Robust optimization in heat exchanger network synthesis

J. L. Miranda [(1)], M. A. S. Casquilho [(2)]

[(1)] Escola Superior de Tecnologia e Gestão, Instituto Politécnico de Portalegre
Lugar da Abadessa, Apt. 148; 7301-999 Portalegre; Portugal.
+351 245 300 200; jlmiranda@estgp.pt

[(2)] Instituto Superior Técnico, Universidade Técnica de Lisboa
Ave. Rovisco Pais, IST; 1049-001 Lisboa; Portugal
+351 21 841 7000; mcasquilho@ist.utl.pt.

1. Introduction – A robust optimization model aimed at heat exchanger network synthesis is developed, in a Two-Stage Stochastic Programming (2SSP) framework, with the uncertainty formulated through a number of discrete scenarios of heat and cold streams, with the corresponding probability. In the first stage, the model defines the heat exchangers dimensions, with the associated binary decision variables (0/1); in the second stage, after the realization of the random scenarios, it determines the recourse values for the utilities streams. The stochastic Mixed Integer Linear Programming (MILP) model is a sparse model with binary variables in the first stage, and it constitutes a NP-hard computational class problem. So, not being possible to build an exact and polynomial algorithm that treats efficiently the problem, a heuristic procedure is developed that produces good possible solutions, in the range of real utilization of the problem parameters. A post-optimality study is realized, allowing us to analyse the sensitivity of the robust objective function to the penalty parameters of the solution variability.

The heat exchanger network synthesis (HENS) problem usually treated through sequential optimization [1] is incompletely, i.e., sub-optimally solved. Indeed, first minimizing the utilities consumption, then minimizing the number of matches needed, and finally minimizing the total costs including the cost of the transfer area is certainly sub-optimal due to the fact that the efficiency of each decision level depends on the quality of the solution obtained in the previous decision level. Also, the economic analysis of the energetic integration problem should conjugate the various economic issues involved, which is not achieved using the described sequence of partial sub-problems.

It is pertinent to apply methods of Mathematical Programming (MP) that proceed to a simultaneous optimization of the described issues, i.e., which can properly emulate the interactions among the different cost components, the costs of utilities and simultaneously of transfer equipments, considering fixed charge and variable costs. However, with the purpose of reducing the computational effort related to non-convex problems and to discrete decision variables in a rigorous model, the pinch point [2] analysis and the referred sequential methodology remain and are widely used.

A general superstructure was developed [3] and addresses the simultaneous energetic integration of heat and cold streams, without recurring to the sequential approach on utilities consumption, number of matches and total transfer area. The simultaneous optimization model treats both the transfer area and the utilities targeting, and it also considers variability on the heat transfer coefficients between the different streams. The superstructure was modified [4] on the sense of: promoting the determination of the number of temperature intervals on the superstructure, assuming the *transshipment* [5] representation of the heat flows; locating the intervals where the matches within each pair (hot and cold) of streams are possible; generalizing the application of utilities all along the temperature intervals of the superstructure, treating them as hot or cold streams. The objective function thus formulated minimizes the total aggregated costs, by aggregating the variable costs related to the transfer area, which were represented through the only non-convex term occurring in the objective function, and this approximation leads to an underestimation of the area cost.

For several models of HENS, the computational complexity classification was done [6], revealing that the MILP models represent NP-hard class problems and, obviously, the LP models are P class problems.

The formulation treated here aims at a robust optimization [7] of the HENS problem, featuring binary decision variables and probabilistic occurring scenarios in a 2SSP framework. The uncertainty is formulated through probabilistic discrete scenarios of hot and cold streams, and the model selects the heat exchangers discrete dimensions in the first stage, through the allocation of binary decision variables (0/1). In the second stage, after the realization of the random scenarios, the model minimizes the recourse values for the utilities streams, and penalizes both the variability of the expected total cost and the expected non-satisfied temperatures of the outlet process streams.

2. Experimental

The stochastic superstructure is defined, in each scenario at each time period, by the inlet temperatures of the heat and cold streams, defining the temperature intervals in a descending order and specifying a numerical value for the energy minimum approach temperature (EMAT). The outlet stream temperatures are targeted and this permits to define the required stochastic heat flows among the exchanging streams.

The formulation of the problem, aiming at a robust optimization, features:

- a robust objective function, that minimizes the present investment cost associated to discrete dimensions of the exchangers, and penalizes the solution variability and the non-satisfied prescribed temperatures of the outlet streams;
- a probabilistic generalized superstructure, that corresponds to probabilistic *transshipment* [8] sub-problems, in each temporized scenario;
- some specific restrictions on heat flows through each temperature interval of the superstructure, on the number of exchangers, and on the matches allowed or prescribed;
- a linearized estimation of the transfer area, that supposes Maximum Driving Force (MDF).

In the robust objective function, each probabilistic term corresponds to the present cost for each scenario, defined as the present value of the consumption of the hot and cold utilities, plus the (discrete) investment costs (according to the discrete transfer areas for each exchange).

$$
\begin{aligned}
[min]\,\Phi = {} & \sum_{r=1}^{NR} prob_r x_r + ldsv \sum_{r=1}^{NR} prob_r . dsvp_r \\
& + l\,TCns \sum_{r=1}^{NR} \frac{prob_r}{NC.NT} \left(\sum_{j=1}^{NC} \sum_{t=1}^{NT} \left(dTcneg_{jtr} + dTcpos_{jtr} \right) \right) \\
& + l\,THns \sum_{r=1}^{NR} \frac{prob_r}{NH.NT} \left(\sum_{i=1}^{NH} \sum_{t=1}^{NT} \left(dThneg_{itr} + dThpos_{itr} \right) \right)
\end{aligned}
$$

where

NC, NH, NK, NR, NS(*i,j*), *NS*(*cu,i*), *NS*(*hu,j*), *NT* – number of cold streams, *j* (*Cold*) and hot streams *i* (*Hot*), of temperature intervals *k*, of discrete scenarios *r*, of discrete dimensions *s*(*i, j, cu, hu*) for the transfer areas, of time periods *t*;

ldsv, lTHns, lTCns – penalty parameters for variability deviation, for temperature differences (not satisfied) of hot and cold streams;

Ccu, Chu – unit costs (uncertain) of utilities, in each period *t* and each random scenario *r*;

x, dsvp – expected present cost, positive linear deviation from previous;

dTcneg, dTcpos, dThneg, dThpos – temperature differences (negative and positive) for non-satisfied temperatures for the streams (*Cold* and *Hot*), in period *t* and scenario *r*;

prob – probability of each discrete scenario in each time period.

A linear estimator was used to penalize the solution variability, which is defined by the positive deviation of costs with reference to their expected value in each random scenario.

The temperature differences, of negative or positive nature, for any hot or cold stream, are defined for each period of time and each scenario, as the slack of the corresponding constraints (by the difference between the targeted temperature of the outlet stream and its effective value).

For each random scenario at each period of time, it should be verified that *transshipment* formulation for heat flows are met along the temperature intervals of the superstructure. That is to say that the energy balances for cold streams, cold utility streams, hot streams and hot utility streams are formulated assuming that each temperature interval corresponds to a *transshipment* point located between the temperatures "source" and "destination". Finally, the bounds on the first and last values of residual flows must be considered.

The usual semi-continuous constraints of logic type are imposed, so that the heat flows are zero if one specified match is not selected or else the existing flows must verify their upper bounds. These bounds are set to the smallest of the estimated heat content of the two streams involved. Also, the number of discrete dimensions selected for each match must be one, at most, if the corresponding match is active.

Some specific issues on the heat exchanger network are defined through the setting or bounding of values for variables, or even by adding new constraints: forbidden or required matches are directly imposed by setting the corresponding binary variables to the values 0 or 1, respectively; the total number of equipment units (exchangers, boilers, coolers) may be set or bound by majoring the sum of the associated binary variables. The number of stream partitions can be bound through the number of exchanges in each temperature interval or even forbidden if one and only one exchange is required on each stream for temperature interval.

Assuming one exchange, at most, within each pair of streams, the discrete transfer area was formulated through a linearization of the logarithm-mean temperature difference (LMTD) developed through a multivariable Taylor expansion of first order.

To accomplish the referred proposal, the semi-continuous variables are obtained from the multiplication of the continuous variables (corresponding to the heat flows) by the binary ones (corresponding to the matches), and their values will be zero if the match is not selected or have an upper bound otherwise. This way, the linear LMTD estimation is performed assuming known the inlet temperature values, in conjunction with the MDF assumption.

3. Results and Discussion -

The model promotes the robustness in the solution, by decreasing variability for the number of scenarios envisaged. Also, the robustness in the model is enhanced considering that it permits to decease the expected temperature differences, and thus making outlet stream temperatures closer to the target defined.

The number of time periods and the number of random scenarios directly affect the problem size, in spite of the underlying linear nature. Indeed, the number of binary variables is prominent, and thus the computational difficulty is high. Approximative or heuristic procedures are envisaged, not excluding the recourse to decomposition methods.

The developed linearization of LMTD, an approximative procedure based on Taylor series, works satisfactorily in the neighbourhood of the target temperatures, is, anyway, of a similar quality to other approximations usually found, and any method would have to cope with the ill-conditioning of the function itself.

It must be noted that MDF assumes that for processing heat transfer, the exchanger inlet temperatures are equal to the stream inlet temperatures and it also assumes that the matches occur within a single heat exchanger. This would be true only for single equipment unit, parallel heat transfer, and is an overestimation of the temperature driving forces and thus an underestimation of the area. The total area cost accounts for the variations on technical coefficients, namely, on the overall heat transfer and area cost coefficients. Assuming MDF and estimating the area value, the exchanger outlet temperatures are then related to the total heat transferred. This model is accurate in the described condition, so for several units in series the available driving forces for a given heat load are greatly overestimated.

4. Conclusions -

A robust optimization model is developed to explicitly treat the uncertainty on the inlet temperatures of the streams, in a simultaneous energetic integration framework: it minimizes the expected cost of utilities and transfer area, considering fixed and variable components; it promotes the solution robustness, penalizing the variability of the stochastic solution; it promotes the model robustness, due to the penalization of the non-satisfied outlet streams temperatures.

The Two-Stage Stochastic Programming model presents discrete values of the transfer area, the values being allocated through binary decision variables, thus representing an NP-hard problem. Also, the superstructure built has a probabilistic nature, and the robust objective function leads to the assessment of proper economic estimators.

Several extensions of the model are in sight, namely: considering the further generalization of the superstructure; assuming multi-period economic formulation (timely dynamic); and promoting the numerical resolution of large instances of the robust HENS through the development of specific heuristics.

5. References

[1] Floudas, C.A., Ciric, A.R., Grossmann, I.E., Automatic Synthesis of Optimum Heat Exchanger Network Configurations, *AICHE Journal* **32** 2 (1986) 276-290

[2] Linnhoff, B., Hindmarsh, E., The Pinch Design Method for Heat Exchanger Networks, *Chemical Engineering Science* **38** 5 (1983) 745-763

[3] Yee, T.F., Grossmann, I.E., Simultaneous Optimization Models for Heat Integration–II. Heat Exchanger Network Synthesis *Computers and Chemical Engineering* **14** 10 (1990) 1165-1184

[4] Daichendt, M.M., Grossmann, I.E., Preliminary Screening Procedure for the MINLP Synthesis of Process Systems–II. Heat Exchanger Networks *Computers and Chemical Engineering* **18** 8 (1994) 679-709

[5] Papoulias, S.A., Grossmann, I.E., A Structural Optimization Approach in Process Synthesis–II. Heat Recovery Networks *Computers and Chemical Engineering* **7** 6 (1983) 707-721

[6] Furman, K.C., Sahinidis, N.V., Computational Complexity of Heat Exchanger Network Synthesis, *Computers and Chemical Engineering* **25** (2001) 1371–1390

[7] Malcolm, S.A., Zenios, S.A., Robust optimization for power systems capacity expansion under uncertainty, *Journal Operations Research Society* **45** (1994) 1040-1049

[8] Cerda, J., Westerberg, A., Synthesizing Heat Exchanger Networks Having Restricted Stream/Stream Matches Using Transportation Problem Formulations, *Chemical Engineering Science* **38** 10 (1983) 1723-1740