Novel Optimization Approaches for Targeting Heat Exchanger Networks*

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Received 2 March 2001

The work deals with recent developments in heat exchanger networks (HENs) targeting. The following issues were addressed: minimum utility cost calculation by generalized transshipment model for nonpoint utilities; targeting approach for minimum area of counter-current (1-1) and multipass (1-2) heat exchangers; and minimization of number of matches at targeting stage by generation of near-balanced subsets of streams. These problems have been solved using novel optimization models. A description of the methods and some examples of applications are given.

Process System Engineering (PSE) has emerged several years ago as a new research field in frames of chemical and process engineering. One of the main issues in PSE is designing a totally heat-integrated chemical complex. In such a complex, heat energy is recovered from the process streams in heat exchanger network (HEN). Nowadays, the optimal design of HENs has reached quite mature state. In this study, we limited a discussion to targeting stage only.

The targeting approaches most often applied in practice are those based on the Pinch Technology (PT). The principles and computation techniques have been described in numerous papers and also in monographs [1—3]. PT methods are easy to use and provide illustrative graphical representations. Hence, they give a user deep insights into the complex problems and allow him to keep the design process under control. However, due to inherent simplifications, PT approaches do not account rigorously for certain problems important in practice such as *e.g.* restricted matches.

Another class of targeting approaches relies on mathematical programming. Linear and nonlinear models were developed to calculate targets for HENs. These methods, though more rigorous than PT ones, feature some limitations that are discussed in the following.

We have developed some novel optimization-based methods to solve certain problems at targeting stage of HENs design. They are more rigorous and general than those from Pinch Technology and, also, do not feature limitations of existing optimization approaches. In particular, the methods for solution of the following issues are presented:

1. Minimum utility cost calculation by a generalized transshipment model for nonpoint utilities.

2. Targeting approach for the minimum area of true counter-current (1-1) and multipass (1-2) heat exchangers with the use of a linear transportation model.

3. Minimization of number of matches at targeting stage by generation of near-balanced subsets of streams with the use of mixed-integer linear programming (MILP).

RESULTS AND DISCUSSION

Transshipment and Transportation Models

Both formulations are applied to calculate a minimum cost of utilities and heat load distributions in a HEN – see *e.g.* [4, 5]. Only a novel transshipment model, which is more general compared to the transshipment model from [4] (referred to as the standard model) is represented graphically in Fig. 1. A difference in comparison with the standard transshipment model is that an additional fictitious utility (hf) was added, and that the hot utility *s* has residual flows.

Let both process and utility streams be divided

*Presented at the 28th International Conference of the Slovak Society of Chemical Engineering, Tatranské Matliare, 21—25 May 2001.

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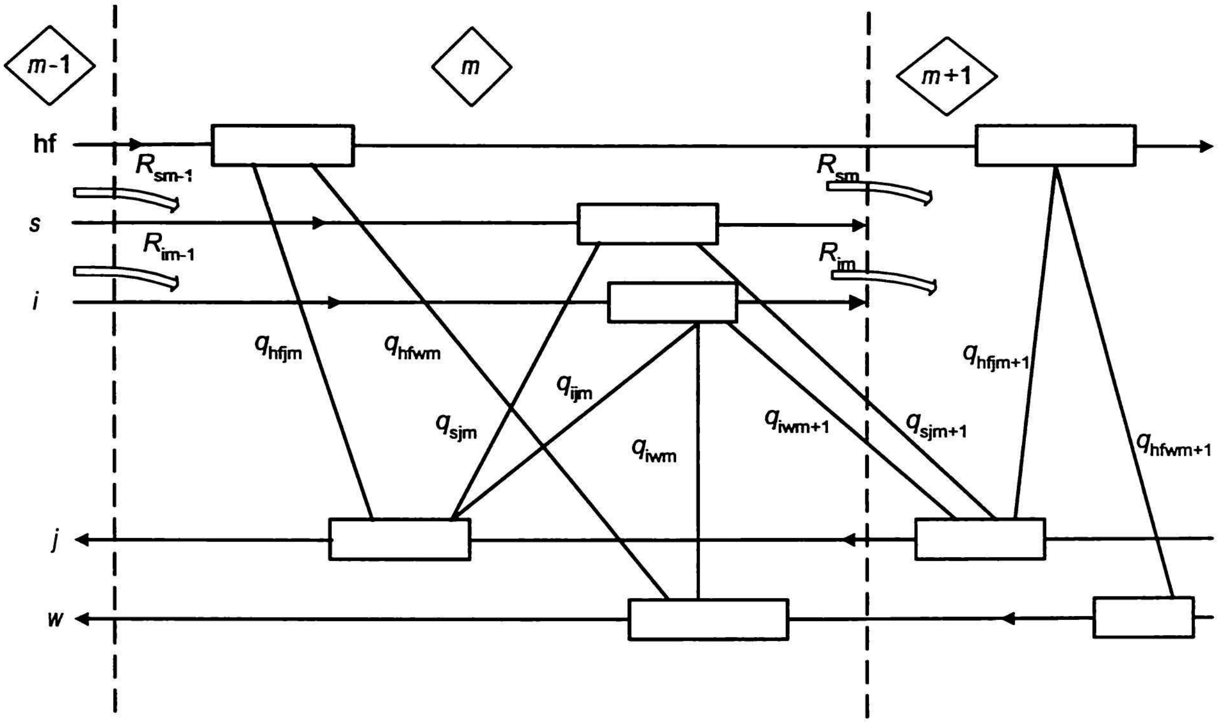

Fig. 1. Graphical representation of generalized transshipment model. Solid horizontal lines illustrate streams; lines connecting rectangles show potential matches; vertical dashed lines show borders of temperature intervals; arrows crossing borders of intervals illustrate residual flows.

at their inlet temperatures into temperature intervals (TI). They are in shifted temperature scale, for instance temperature of hot streams is decreased by HRAT (Heat Recovery Approach Temperature) in case of heat recovery calculations or by EMAT (Exchanger Minimum Approach Temperature) for other targets. In our representation we used both inlet and outlet temperatures for creating TIs in order to capture some additional information to construct the so-called Utility Grand Composite Curve (UGCC) plot. Due to space limitation this issue is not considered here and one can use inlet temperatures for the minimum utility cost target.

In order to meet thermodynamic constraints, heat exchange is feasible if and only if a hot stream transfers heat to a cold stream from the same or lower temperature interval TI, *i.e.* to TIs with the same or higher number. In consequence, the optimization problem can be formulated as linear one. The variables in original transshipment model are:

q_{ijm} – heat loads of matches between hot streams i and cold streams j in the interval m. It is important to note that if a hot stream ceases to exist in the next TI, it can exchange heat with cold streams existing in TI of lower temperature, too. Matches are shown in Fig. 1 as rectangles connected by lines similarly to grid representation in PT.

R_{im} – residuals of hot streams i that transfer heat from TI no. $(m-1)$ to TI no. m. Residuals are shown in Fig. 1 by arrows crossing borders of TIs.

It is interesting to note that the well known Problem Table method formulation from PT presented first in [6] is in fact embedded in the transshipment model. For single utilities, *i.e.* for one hot and one cold utility without restrictions on matches, the transshipment model has one degree of freedom and can be solved using the Problem Table method found in literature [6] or procedure published in [7].

An objective function depends on the problem formulation. In the Problem Table approach this is a minimum heat load of utilities. In the case of minimum utility cost, the objective function involves the heat loads of matches with utilities multiplied by the utility unit price or some weights. Constraints in optimization model consist of heat balances for each process stream in each TI. They have to ensure that required enthalpy change of a process stream in each TI is met in matches chosen by the optimization procedure. In consequence, the constraints ensure that the final temperatures of streams are also met.

Generalized Transshipment Model for Non-point Utilities

Motivation and Prerequisites for a Method of Solution

All the models mentioned have similar limitations. The standard transshipment model considered a general and efficient tool (see *e.g.* [1—3]) is, in fact, valid for point utilities such as steam. It is commonly employed for nonpoint utilities (such as flue gas, hot oil, cooling water, *etc.*) too, but the model treats them as a sequence of point utilities in consecutive temperature intervals. Such "pseudo-point utilities" in the standard transshipment model are not related to each other by mass flow rates values. Moreover, during the model formulation stage, it has to be taken into account that a nonpoint utility spans over more than one temperature interval. Hence, to determine if a utility is of point or nonpoint type one has to construct temperature intervals such as in Fig. 1.

Other existing methods exhibit similar shortcomings as noticed first in [8]. Since the standard model does not provide information on sufficient flow rates of nonpoint utilities, its application in practice is limited. Moreover, by fixing a "wrong" value of outlet temperature of nonpoint utility (notice that final temperatures have to be given), one can pay a double penalty. It results from the fact that for a nonpoint utility such a final outlet temperature can be given in data that cause excess load on this utility. We referred to this as to pinch-crossing utility and pinch-crossing load. Since one utility is in excess (*e.g.* hot utility), the opposite type of utility (cold one) has to be applied in excess, too. It is important that it is impossible to determine beforehand if the utility is in excess due to the incorrect final temperature given by the designer in data. Even the knowledge of process pinch is insufficient since pinch-crossing utility can result also from utility pinches that are known only after solving the standard model. This will be illustrated by Example 1.

An iterative approach for redistributing flow rates of nonpoint utility into intervals has been developed in [8]. However, the computation load can be overwhelming in case of many utilities and the approach does not account for restricted matches. On the other hand, the idea applied in [8] that in order to meet the maximum heat recovery one should adjust properly outlet temperatures of nonpoint utilities is valid and applied also in the approach presented in this paper.

The method developed in this work employs cost of utilities as objective function but accounts also for minimization of flow rates of nonpoint utilities. To account for temperature-dependent C_p values, nonpoint utilities can be divided into segments of "near-constant" C_p values. Moreover, the model handles the point utilities explicitly as limiting case of nonpoint utilities. Constraints of fixed, outlet temperatures can also be accounted for, if forced by industrial requirements. The minimum (for hot utilities) and the maximum (for cold utilities) outlet temperatures that ensure maximum heat recovery are computed. The model accounts directly for multiple utilities and constrained matches, and fulfils the requirement that its solution should provide explicit information whether given utilities have sufficient inlet temperatures or not. Existing approaches will fail to detect such cases.

Modifications in the Standard Transshipment Model Formulation

The changes in the standard transshipment model formulation are:

1. To provide constant C_p value of a segment of nonpoint utility in its entire temperature range the continuity relations for C_p are added for each segment of the utility: C_p =*const. for all temperature intervals the utility segment enters or can cascade heat.*

2. To provide constant mass flow rate (MF) for all segments of a particular utility the continuity relations are added: MF =*const. for the interval where segment no. i ends and segment no.* $(i + 1)$ *starts.*

3. Fictitious hot utility (hf) that can transfer heat to each temperature interval is added to the standard model. This fictitious hot utility can be matched with all cold process streams and cold utilities as well – see Fig. 1. The heat loads of matches of fictitious hot utility with the cold nonpoint utilities encapsulate information on the excess heat of cold utilities that is not useful in a process. Matches of fictitious hot utility with cold process streams are necessary to determine whether inlet temperatures of hot utilities given in data are sufficient.

4. We allow for nonzero residual heat flow from the last intervals for hot utilities and process streams as well. This is to get information on excess (not useful in a process) heat of hot utilities and insufficient (as for temperatures) cold utilities.

5. The goal function contains weight of all matches multiplied by their heat loads and also weight of residual flows from the last temperature intervals of hot utilities multiplied by their values. This is because residuals act as fictitious cold utilities and have the unit price of these utilities. The terms with heat loads of matches with hf and these with residual flows act as penalty terms. Moreover, they ensure that an information on excess utility load, that has to be applied in case of incorrect final temperatures of utilities in data, is available in the results.

With standard weights applied in the standard model the generalized new model will integrate also "excess" utilities into a process. Therefore, novel weights scale should be applied at last to account for the pinch-crossing utilities as follows:

– matches of fictitious hot utility with cold utility $w \in W$: $c_w(1 + \delta)$

– last residuals of hot utilities $s \in S$: $c_s(1 + \delta)$

Parameter δ has to meet the following conditions

$$\delta < \min_{s \in S}(c_s) \tag{1}$$

$$\delta < \min_{s \in S}(c_s) / \max_{w \in W}(c_w) \tag{2}$$

$$\delta < \min_{w \in W}(c_w) \tag{3}$$

$$\delta < \min_{w \in W}(c_w) / \max_{s \in S}(c_s) \tag{4}$$

Also, in order to ensure the aims of the methods, weights for matches of process-process streams are any longer zero as usually in the standard model but they have to meet the following conditions

$$c_{\text{pr}} < -\delta[\max_{s\in S}(c_s) + \min_{w\in W}(c_w)] \qquad (5)$$

Simultaneously, the weight for matches of process streams with fictitious hot utility is set at value lower than a weight of forbidden matches and higher than the weights for matches of process stream utilities (the same weights as in the standard model, c_s and c_w). A detailed mathematical formalism of the extended transshipment model and a proof that the conditions for weights given by eqns (*1—5*) are necessary and sufficient to ensure the maximum heat recovery for pinch-crossing utilities, as well as the graphical representation of results (UGCC plot) can be found elsewhere [9].

Example 1

The problem is taken from [8] and data are gathered in Table 1. Outlet temperature of hot utility is treated as a minimum admissible value, not necessarily as fixed one. For $\Delta T^{\min} = 10$ °C energy targets, *i.e.* optimal heat loads of utility calculated for point utilities are: $Q(s) = 453.5$ kW and $Q(w) = 0.0$ kW.

The solution from the model developed in this study:

– Useful hot utility load is $Q(s) = 453.5$ kW while the pinch-crossing load of 856.5 kW is needed. Target temperature of hot utility, *i.e.* temperature that ensures useful load or the minimum heat load that does not cause pinch-crossing effect, is 225 °C. Hence (MF × C_p) value is 10.08 kW/K.

– Cold utility heat load is 0.0 kW.

– For the fixed hot utility outlet temperature of 140 °C, the hot utility total load of 1310 kW is needed. This is the sum of useful load and pinch-crossing load from our solution. Additionally, to meet energy balance the cold utility of load 856.5 kW, *i.e.* pinch-crossing heat transfer for hot utility, has to be used, too. This is the penalty for fixing the hot utility outlet temperature at 140 °C.

The results obtained by the new model are the same as those published in [8], however, determined directly without tedious, iterative computations.

Table 1. Data for Example 1

Stream	TS/°C	TT/°C	MF · C_p/(kW K^{-1})
H4	249	138	10.55
H2	160	93	8.79
C1	60	160	7.62
C3	116	260	10.08
Steam	270	140*	–
Water	38	82	–

*Minimum value.

Targeting Approach for Minimum Area of Heat Exchanger Networks

PT methods based on certain modifications of the so-called Bath formula [10], though commonly applied for area targeting, do not ensure accurate results in case of different heat transfer coefficients of streams. They, also, do not account for restricted matches. More rigorous optimization methods [11, 12] require nonlinear optimization problem solution and do not apply for multipass (1-2) heat exchangers common in industry. The notable exception is the approach that combines mathematical programming and some insights from Pinch Technology and is valid for 1-1 and 1-2 heat exchangers [13]. However, this model is very complex and requires involved data preparation.

The approach proposed in this paper is based on the solution of a linear programming problem modelled as a transportation task. The use of this formulation results from the necessity of accounting for heat transfer coefficients of streams. This can be easily done since, in opposite to the transshipment model, the transportation formulation does not apply residual heat flows. The developed linear optimization model is easy to solve with widely available optimization solvers and local optima traps are eliminated. It is worthwhile noting that the model uses temperature intervals instead of enthalpy intervals from composite curves applied in other approaches. The temperature intervals are similar to those in the transshipment model shown in Fig. 1 but denser division is necessary. The use of temperature intervals enables an extension of the method for simultaneous targeting for minimum total cost and in consequence generating optimal and sub-optimal HENs, see Ref. [14].

The aim of optimization is to minimize the total area of all matches between streams in temperature intervals, *i.e.*

$$\min \sum_{m=1}^{M}\sum_{n=1}^{M} 1/(\text{Ft} \times \text{LMTD})_{m,n} \cdot \sum_{i\in C_{jn}}\sum_{i\in H_{im}} q_{im,jn}/(h_j + h_i) \qquad (6)$$

where m, n are the numbers of temperature intervals; $m = 1, \ldots, M$, $n = 1, \ldots, M$, $q_{im,jn}$ is the heat load of match between hot stream i in interval m and cold stream j in interval n, C_{jn} the set of cold streams j in interval n, and H_{im} the set of hot streams i in interval m.

To keep the optimization model linear it is necessary to fix corrections factors for 1-2 heat exchangers (Ft) and logarithmic mean temperature approaches (LMTD), *i.e.* their values have to be given in data. They are approximated by using well-known equations with temperature values taken as borders of temperature intervals. For instance, $(\text{LMTD})_{m,n}$ is calculated using border temperatures of intervals m and n, respectively. Hence, values of Ft factors and temperature differences LMTD can be calculated beforehand. To ensure accurate results a size of TI has to be small, but not too small to keep number of variables in reasonable limit. Based on extensive tests, an algorithm for appropriate division into temperature intervals was developed as follows:

Let the size of the smallest TI after preliminary division at inlet and outlet temperatures be dT^{min}. Find the mean size (dT^{mean}) of an interval from

$$dT^{mean} = \max[3\,dT^{min}, 10] \quad (7)$$

Find all intervals $k \in K$ so that their sizes dT^k are higher than dT^{mean}. Divide each interval $k \in K$ into N^{ad} intervals, where N^{ad} is given by

$$N^{ad} = \text{entier}[dT^{mean}/dT^k];\ k \in K \quad (7a)$$

where entier(a) means the nearest integer value of a not less than a.

Example 2

Table 2 contains data for an example taken from literature [11]. Table 3 presents the results obtained by the model developed in this study and their comparison with results calculated by other approaches.

The linearization used in the model is of heuristic type. Its validity can only be proved by numerical tests that were performed for many various examples published in literature to date. The tests proved the accuracy of results. The accuracy of about 1.0 % was obtained comparing to results for area of 1-1 apparatus computed by the most rigorous NLP approach [11]. We have not found important limitations of the approach except the cases where very small value of EMAT, of order 2 K or less, was applied for creating temperature intervals. However, such small EMAT are not used in industry, especially for multipass heat exchangers.

Table 2. Data for Example 2 ($\Delta T^{min} = 10$)

Stream	TS/K	TT/K	$C_p \cdot MF/(kW\ K^{-1})$	$h/(kW\ m^{-3}\ K^{-1})$
H1	395	343	4	2.0
H2	405	288	6	0.2
C1	293	493	6	2.0
C2	353	383	10	0.2
Steam	520	519	–	2.0
Water	278	288	–	2.0

Targeting for Minimum Number of Matches by Determination of Near-Independent Subsets

A given set of process streams and utilities in any HEN constitutes heat balanced set of streams. Sometimes, a total balanced set consists of independent subsets that are in heat balance, too. In such cases, HEN system consists of independent subsystems, one subsystem for one subset of streams. Identification of subsystems existing in HENs is important because of two reasons. First, the heat exchanger networks synthesis requires setting up targets for minimum number of heat exchange units. According to eqn (*8*) (see *e.g.* [15]), evaluation of absolute minimum number of units (N_{min}) for a given set of process and utility streams requires the number of independent subsystems N_{sub}.

$$N_{min} = N_{str} - N_{sub} \quad (8)$$

where N_{str} is the number of all streams. In the absence of a method able to calculate the number of independent subsystems, it is often approximated to unity. This guess may lead to inaccurate targets.

Second, for large industrial-size problems, an explicit knowledge of the process and utility streams that constitute a subsystem can help to reduce the complexity of the design, operation and controllability of the HEN. In this contribution, a rigorous approach for subsystems identification in a given set of process and utility streams was developed. Furthermore, the method finds the maximum number of subsystems, thus giving a truly minimum number of matches according to eqn (*8*).

The truly independent subsystems, *i.e.* subsets of streams in perfect heat balance, are relatively rare. Therefore, the algorithm developed in this study identifies near-independent subsystems using temperature-based tolerances on streams, *i.e.* near-independent subsystem is near-heat balanced within limits of user given tolerances. In industrial applications this is acceptable since some outlet temperature values are more or less "weak" constraints, *i.e.* they

Table 3. Comparison of Area Targets for 1-1 Apparatus for Example 2

Our approach		Solution from [11]		Solution from [12]		Bath formula (PT method)	
A_1/m^2	$\Delta^*/\%$	A_1/m^2	$\Delta^*/\%$	A_1/m^2	$\Delta^*/\%$	A_1/m^2	$\Delta^*/\%$
260.6	0.69	258.8	0.0	263.6	1.85	295.7	14.2

*Relative error in comparison with solution from [11].

can vary in certain limits as *e.g.* streams to tanks. Also, small deviations for given in data fixed outlet temperatures are, in fact, meaningless for practice since the calculations are performed at synthesis stage of the process design.

The transshipment MILP model approach for calculating optimal heat load distributions [4] is not able to determine near-independent subsets, though calculates perfectly balanced ones. The only method that tries to cope with the problem is that published by *Mocsny* and *Govind* [16]. Their combinatorial method requires generating all possible $2^{N_h}2^{N_c}$ options (where N_h and N_c are the numbers of hot and cold streams, respectively). Then, an exhaustive comparison of unbalanced loads on them is necessary to find such that meet given limits.

In the present paper, a MILP model was developed that minimizes the number of streams that satisfy the heat balance constraints within given tolerances. The streams form a minimal subset, *i.e.* subset with minimal number of streams in "near balance". The goal function accounts for minimization of unbalanced loads on subsystems. Hence, not only given temperature tolerances are satisfied, but also they are minimized. The heat balance constraints are formulated in such a way that they embed the transshipment formulation for minimum utility cost. They ensure thermodynamic feasibility including pinch principle of the subsystem. Binary variables are applied to differentiate among streams that are in the subsystem and those which are in its complement. Therefore, the number of binary variables is equal to number of process and utility streams. Even for industrial problems this is quite moderate value.

The solution of the MILP problem is the minimum near-independent subsystem (SS^{min}) and its complement (SS^{comp}), both meeting temperature tolerances, that is both subsets are near-balanced in the sense of the definition. As mentioned above, the deviations from fixed temperatures (if any) are forced to a minimum. The generation of all near-independent subsystems in the problem lies then in sequential solutions of the MILP formulation. First, the model is solved for the entire problem. The solution yields an independent subsystem with the smallest number of streams (SS^{min}) and its complement (SS^{comp}). In subsequent steps, the MILP formulation is applied on the complement that was generated in a preceding step. The process concludes when no more independent subsystems are found, *i.e.* solution of MILP formulation does not contain two subsets.

Fig. 2 illustrates the procedure. The solution is represented by set of minimal subsets SS_i^{min} at each level i of the procedure and the complement from the last level (SS_k^{comp} in Fig. 2). This set contains the maximum number of subsets that are in heat balance within given tolerances. Based on knowledge of this set, the HEN could be designed. Usually, subsets contain a small number of streams and a simple method such as PDM approach [17] is sufficient to synthesize a network consisting of minimal number of matches.

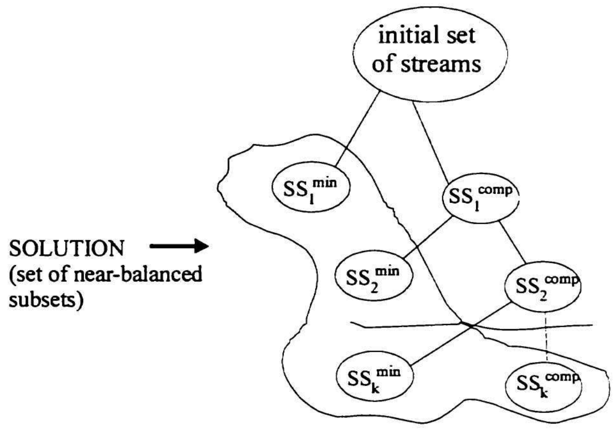

Fig. 2. Illustration of the method for generating subsets.

The approach has been applied to some large-scale problems from the literature. Many times, several sets of independent subsystems could be found, thus reducing greatly the number of units in the entire HEN. The number of independent subsystems depends on temperature tolerances. Example 3 was taken from [16]. Temperature-based tolerance of 1 % of the difference between the inlet and outlet temperature of a stream was assigned to each stream.

Example 3

This problem has 23 process streams and one hot utility, *i.e.* this is threshold task for the ΔT^{min} specified. The heat load of the hot utility is 2553.7 kW. Using the method of generating subsystems 7 near-independent subsystems were found. Hence, according to eqn (*8*) a total HEN will require only 17 units instead of 23 identified by this equation for N_{sub} set at 1. This gives substantial reduction of fixed cost of the heat exchangers network. The solution features: two subsystems with two streams, three subsystems with three streams, one subsystem with four streams, and one subsystem with seven streams.

The temperature deviations from outlet temperatures, providing that they must be considered as fixed values, are equivalent to 124.7 kW on heat load basis. This shows the effect of temperature deviations minimization by the method. Thus, the HEN design task is simplified and relatively small-sized problems remain to be solved. Since heat is exchanged within an independent subsystem, we can also ensure that the operation and control of the entire HEN is simplified.

Several other sets of subsystems were obtained for this example with smaller number of subsystems, depending on the integer cuts in MILP optimization formulation. The solutions differ in total cost and operability of the HEN. Therefore, several options should be considered in detail in order to meet specific industrial requirements.

CONCLUSION

This contribution presents some of the novel mathematical formulations applied in HX-NET software of AEA Technology Engineering Software. They all are used at targeting stage of HEN design. It is important to note that linear models developed allow for reaching global optimum even for large, industrial-scale problems. The approaches extend applications of HENs targeting for difficult industrial cases. Some of them, as *e.g.* the method for targeting, were basis for developing approaches for designing optimal HENs (see [14]).

SYMBOLS

A_1	HEN heat transfer area of 1-1 heat exchangers
C_p	heat capacity
c_{pr}	weight for matches of process streams
c_s/c_w	unit price of utility s/w (per unit of energy)
EMAT	exchanger minimum approach temperature
Ft	correction factor for LMTD for multipass heat exchangers
h	heat transfer coefficient
HRAT	heat recovery approach temperature
i/j	cold/hot process stream
LMTD	logarithmic mean temperature difference
M	total number of temperature intervals
MF	mass flow rate
q	heat load of a match
$Q(s)/Q(w)$	heat load of hot utility s/heat load of cold utility w
s/S	heating utility/set of available heating utilities
SS	near-balanced subset (independent subsystem)
T	temperature
TS/TT	inlet/target temperature of a stream
w/W	cooling utility/set of available cooling utilities
$\Delta T^{\min}$	minimum temperature approach for heat recovery calculations
δ	parameter for calculating weights of matches in generalized transshipment model

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