what happens when we teach McCabe−Thiele diagrams to understand distillation, but we would be using inside out methods in simulators to solve MESH equations.

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Notes

The authors declare no competing financial interest.

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DOI: 10.1021/acs.iecr.9b02611
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