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Challenges in Replacing Heuristics-Based Trial-and-Error Procedures by Mathematical Optimization for Basic Equipment Design

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Abstract

Even though the last decades have seen an explosion of simulation and optimization tools in Process Systems Engineering, this has not had a significant impact in the basic design of equipment such as heat exchangers, condensers, reboilers, distillation columns, absorption, adsorption columns, etc. To this date most mainstream textbooks advocate the use of trial and error procedures, while scattered work has been done using MINLP methods. In addition, these methods are most of the time local and/or do not converge if no good initial points are provided. We provide here alternatives to formulate global and robust rigorous models, sometimes linear. In this paper, we discuss the challenges that this quest is presenting.

Keywords: Process Equipment Basic Design, Optimization Models

1. Introduction

Practitioners employ computational tools for equipment design, but they are limited to analyze the behavior of proposed solution alternatives in a task that is highly dependent on the engineer experience. Despite the wide utilization of modern simulation tools, the rationale of the basic design procedure is usually based on trial-and-error procedures guided by heuristic rules and rarely search optimality. This philosophy is the established mainstream paradigm in design books for education and in many specialized texts. For example, in the area of heat exchanger design, the procedures recommended in current textbooks are based on the aforementioned trial-and-error schemes. These procedures contain rules of thumb or heuristic options that usually end when a solution unit performs the desired heat transfer task with an acceptable pressure drop, but without a focus on cost minimization. These procedures require the intervention of knowledgeable personnel to make good choices during the search. Heat exchanger rating software employ distributed models and up-to-date correlations, but the design solutions are obtained using simple search algorithms with several limitations. The same can be said about the design of separation vessels and distillation columns.

Advances of optimization models and mathematical programming algorithms have been made by the PSE community, but they are seldom used in the solution of equipment design problems in practice and remain difficult to solve in general. In the area of heat exchangers is where MINLP models, in many cases difficult to solve, even locally, have proliferated.

This paper presents a discussion about the drawbacks that restrain the utilization of mathematical programming for the solution of design problems, such as: a) The utilization of simplified models obtained through analytical solutions; b) Convergence problems originated from nonlinear (MINLP) formulations. Aiming to circumvent these problems we propose some possible solutions involving: 1) The introduction of discrete variables, and reformulations to attain simpler models; 2) The need for models that represent transport properties as a function of local conditions expressed through state variables (temperature, pressure, concentration), as opposed to overall averages through the equipment. To illustrate the ideas, we show examples of simple MINLP models, MILP and IP models for the design of heat exchangers as compared to heuristics, and how global optimization can be implemented in the case where the resulting models cannot be completely and rigorously reformulated to be linear.

Finally, we clarify that the reformulations we are proposing are such that no approximations, 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.

2. Heuristic-based Trial and Error Procedures

Consider the case of the design of shell-and-tube heat exchangers. Heuristic procedures, presented in most design books (Towler and Sinnot, 2012, for example) and heat transfer books (Serth, 2007; Cao, 2010), are based on trial-and-error schemes, such as the set of steps presented below:

(1) Make initial specifications, such as fluid allocation (tube-side x shell-side), shell and head types, and heat exchanger configuration (e.g. number of tube and shell passes). Pick a combination of tube diameters, tube lengths, baffle spacing, etc; (2) Start estimating the area using some good estimate of the overall heat transfer coefficient (U^{est}), that is

$$A^{est} = \frac{\hat{Q}}{U^{est}\widehat{\Delta T}_{lm}\,F} \tag{1}$$

where $\hat{Q}$ and $\widehat{\Delta T}_{lm}$ are given according to the thermal task; (3) Pick a number of tubes, compatible shell diameter, such that the area matches closely to A^{est}; (4) Calculate heat transfer coefficients for the tube side and the shell side and with a recommended fouling coefficient, calculate a new overall heat transfer coefficient, and the pressure drops resulting from using the above geometric choices; (5) If the overdesign is acceptable, and the pressure drops are below recommended maximums, then the design is usually finished. Otherwise, some clever adjustments are made based on the analysis of the current trial, aiming at fixing the problems observed. After that, a new evaluation of the new solution candidate is executed (return to Step 4).

Little is said by these procedures, as to how the iteration is handled, when a new trial is needed, neither recommendations are given for the cases where the new calculated value of overall heat transfer coefficient is excessively larger that the value estimated. This is handled by somebody with expertise. One can see a similar approach for the case of designing vertical and horizontal flash-units, distillation column tray design, etc.

In conclusion: most recommended procedures do not incentivize iterative procedures, only trial and verification, that is they provide heuristics and require expertise to obtain a feasible answer, not an optimal one.

The limitations of the traditional design approaches present an opportunity for mathematical programming to contribute with solutions. Despite the number of papers published that tries to fill this gap, there are important limitations that hinder the utilization of such approaches for practical problems, as discussed in the next section.

3. Optimization Models

In the last few decades, several authors started to present different optimization approaches to the design of heat exchangers. Nowadays, the two main approaches employed are stochastic methods and mathematical programming. The utilization of mathematical programming efforts has been dominated by nonconvex formulations, encompassing older nonlinear programming approaches (Jegede and Polley, 1992) or more recent mixed-integer nonlinear programming solutions (Ravagnani and Caballero, 2007). Of all the above approaches, mathematical programming is only one that has any chance of achieving and guarantee globally optimal solutions.

A more detailed analysis of the literature about the utilization of mathematical programming techniques for solving the design problem of shell-and-tube heat exchangers indicates several aspects that limit the utilization of these approaches for practical applications:

a) The utilization of nonlinear formulations that are associated to convergence problems and multiple local optima with different values of objective function. The lack of robustness is an important barrier for the acceptance of this kind of tool by a broader audience, including practitioners;
b) Utilization of heat exchanger models based on analytical solutions where the heat transfer coefficients have a uniform value along the heat transfer area. This problem is particularly important for services with phase change (vaporization or condensation), where the conditions along the flow can change considerably.

In the next sections, we discuss how these challenges have been addressed in our group.

4. Use of Discrete Variables

Our proposal is to use a set of discrete values for geometric variables, thus allowing a representation of the design solution closer to the engineering practice. Additionally, having the design variables in a discrete space allows reformulation to a linear form.

For example, heat exchanger tubes come in discrete options (3/4”, 1”, 1 ¼”, 1 ½”, 2”) with different wall thickness dictated by pressure (BWG 12, 14, 16, etc.) and different discrete options for length. The same can be said for shell diameters and other geometric variables that have been standardized (TEMA). A similar case can be made for other equipment. Thus, the diameter is expressed in terms of discrete options as follows:

$$dti = \sum_{sd=1}^{sdmax} \widehat{pdti}_{sd}\, yd_{sd} \quad (2)$$

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

$$\sum_{sd=1}^{sdmax} yd_{sd} = 1 \quad (3)$$

Consider now for example the calculation of the heat transfer coefficient for the tube-side flow using the Dittus-Boelter correlation:

$$ht = \frac{0.023\, Ret^{0.8} \widehat{Prt}^{n}\, \widehat{kt}}{dti} \quad (4)$$

Assuming one tube-side pass, the expression of the Reynolds number in relation to the mass flow rate is:

$$Ret = \frac{dti\, v\, \widehat{\rho t}}{\widehat{\mu t}} = \frac{4\ \widehat{mt}}{Ntt\, \pi\, \widehat{\mu t}\, dti} \quad (5)$$

Thus, substituting, one obtains:

$$ht = \frac{0.023\left(\frac{4\,\widehat{mt}}{\left[\sum_{sNtt=1}^{sNttmax} \widehat{pNtt}_{sNtt}\, yNtt_{sNtt}\right] \pi\, \hat{\mu}\, \sum_{sd=1}^{sdmax} \widehat{pdti}_{sd}\, yd_{sd}}\right)^{0.8} \widehat{Prt}^{n}\, \widehat{kt}}{\sum_{sd=1}^{sdmax} \widehat{pdti}_{sd}\, yd_{sd}} \quad (6)$$

Note that we replaced the total number of tubes by a sum of discrete options. The above expression is nonlinear in the binary variables and requires reformulation if it is run by most commercial MINLP.

5. Reformulation

We first 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:

$$[\sum_i \widehat{pd}_i\, yp_i]^{n1}\, [\sum_j \widehat{qd}_j\, yq_j]^{n2} .. [\sum_k \widehat{zd}_k\, yz_k]^{nm} = p^{n1} q^{n2} \cdots z^{nm} = \sum_{i,j,..k} \widehat{pd}_i^{\ n1} \widehat{qd}_j^{\ n2} .. \widehat{qd}_k^{\ nm}\, yp_i\ yq_j \ldots\ yz_k \quad (7)$$

Thus Eq.(6) can be rewritten as follows:

$$ht = 0.023\, \widehat{Prt}^{n}\, \widehat{kt}\, \left[\frac{4\,\widehat{mt}}{\pi\, \hat{\mu}}\right]^{0.8} \sum_{sd=1}^{sdmax} \sum_{sNtt=1}^{sNttmax} \frac{yNtt_{sNtt} yd_{sd}}{\widehat{pdti}_{sd}^{\ 1.8}\, \widehat{pNtt}_{sNtt}^{\ 0.8}} \quad (8)$$

A generalized expression for this equation, valid for any number of tube passes, including the relations associated to the tube count in relation to the shell diameter can be find in Gonçalves et al. (2016). We emphasize again that we arrive at Eq.(8) by rigorous reformulation, that is without making any approximation of any sort.

In general, we expect, products of binaries and continuous variables as well as fractional terms, which we know can be easily and rigorously linearized (Williams, 2013). The resulting formulation can be MILP or even IP (Gonçalves et al., 2017). Now, we are exploring this approach for other alternatives of heat exchangers, such as double-pipe, air coolers, plate-and-frame, and plate-and-fin; there are also investigations using a similar approach to the design of the internals of distillation columns, flash units and separators.

Another alternative for representation of the discrete variables is the utilization of a table that contains all combinations of the discrete values, i.e. each row of the table is a solution candidate. Therefore, instead of using several sets of binary variables, this formulation employs a single set, associated to the table rows. Numerical tests indicated that this approach can bring large reductions of the computational effort (Gonçalves et al., 2017).

6. Global Optimization

Sometimes, the resulting model contains continuous variables participating in non-linear terms that are not amenable to be discretized. We illustrate this with the case of an air cooler. Hitherto, we solved this problem using a fixed air flow rate, which yielded an IP problem (Souza et al., 2017). Now, we are exploring the case of variable air flow, which leads to a model that is nonlinear in only one continuous variable (the air flow rate). The air flow rate participates in several expressions used to calculate the Reynolds number and consequently the overall heat transfer coefficient. This can be solved using any global optimizer (we tried Baron, Antigone and Rysia (Faria and Bagajewicz, 2012)). One can think of just using different flow rates and solve the IP fixed flow problem repeatedly, by using several discrete values of flow, or incorporate such discretization to the model and reformulate. Both options are mathematically not rigorous, but practically sound.

We also find the same situation in the case of heat exchangers with fouling being modelled. 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 (Lemos et al., 2017). 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.

7. Local models

One of the challenges ahead is to move away from simplified models based on analytical solutions (e.g. LMTD method) and address the optimization problem using discretized portions of the equipment where local properties are calculated using conservation equations. 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 vapour and the outlet stream is saturated liquid). Instead of only use the end temperatures, the model will contain equations related to the set of temperatures distributed along the flow path.

8. Implications for Process Design/Retrofit

The current paradigm in PSE regarding process design and/or retrofit is one where one first use approximate models to determine structure and then eventually perform basic equipment design. The alternative is to incorporate detailed equipment models into the whole optimization. We believe that the PSE community needs to move in the latter direction and increasing computing power will render 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. The only chance address it is to include the detailed exchanger design into the modelling. This thought is extended to the whole process design.

9. Conclusions

PSE has been attained remarkable advances in the last decades, providing a myriad of computational tools to solve chemical 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-error approach.

Possible reasons that hinder the direct utilization of PSE tools to solve real design problems were discussed along this paper. The lack of robustness and the simplified physical modelling are two aspects that hinder the utilization of the optimization tools for solving design problems. 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. We are also investigating solutions for the latter issue 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).

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