CHEMICAL ENGINEERING TRANSACTIONS

VOL. 61, 2017

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Petar S Varbanov, Rongxin Su, Hon Loong Lam, Xia Liu, Jiří J Klemeš

ISBN 978-88-95608-51-8; **ISSN** 2283-9216

DOI: 10.3303/CET1761228

A Hybrid Meta-Heuristic Approach for Multi-Objective Optimization of Heat Exchanger Networks considering Costs and Environmental Impacts

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Heat Exchanger Networks (HEN) are able to reduce the operating costs in an industrial plant. Cost-optimal HEN generally leads also to a substantial reduction in pollutant gases emissions. However, HEN synthesis approaches are based generally on the optimization of total annual costs (TAC) only. In that manner, this work aims to address environmental impacts (EI) more directly. The EI were converted into an objective function by using a Life Cycle Assessment (LCA) methodology. With two objective functions (EI and TAC), a multi-objective optimization (MOO) may be performed. A meta-heuristic approach is adapted to handle MOO in the formulation proposed. As expected, a conflictive behaviour was noticed. The approach proposed was able to yield Pareto fronts efficiently, providing good intermediate solutions that could be used by decision-makers in search of a trade-off HEN configuration which is able to present low costs and is also environmentally friendly. The results reported in the case study also demonstrate the method reliability with intermediate solutions that are much more environmentally friendly than the cost optimal configurations, presenting costs only marginally higher.

1. Introduction

Heat Exchanger Networks (HEN) are an extensively investigated field in process engineering. An efficiently heat-integrated industrial plant is able to yield massive reductions in operating and capital costs, as well as in pollutant emissions. In that manner, designers and researchers have developed several methods aiming for costs-optimal HEN designs. Aiming for an automated synthesis, methods based on mathematical programming formulations were proposed, such as the stagewise superstructure (Yee and Grossmann, 1990) which has simplifying assumptions such as isothermal mixing and a single piece of equipment per branch of stream split. Despite such considerations it can lead to efficient solutions and is still widely used and taken as basis for HEN models comprising other features, such as multi-period operation (Kang et al., 2015). The reader is also referred to the work of Fraser et al. (2016), where a comprehensive performance analysis regarding HEN synthesis models is presented. HEN synthesis mathematical formulations are complex to solve, given the problem combinatorial nature, nonlinearities, non-convexities and the large number of local minimum solutions. A recent trend is the use of hybrid meta-heuristic based methodologies in the search for HEN promising designs, such as two-level methods, which separate meta-heuristic methods for the combinatorial and the continuous levels of the problem, and variations. For instance, GA with Particle Swarm Optimization (Pavão et al., 2016) or Simulated Annealing (SA) with Rocket Fireworks Optimization (RFO) (Pavão et al., 2017), the method that serves as basis to this work.

Although global optimality in the HEN synthesis problem is difficult to guarantee given the already mentioned difficulties, the methods are continuously evolving and progressively better solutions to benchmark problems are being reported in the literature.

However, although costs-optimal solutions might reduce greenhouse gases emissions as a natural consequence of diminishing utilities generation requirements, only few works in the literature address directly

Please cite this article as: Pavão L.V., Costa C.B.B., Jiménez L., Ravagnani M.A.S.S., 2017, A hybrid meta-heuristic approach for multi-objective optimization of heat exchanger networks considering costs and environmental impacts, Chemical Engineering Transactions, 61, 1381-1386 DOI:10.3303/CET1761228

the environmental aspect of HEN synthesis. López-Maldonado et al. (2011) proposed a bi-criteria formulation for TAC and EI arisen from the use of utilities in HEN. Vaskan et al. (2012) presented a model where EI from heat exchanger construction was also considered. The authors also made an analysis of several impact categories in different plant lifetimes. In both works (López-Maldonado et al., 2011; Vaskan et al., 2012), EI quantifying was performed using the Eco-indicator 99, and the mathematical formulations solved with DICOPT, CONOPT and CPLEX in GAMS.
Since a bi-criteria optimization of the HEN synthesis problem increases problem complexity, aforementioned works presented solutions to small case studies only. Aiming to handle larger and more difficult HEN synthesis cases, this work adapts an efficient meta-heuristic HEN synthesis method (SA-RFO) recently proposed in Pavão et al. (2017) to a MOO approach in order to handle trade-offs in TAC and EI of medium-to-large scale HEN problems. The SA-RFO methodology was able to outperform other methods presented in the literature based both on deterministic approaches aided by commercial solvers or on meta-heuristics. The adapted method presents a Pareto front with several interesting efficient solutions, providing decision-makers with options that better fit their economic and environmental goals. The LCA methodology is also used by means of ReCiPe (Goedkoop et al., 2013), a reliable indicator for environmental impacts.

2. Formulation

In order to perform TAC and EI multi-objective optimization of a HEN and find the Pareto solutions, the problem has to be modelled with a mathematical programming formulation. The cost function is based on the widely used stagewise superstructure (SWS) (Yee and Grossmann, 1990).
The formulation divides the HEN in stages, each comprising every possible heat exchange match, one per process stream branches (i.e., the model has stream splitters and mixers). Heaters and coolers are placed at the end of each stream. In the original formulation the authors assumed that the heat exchangers outlet temperature in a single stream were equal, in order to avoid an energy balance in the mixers and make the formulation simpler to solve. In this work, however, the model is adapted to perform the mentioned mixers energy balance, not adopting the isothermal mixing assumption of the original work. The costs function is presented in Eq. (1).

$$\begin{aligned} TAC = & \sum_{i \in N_H} Ccu \cdot Qcu_i + \sum_{j \in N_C} Chu \cdot Qcu_j + \sum_{i \in N_H} \sum_{j \in N_C} \sum_{i \in N_S} z_{i,j,k} (B + C \cdot A_{i,j,k}^{\beta}) + \\ & \sum_{i \in N_H} zcu_i (B + C \cdot Acu_i^{\beta}) + \sum_{j \in N_C} zhu_j (B + C \cdot Ahu_j^{\beta}) \end{aligned} \tag{1}$$

Where *Ccu* and *Qcu* are the costs and total heat loads for cold utilities, *Chu* and *Qhu* are analogous for hot utilities. The *z* variable is of the binary type and represents the presence or not of a given *i,j,k* match, defining the HEN topology. The parameters *B, C and β* are the fixed cost for a heat exchanger, the cost factor, and the costs exponent. The variables *A*, *Ahu* and *Acu* are the areas for heat exchangers, heaters and coolers. Finally, subscripts *i*, *j* and *k* represent hot and cold streams and stage of a match. The reader is referred to Pavão et al. (2016) for more information on the non-isothermal mixing, temperatures and areas calculation, as well as other equations and constraints of this adaptation of the SWS.
In order to quantify environmental impacts, a LCA method can be used. This work employs the ReCiPe method in order to address the environmental impacts yielded by utilities production in the plant, as well as the heat exchangers construction. In such method, the quantifying is presented in the form of "ecopoints", or simply "points" which are here referred to, in short form, as "pts".
ReCiPe defines impacts into 18 midpoint impacts categories under three great endpoint groups: ecosystem diversity, resource availability and human health. According to the LCA methodology, impact categories have to be weighted in order to be quantified. In this work, data from the ReCiPe methodology were weighted under one of the perspectives from the "Cultural Theory", by Thompson et al. (1990): the Hierarchist. Such perspective is often used in scientific models, being somewhat a middle-ground between the less and the most precautionary perspectives (Individualist and Egalitarian) regarding to time-frames and damages avoidance. The data is obtained from EcoInvent v3.2, an online database for LCA.
The impacts here considered are related to the production of hot and cold utilities as well as the quantities of stainless steel needed for the heat exchangers construction. The data retrieved and converted to units of ecopoints per kilowatt year (pts/(kWy)) in the utilities production case are presented in Table 1 with the same number of significant digits from the database. Further extrapolations to this data are presented in the case study. The EI objective function, which has to be optimized simultaneously with TAC, is presented in Eq. (2). In the referred equation, *EPcu*, *EPhu and EPss* are environmental impacts from cold utilities, hot utilities and stainless-steel production and *m*, *mcu* and *mhu* represent the mass of heat exchangers, heaters and coolers,

in kilograms, calculated as the product of unit area (variable, m^2), stainless steel density (7,900 kg/m^3) and thickness (5.0×10^{-3}m).

Table 1: LCA data from ReCiPe

	Cooling, pts/(kW y), raw electricity, high voltage	Heating, pts/(kW y), - steam, eff. 74%	Stainless steel, pts/kg
Ecosystem diversity	5.1792	4.4379×10^{1}	1.0546×10^{-1}
Human health	9.2743	8.5014×10^{1}	3.2023×10^{-1}
Resources availability	7.4337	9.4980×10^{1}	7.7904×10^{-1}
Total	2.1887×10^{1}	2.2438×10^{2}	1.2047

$$EI = \sum_{i\in N_H} EPcu\cdot Qcu_i + \sum_{j\in N_C} EPhu\cdot Qcu_j + \frac{EPss}{LT}\left(\begin{array}{l}\sum_{i\in N_H}\sum_{j\in N_C}\sum_{i\in N_S} z_{i,j,k}(B + C\cdot m_{i,j,k}) + \sum_{i\in N_H} zcu_i(B + C\cdot mcu_i) + \\ \sum_{j\in N_C} zhu_j(B + C\cdot mhu_j)\end{array}\right) \quad (2)$$

3. Solution method

The MOO method proposed in this work is an adaptation of a meta-heuristic approach over the well studied ***ε***-constraint method (Ehrgott, 2005). In this methodology, the optimal solutions regarding both objectives have to be found first. Then, the range between the two previously obtained extreme solutions is divided in equal smaller intervals, according to the desired number of Pareto solutions to be obtained. One of the objectives is then is set as an auxiliary constraint, and the values of the bounds of the aforementioned intervals are imposed to it. Such bounding values are called ***ε***. To each ***ε*** value imposed to the secondary function, the primary one is optimized in a single-optimization problem, respecting the ***ε***-constraint. Figure 1 presents the method block diagram.

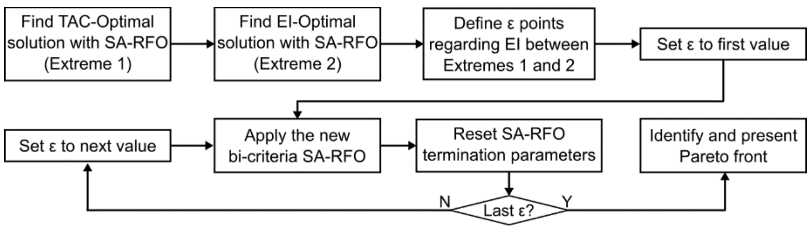

Figure 1: Solution method block diagram

The meta-heuristic method for HEN synthesis which serves as basis to the MOO method developed in this work uses Simulated Annealing (SA) on the combinatorial level and the Rocket Fireworks Optimization (RFO) in the continuous level to find optimal HEN heat loads and stream fractions. It is implemented in C++ and is able to achieve good near-optimal solutions for medium and large-scale cases. SA, originally proposed by Kirkpatrick et al. (1983) is used in the first (combinatorial) level with a simple move of adding one random heat exchanger at a time. That means a new topology is proposed which needs to be optimized with a continuous optimization approach. Rocket Fireworks Optimization (RFO) consists in two steps. Firstly a modification of the original Simulated Annealing to handle continuous spaces (CSA) is applied in order to find a promising solution, which is incorporated to a set of random solutions. These become particles in Particle Swarm Optimization (PSO) (Kennedy and Eberhart, 1995), which performs better with the incorporated CSA solution. Moreover, the reader is referred to the original work in which SA-RFO is presented (Pavão et al., 2016) for details related to other strategies of the method such as the identification of interdependent matches and constraint handling schemes. In order to adapt the SA-RFO method to handle HEN multi-objective optimization with the ε-constraint method, costs are defined as primary function, while environmental impacts are set as the constraint. The optimization method must, then, find the minimal TAC to each of the ***ε*** values assigned to EI. The first challenge is to find solutions that satisfy the constrained EI while costs are minimized. Some rules are then implemented in the SA-

RFO program routine. In this approach, solutions are initially guided only by EI, and the search is guided only for more environmentally friendly solutions. Following, once the method is able to find one solution that satisfy *ε* value, the search rules are changed, and cost optimal solutions are sought. However, that might lead the solutions back to the area with invalid *ε* values. In order to forbid that from happening, a rule is implemented, so that if, during the search, a solution with an invalid value for EI is found, it is never accepted. All constraint handling routines are implemented and applied to the CSA solution as well as to all particles in PSO. An illustration of the solutions evolution during the continuous optimization is depicted in Figure 2 (a). It is possible to notice that once the solutions pass through the *ε* "barrier", they are not allowed to go back to the invalid *ε* region. In that illustration, the method finds a solution, which is dominated, by the current best solution from the combinatorial SA, and the acceptance rules are applied to decide whether this solution is accepted as the new solution or not. In Figure 2 (b), the final Pareto front obtained for a problem is shown together with all solutions achieved in the method. Each point in Figure 2 (b) is a solution achieved by the aforementioned continuous optimization method depicted in Figure 2 (a).

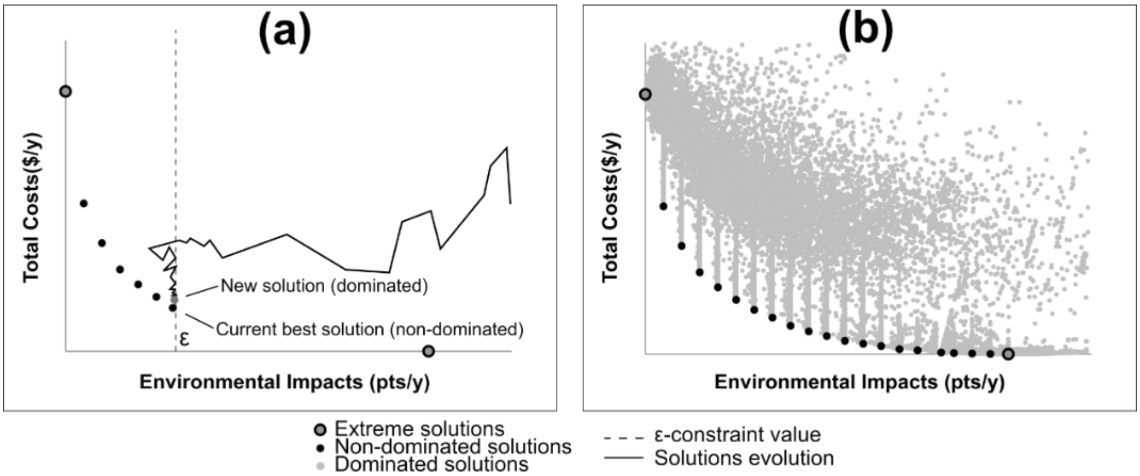

Figure 2: (a) Obtaining of one solution with the ε-SARFO method (b) Overview of all solutions during the application of the method

4. Case study

In order to verify the developed method performance, it was applied to a slightly modified version of a well-studied case from the literature. The problem has 10 streams, being six hot and four cold. The original case was proposed by Ahmad (1985), who used it to present Pinch technology features. The case has served as a benchmark to the HEN synthesis scientific community ever since, e.g. Ravagnani et al. (2005) who applied a Genetic Algorithm to the problem. The case has many interesting local minimal solutions to be explored, and no method has been yet able to guarantee a solution of global optimal TAC. The original case study, however, has no fixed costs for heat exchangers, which leads solutions to have a large number of units. Such solutions might be undesirable in some cases, from the design and control point of view, and costs presented may also be unrealistic. Such drawbacks were handled by Huang and co-workers by proposing an adapted formulation in which $8,000/y is considered as unit fixed deploying costs (Huang et al., 2012). They used an approach based on Outer Approximation with the commercial solvers CPLEX, CONOPT and BARON in GAMS for costs optimization using the SWS formulation without the isothermal mixing assumption. The problem was solved also in (Huang and Karimi, 2014) with a more complex superstructure and a better solution was found. As expected, by considering heat exchangers fixed costs slightly more expensive solutions were achieved. However, these were more feasible configurations, with less units. The modified cost formulation was also used by Pavão et al. (2016), where a solution with costs a bit lower was achieved. That cost formulation is also used in this work and the reader is referred to Pavão et al. (2017) for process streams data. Differently from previous studies on this case, MOO of TAC and EI is here performed. The plant proposed in the case study uses steam as hot utility. Thus, the value for eco-points used (*EPhu*) can be that presented in Table 1 (2.2438×10^2 pts/ kWy). Cold utilities need some extrapolation though. The temperature range for cold utilities in this plant is 15 – 25 °C. It is considered that utilities come from cooling towers and chillers. The former is assumed to operate in the range of 20 – 25 °C, while the latter covers the lower temperatures range of 15 - 20°C. Both pieces of equipment require electricity, whose data is in Table 1. The cooling efficiency of 70.3 kW_r/kW_e (kW of refrigeration per kW of electricity) is considered for cooling towers and 7.03 kW_r/kW_e for and chillers. By assuming 50% of the utilities coming from each kind of cooling equipment, given their temperature operation ranges, the *EPcu* is 3.0095×10^{1} pts/kWy.

The ε-SARFO method is then applied to firstly achieve the TAC-optimal solution, then, the algorithm guidance becomes the EI, and the most environmentally friendly configuration is achieved. It is worth pointing out that the TAC-optimal solution achieved presents lower costs than those achieved with the deterministic methods used by Huang and Karimi (2014). Extreme solutions configurations and their data are presented in Figure 3 (a), in a form derived from the SWS (Yee and Grossmann, 1990) model representation adopted in Ravagnani and Caballero (2007) and more recently Pavão et al. (2017). A set of 60 Pareto solutions is obtained. Figure 3 (b) presents the front, as well as hot and cold utilities used, total areas of heat exchangers, heaters and coolers. Please note that the abscissas in the three plots are the same, and each point from the Pareto front has correspondent points in the other two plots below it.

Some aspects are worth noting in extreme solutions. The environmentally-optimal configuration makes use of equipment with high areas in order to reduce the use of utilities, which weight more to the environmental impacts than the heat exchangers material of construction. The costs optimal solution presents more balanced values between utilities and area. However, such trade-off is not ideal regarding environmental impacts.

With a reasonable set of solutions, decision-makers have a good source of information and are able to choose a configuration that better satisfies their necessities. The solution of optimal EI is too expensive, but there are configurations able to reduce much of the impacts while costs are not too affected. Some good solutions can be compared to the costs-optimal solution, e.g., one of the configurations obtained has TAC of $5,847,849/y with EI of 4,989,262 pts/y, yielding impacts reduction of 10.3 % (compared to cost-optimal configuration), while costs increase only 2.4 %. If a configuration with better costs is required, another of the solutions has TAC of $5,737,321/y and EI of 5,370,371 pts/y (cost 0.42 % higher with impacts 3.43 % lower than the cost optimal).

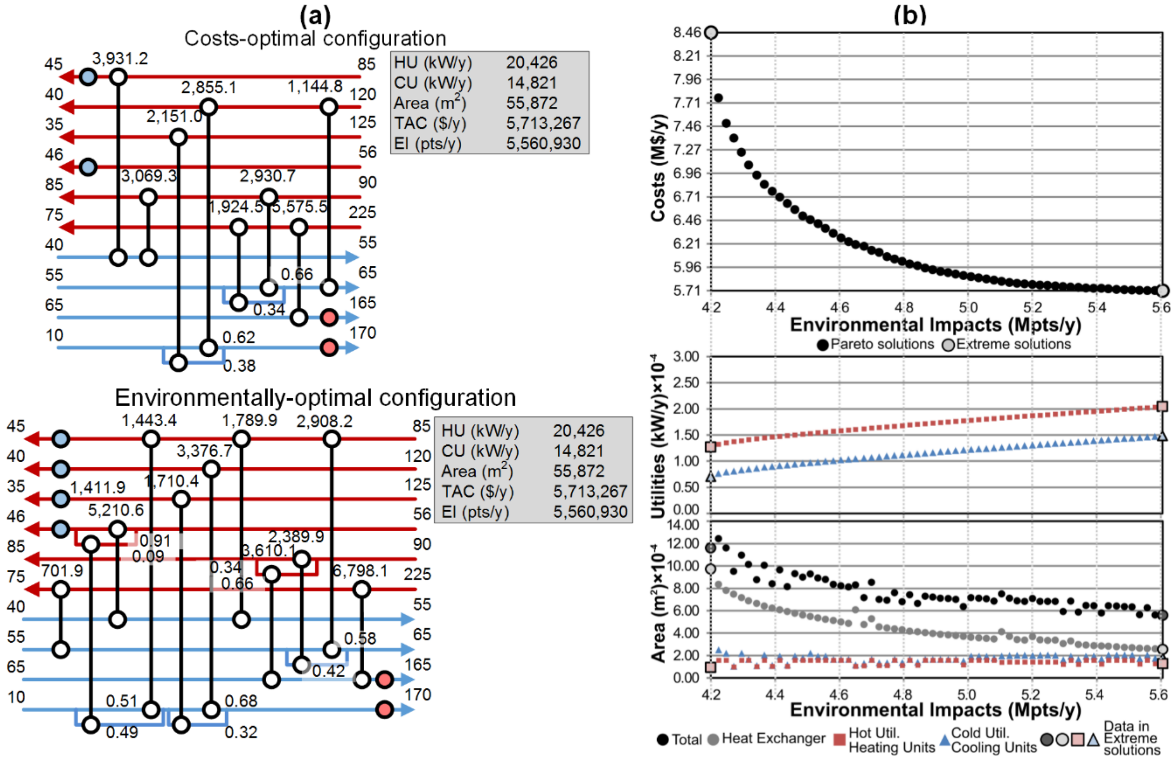

Figure 3: (a) Costs-optimal and Environmentally-optimal solutions (b) Pareto front, utilities and areas for each solution obtained to the case study

5. Conclusions

A method able to handle the multi-objective optimization of HEN total annual costs and environmental impacts was presented. The SA-RFO approach for HEN synthesis, which is a meta-heuristic scheme, was adapted to perform the ε-constraint method in order to find a set of Pareto solutions. The strategy was applied to a modification of a well-studied benchmark case study, to which EI indicators based on the ReCiPe LCA methodology were employed. With the Pareto front, it was possible to observe the *trade-offs* in TAC *versus* EI. More environmentally friendly solutions are likely to present reduced utility requirements, but the total heat exchange area is greatly increased, making solutions more expensive. However, the method demonstrated reliability in finding good intermediate Pareto solutions, which are environmentally friendly with relatively low costs, being able to serve as options for decision-makers to make choices based on their needs.

Acknowledgments

The authors acknowledge the financial support from the Coordination for the Improvement of Higher Education (CAPES, Brazil) and the National Council for Scientific and Technological Development (Processes 400741/2013-0 and 210318/2015-5, CNPq, Brazil). L. Jiménez thanks the Spanish Ministry of Education and Competitiveness for their financial support (CTQ2016-77968-C3).

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