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**Mathematical Methods for Heat Exchanger
Network Synthesis**
Ignacio E. Grossmann
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Mathematical Methods for Heat Exchanger Network Synthesis

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Abstract

This paper gives an overview of the evolution of mathematical methods for heat exchanger network synthesis over the last 25 years. Two major developments have been methods for targeting and methods for automated synthesis through simultaneous optimization. The former have helped to expand the scope and increase the accuracy of pinch based methods; the latter have provided a framework to automate the synthesis of networks while explicitly accounting for trade-offs between energy consumption, number of units and area. Basic ideas behind these methods are discussed, as well as their capabilities and implementation in computer software. Several application examples are also presented. The paper concludes with the major lessons that have been learned in developing these methods, as well as future directions and prospects for automated synthesis capabilities which can greatly enhance the productivity of design engineers and the quality of their designs.

Introduction

Given that industrial applications for heat exchanger network (HEN) synthesis have proved to be very successful (e.g. see Linnhoff and Vredeveld, 1984; Gundersen and Naess, 1987) one may wonder as to why there is a need to investigate and develop synthesis techniques that are based on mathematical methods. Is this just an interesting academic exercise, or are there in fact capabilities in these methods that cannot be accomplished with the largely graphical and manual techniques of pinch based methods? Furthermore, to what extent do mathematical methods replace or complement the decision making process of engineers in the synthesis of these networks?

The above questions, which were prevalent in the early 80's, have to a large extent been resolved with the research work that has been done and over the last 10 years. Mathematical methods for the synthesis of HEN's have shown that they can play an important role in terms of automating the search among many design alternatives, while explicitly accounting for economic trade-offs between investment and operating costs. Furthermore, it has been shown that these methods can be used effectively by engineers without having to be experts in optimization, and in a way where their productivity can be enhanced, while allowing them to retain control of the synthesis process. Mathematical methods in fact are complementary in nature to the ones based on physical insights. It has also been shown that aside from the fact that mathematical methods can produce innovative solutions, they can also be extended beyond HEN synthesis so as to perform process flowsheet optimization simultaneously with heat integration which can produce substantial economic savings. Despite these advances it is clear that not all the issues have been solved with mathematical techniques; for instance, problem size and nonconvexities are still problems that await for improved solutions.

It is the main purpose of this paper to provide a general overview of mathematical methods giving a brief account on how they have evolved, emphasizing the most recent developments. Due to space limitations in this paper, we will not dwell into the detailed mathematical formulations of the various models that have been proposed. Instead, we will

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highlight the main ideas and show the application of the techniques with several example problems. Finally, current limitations and future directions will be discussed.

Assumptions **and** basic equations

Mathematical optimization models have commonly relied on the following assumptions for synthesizing HENs:

- a) Constant heat capacity flowrates
- b) Fixed inlet and outlet temperatures
- c) Constant heat transfer coefficients
- d) Single-pass countercurrent heat exchangers
- e) Layout and pressure drop costs are neglected
- f) Operating cost is given in terms of the heat duties of utilities
- g) Investment cost is given in terms of the areas of the exchangers.

A number of the above assumptions can in fact be relaxed with some of the methods, although often at the expense of significant computational expense- Also, it should be noted that while initially fixed minimum temperature approaches had to be assumed, (HRAT heat recovery approach temperature, EMAT individual exchanger approach) this is no longer required in the most recent methods as will be discussed later in the paper.

Based on the above assumptions, the three basic modules or units for HEN's are modelled as follows (see Fig. 1):

- a) Splitter - mass balance

$$F_i - F_j + I = F \quad (1)$$

which gives rise to linear equations.

- b) Mixer - heat balance

$$F_i T_i = F_j T_j + F_u T_u \quad (2)$$

which gives rise to nonlinear (bilinear) equations.

- c) Heat exchanger - heat balance, design equation

$$Q = F_i (T_j - T_i) \quad (3)$$

$$Q = U A \left(\frac{T_i + T_j}{2} - t_j \right)$$

which again gives rise to nonlinear equations.

Finally, the cost functions are modelled as follows:

$$\text{Area: } C_F + \alpha A^{\beta} \quad (4)$$

$$\text{Utilities: } C_{HU} Q_{HU} + C_{CU} Q_{CU}$$

where the area cost is again generally nonlinear ($0 < \beta < 1$) with a fixed cost C_F , and the utility costs are linear.

Equations (1) to (4) constitute the basic equations that are used in mathematical models for synthesis. Although simple in form, the main complication that arises is due to the nonlinearities. Firstly, the area cost in equation (4) is concave for $0 < \beta < 1$ with infinite derivative at zero area ($A = 0$). Secondly, the heat balance equations in (2) and (3) are bilinear and therefore nonconvex. Finally, the design equation in (3) is nonlinear and also nonconvex. Since mathematical optimization techniques rely largely on convexity assumptions and have only achieved great speed and robustness for the case of linear programming, it is no surprise that it has taken considerable research effort to formulate and solve the synthesis of HEN's as optimization problems.

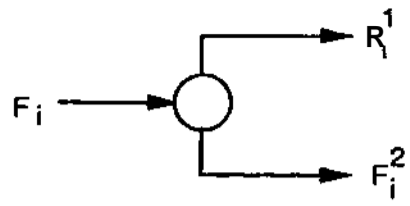
Furthermore, the above equations do not completely describe the discrete selection of stream matches and their corresponding exchangers which define the topology of the network. A second major complication is the development of representations to generate these network structures. The two major approaches have been on the one hand to use tree search methods to gradually build-up the network configuration, and on the other hand to use "superstructures" that have embedded all the alternatives of interest, and where the structures are obtained by "deletion" of units and streams.

In summary, the nature of the nonlinearities, the discrete decisions and systematic representation of alternatives have constituted the major bottlenecks in the development of mathematical networks for HEN synthesis. Some of these issues, however, have been overcome over the last few years. The next sections in the paper give first a brief account of initial work, followed by the development of targeting models and finally by automated synthesis models.

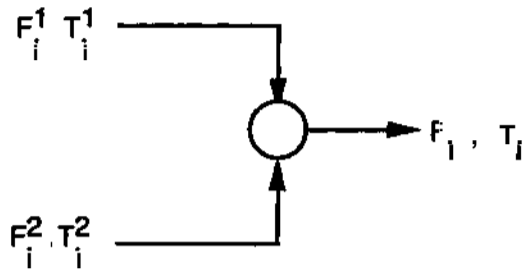
Initial work

Hwa (1965) was among the first researchers that reported an optimization approach for selecting the topology and the areas, heat loads, temperatures and flows for HEN's. His problem representation consisted of specifying a superstructure that resulted from combining several alternative network structures. For example, as shown in Fig. 2, the two networks (a) and (b) were combined into a single network superstructure which was then modelled as a nonlinear programming problem (NLP) using the equations (1) to (4) (without the fixed cost for the exchanger cost) to define the objective function and constraints. Note that by creating this superstructure one is in fact creating additional alternatives. The idea in this approach was then to solve the NLP which would then "delete" exchangers or streams yielding the minimum cost network structure. Aside from the problem of dimensionality (as least for 1965 standards), Hwa found that his approach would often be trapped into local solutions and that numerical difficulties were encountered as the areas approached values of zero. Furthermore, another major question was how to construct the superstructure so as to guarantee that the optimum design would not be excluded.

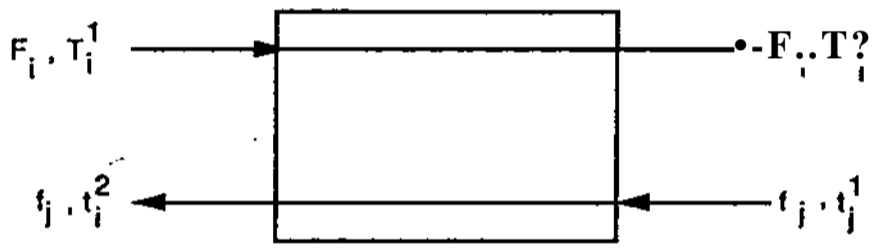
A next major attempt came from Kesler and Parker (1969) who managed to formulate the synthesis problem as a linear programming (LP) problem; more specifically, as an assignment problem. The idea was to use a representation based on the heat content diagram F_{cp} vs. T in which the utility consumption was fixed. The heat content of each stream was subdivided horizontally into small chunks of heat. For each of these, the potential "assignment" or match from a given hot chunk to a given cold chunk was modelled with a heat flow variable. To account for the cost, each of these variables was assigned a cost coefficient inversely proportional to the heat transfer coefficient and temperature difference. The difficulty that was encountered with this approach is that the model did not recognize the benefits of assigning adjacent heat chunks for the same match, and therefore produced complex network structures with many heat exchange units.



(a) Stream splitter

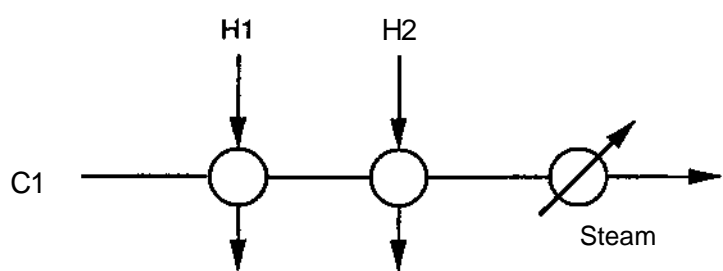


(b) Stream mixer

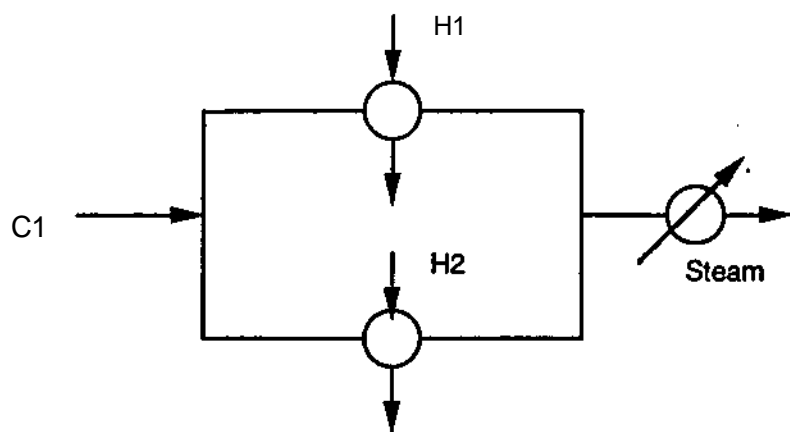


(c) Heat exchanger

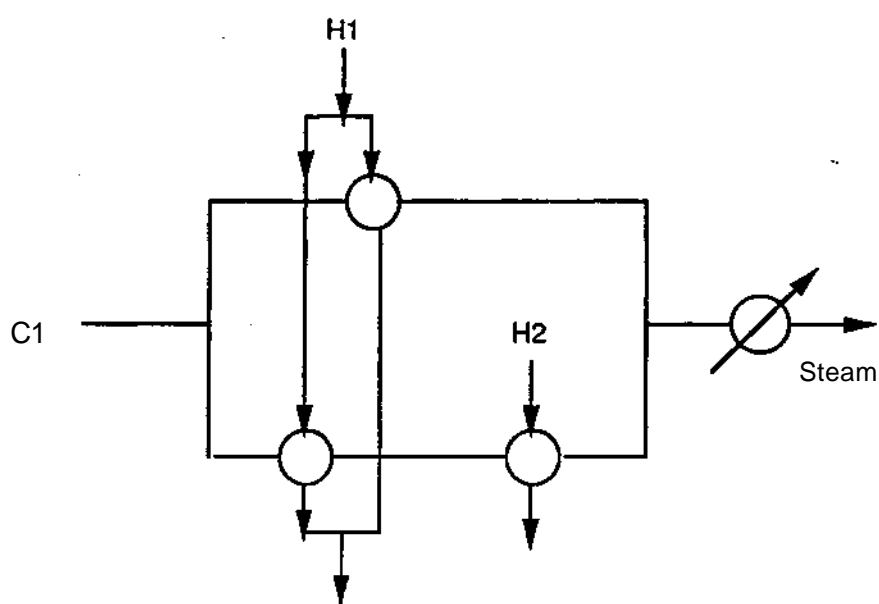
Figure 1. Basic modules for HEN



(a) Alternative 1

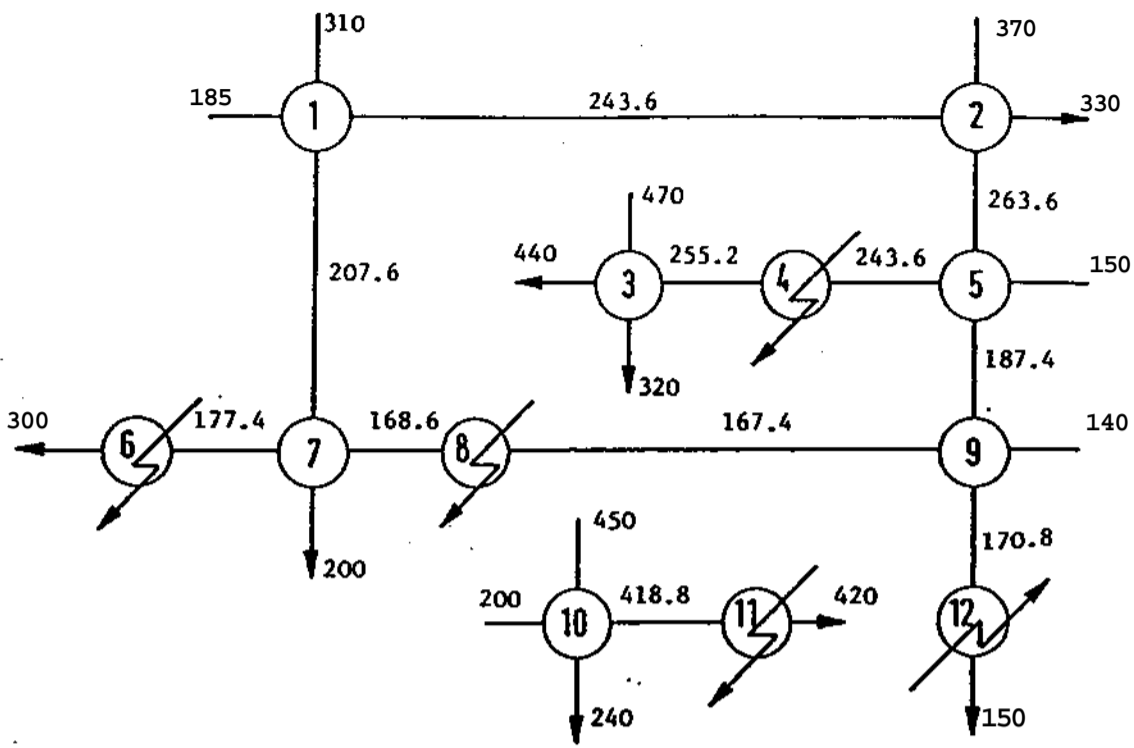


(b) Alternative 2



(c) Superstructure

Figure 2. Generation of superstructure for selected alternatives in HWA's approach.



(a) Network synthesized by branch and bound

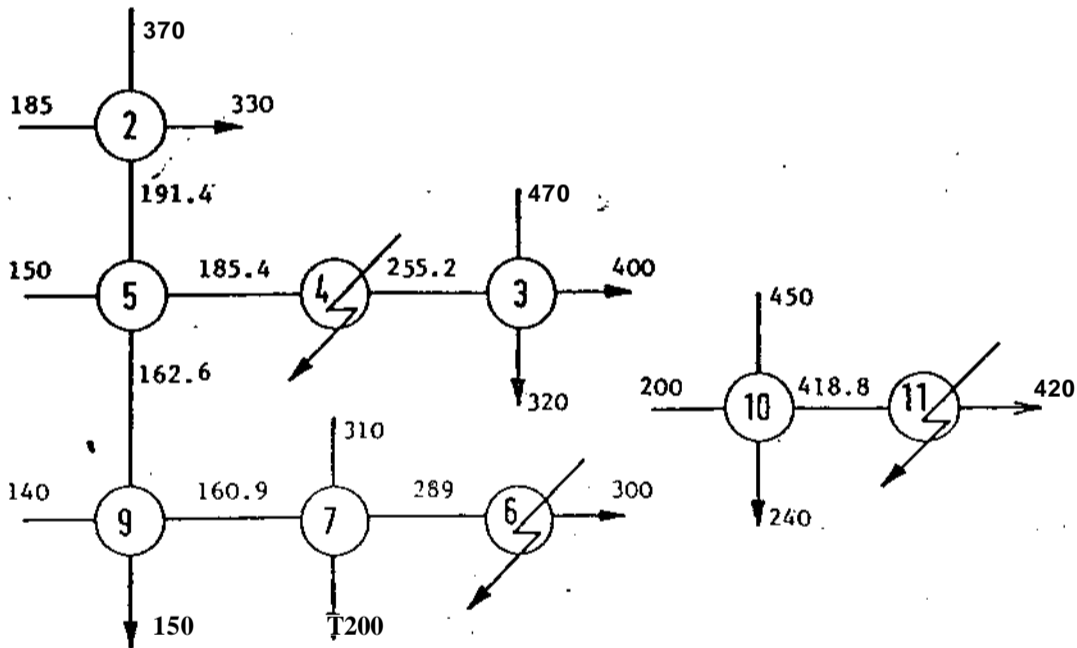


Figure 3. (b) Network optimization by NLP (Grossmann, 1977)

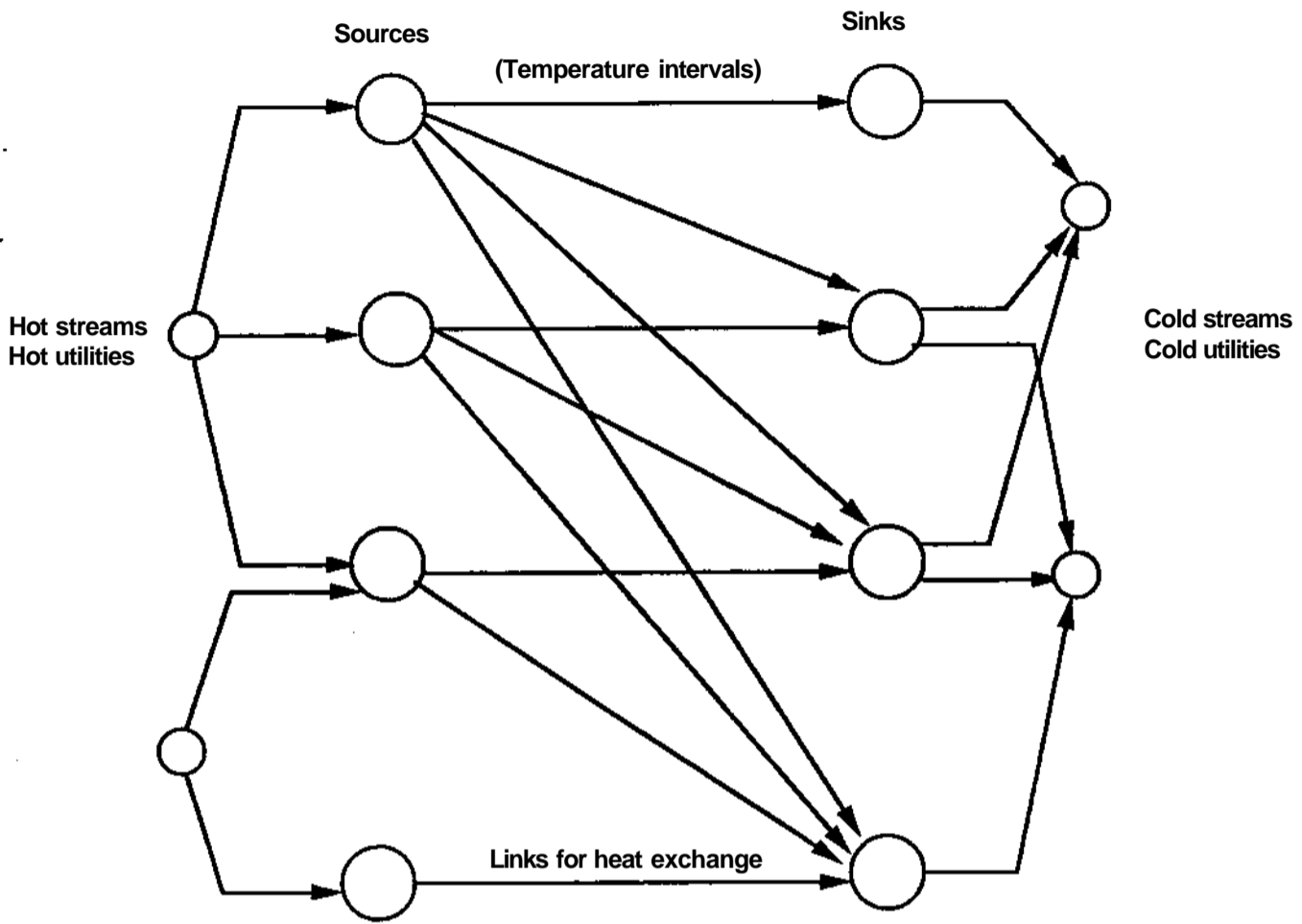


Fig. 4 Representation of transportation model.

The experience of Hwa (1965) and Kesler and Parker (1969) motivated the need for methods that could explicitly handle discrete decisions. This led to tree search methods some of which were solved through the branch and bound optimization procedure. The idea here was to generate network alternatives by a sequence of stream matches up to the point where the streams would meet their inlet/outlet conditions. In order to avoid the exhaustive enumeration of all the sequences bounds based on cost were used within an implicit tree search enumeration. Lee, Masso and Rudd (1970) were the first to apply this technique, which was then subsequently extended by Rathore and Powers (1975) and by Grossmann and Sargent (1977). The major difficulty encountered in these methods was that by the sequential assignment of matches heuristic decisions had to be made on how much heat to exchange at each match, and the fact that stream splitting was disallowed. Nevertheless, despite these limitations these techniques were at least able to automatically synthesize reasonable network structures, although they did not necessarily meet the target for minimum utility requirements for the specified minimum temperature approach. An example of the type of networks synthesized with such an approach (see Grossmann, 1977) is given in Fig. 3 for a 4 hot-4 cold problem, in which the network obtained by branch and bound in Fig. 3a, was subsequently optimized by nonlinear programming, reducing the cost from \$41,228/yr down to \$31,390/yr (see Fig. 3b). The number of units was reduced from 12 down to 9. The largest problem solved with this method was a 20 stream problem.

Targeting methods

The experience in synthesizing HEN's with various optimization approaches proved that utility costs were the dominant cost item and that optimal or near optimal networks achieved maximum energy recovery for a specified temperature approach. However, no fundamental understanding was achieved as to what was a feasible and realizable target for minimum utility consumption (for fixed HRAT). This important question was answered by the work of Linnhoff and Flower (1978) which uncovered the pioneering work of Hohmann (1971) and the contribution of the pinch concept by Umeda et al (1978). This development gave rise to the basic elements of what nowadays is termed as "pinch technology" which has been pursued vigorously by Linnhoff and coworkers over the last decade.

The basic approach as is now well known for pinch based methodologies consists of the prediction of the following targets:

- a) Minimum utility consumption
- b) Fewest number of units
- c) Minimum total area.

These ideas motivated developments of mathematical methods that could expand the scope and provide more accurate estimates of these targets than the ones provided by simple approximations. The first method was the LP transportation model by Cerda and Westerberg (1983) and Cerda et al (1983) which allowed the treatment of multiple utilities and constrained matches (e.g. forbidden matches) which could not be handled with the problem table by Linnhoff and Flower (1978). The basic idea was to represent the hot streams as sources of heat and the cold streams as sinks of heat at different fixed temperature levels as given by the temperature intervals of Linnhoff and Flower (1978) (see Fig. 4). Variables representing heat flows linking each source and sink were assigned and the equation given by heat balances around each source and each sink. Multiple utilities were simply treated as additional sources or sinks of heat, and forbidden matches were disallowed by assigning very large costs. The significance of this development was to expand the scope of the minimum utility target calculation.

An alternative model was developed by Papoulias and Grossmann (1983) who at that time were concerned with the embedding of the minimum utility target within the MBLP optimization of total processing systems. Their model corresponds to the LP transshipment model which is based on the heat cascade diagram (see Fig. 5). In this case hot streams are also treated as sources and the cold streams as sinks. However, instead of assigning links for each pair, heat flow was treated as a "commodity" that would be transferred through "warehouses" which physically correspond to the temperature intervals. The variables include the heat residuals that are assigned to the flow of heat between these warehouses, and the heat flows for the utilities. For the case of unconstrained matches and multiple utilities the LP model simply consists of heat balances around each temperature interval. For the case of constrained matches the model is expanded by disaggregating flows of heat within each interval in order to track the heat path from a given hot stream to a given cold stream. The advantage of the LP transshipment model is that it leads to a problem that is significantly smaller in size than the transportation problem. This has allowed the effective use of this model to handle the flows of the streams as variables for simultaneous optimization and heat integration as will be discussed later in the paper.

Both the LP transportation and LP transshipment model were extended to predict the target for fewest number of units. The basic idea is to assign 0-1 variables for every pair of streams (either in each subnetwork or in the total network) which gives rise to a mixed-integer linear programming (MILP) model. Due to its smaller size, the transshipment model is more convenient for this extension. The significance of the MILP model is that it predicts not only the fewest number of matches, but it also predicts: (a) which are the streams involved in each match, and (b) their corresponding heat loads. Furthermore, as opposed to the targeting formula by Hohmann (1971) for fewest number of units and its extensions, the MILP model provides an exact target. Fig 6, presents a counter-example for a 2 hot-2 cold threshold problem. The MILP model predicts correctly 4 units while Hohmann's formula predicts 3 units. There is in fact no feasible network that involves only 3 units.

Related work to targeting models includes the LP model by Jones and Rippin (1985) which can generate alternative heat load distributions for fewest number of units without partitioning into subnetworks. Also, Saboo et al (1985) presented extensions of the LP transportation and transshipment models.

Area targets have proved to be more difficult to model. The most recent developments include the NLP transshipment model by Colberg et al (1989) and the NLP model by Yee et al (1990). These models can account for unequal heat transfer coefficients and constrained matches, and they provide more accurate estimates than the Townsend and Linnhoff (1984) formula for which discrepancies of up to 20% have been reported.

Automated sequential synthesis

As was mentioned earlier in the paper, the branch and bound methods provided the first automated synthesis capability for HEN's. Their major drawback, however, was the fact that they were not guaranteed to meet the minimum utility target and that they could not handle networks with stream splitting. Motivated by the mathematical models for targeting, and the time consuming exercise that it is to manually derive detailed network structures by trial and error, there was a clear incentive to reconsider the development of automated synthesis tools for HEN's.

The major development here was by Floudas et al (1986) where the idea was to perform the synthesis of the network through 3 major steps:

1. Prediction of minimum utility cost with the LP transshipment model.

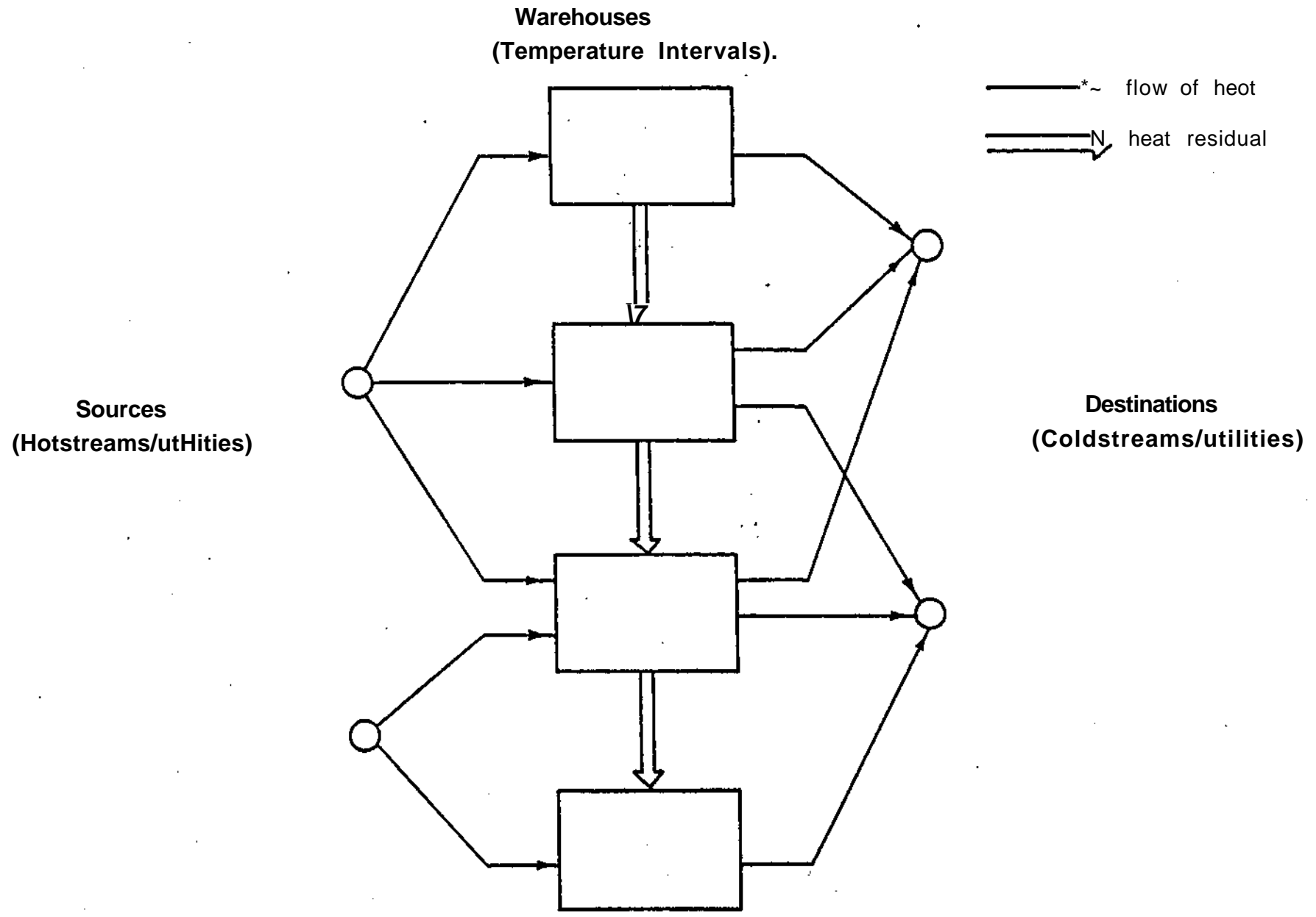


Figure 5. Representation of transshipment model

	$F_{cp}(\text{KW/K})$	T_{in}	$T_{out}(\text{K})$
H1	1	450	350
H2	1.2	450	350
C3	1	320	400
C4	2	350	420

$\Delta T_{min} = 10\text{K}$

Min no. of units

Heuristic estimate = $2 + 2 - 1 = 3$ units

Prediction by MILP transshipment = 4 units

Figure 6. Counter-example to minimum number of units

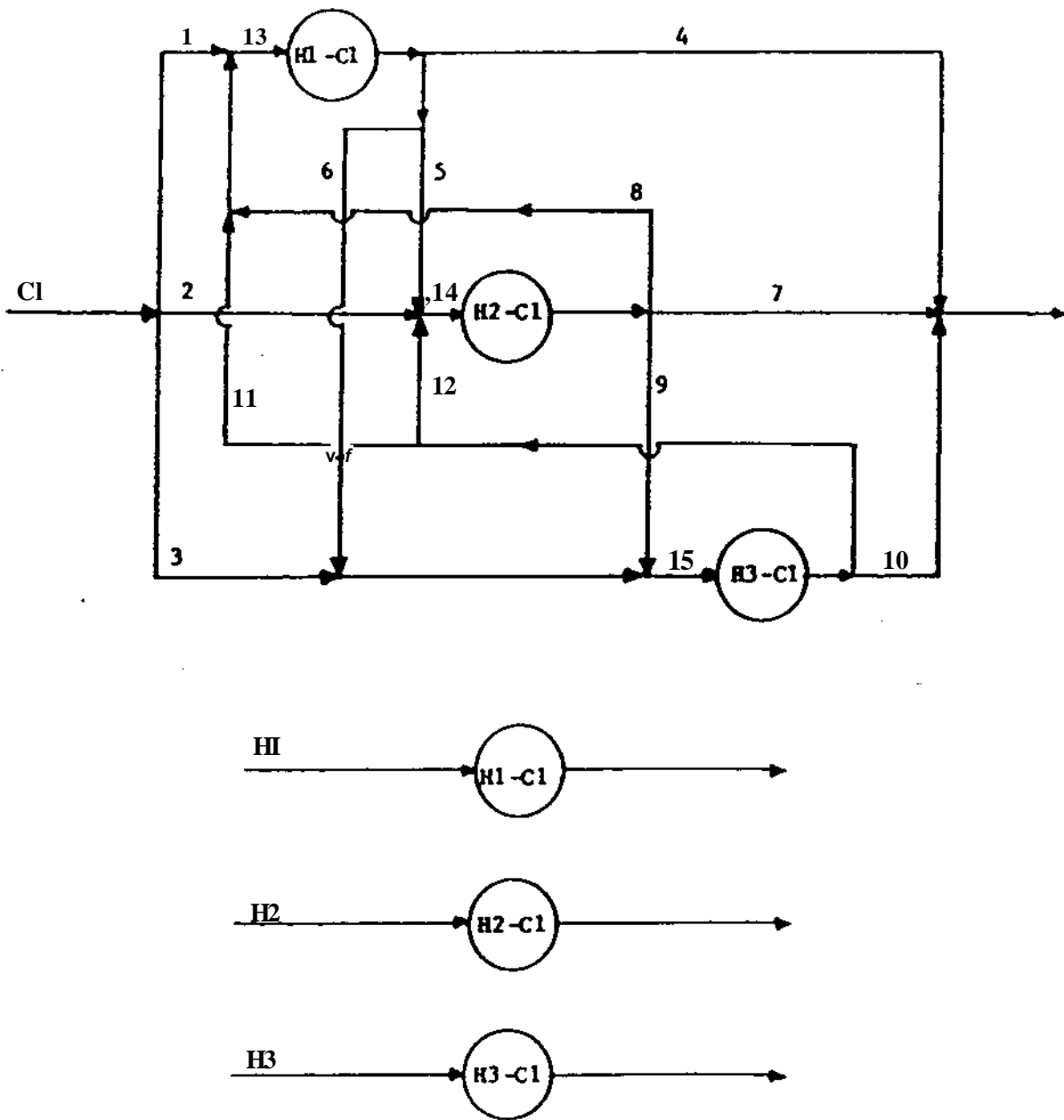
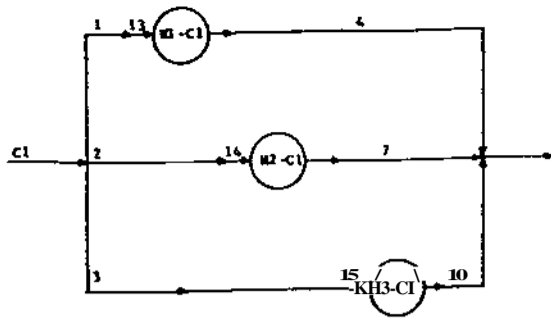
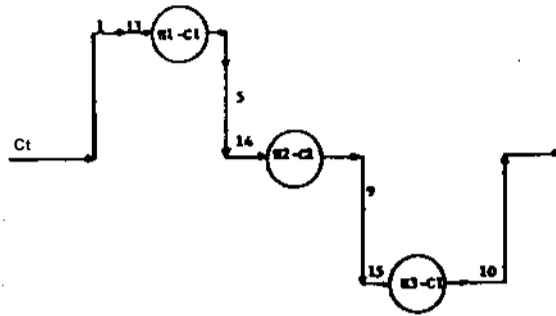


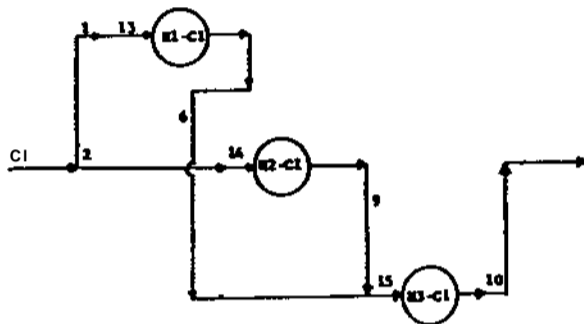
Figure 7. Superstructure by Floudas et al (1986) for 3 matches



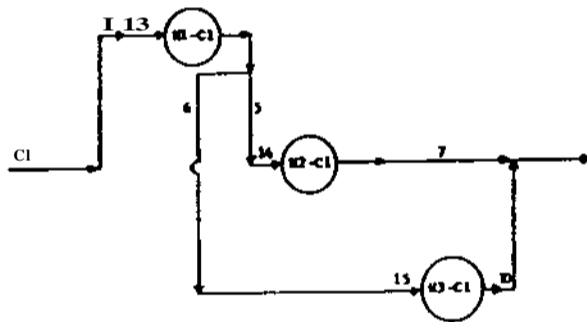
(a) Sequence in parallel



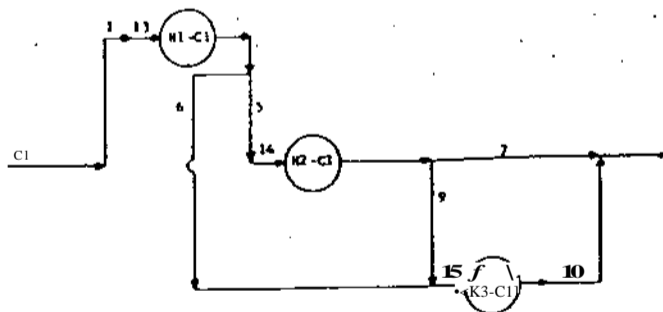
(b) Sequence in series



(c) Sequence in parallel-series



(d) Sequence in series-parallel



(e) Sequence in series-parallel with bypass

Figure P. Alternatives for configuration in Fig. 7

2. Prediction of fewest units and matches with the MILP transshipment model subject to the heat recovery predicted in step 1.
3. Automatic derivation of network structure using an NLP model given the heat recovery and matches predicted in steps 1 and 2. using an NLP model.

The novel aspect was the third step. The idea was to postulate a superstructure for each stream that would include all possible interconnections for the matches (units) predicted in step 2. As shown in the example of Fig. 7, which involves the 3 matches C1-H1, C1-H2 and C1-H3, this superstructure has embedded all possible configurations for the selected matches as can be seen in Fig. 8. The different configurations are obtained by setting to zero values the flows of intermediate streams. The objective function considered is the minimization of investment cost subject to the mass and energy balances as given by equations (1) to (4) which gives rise to an NLP problem. The significance of this development was the fact that this approach produced network structures without or with stream splitting and that would satisfy exact minimum utility and fewest number of units targets.

While the work by Floudas et al (1986) was a major advance, it also had some important limitations that were due to the sequential decomposition approach to the problem. Firstly, the MELP in step 2 has often multiple solutions with different stream matches and heat load distributions for the same number of fewest units. Secondly, although the NLP in step 3 avoids the deletion of units (i.e. zero areas), the problem is still nonconvex and may exhibit local optima. Also, the NLP model does not allow the specification of no stream splitting which is often desired due to practical reasons. Finally, the only way to optimize the heat recovery was to optimize the HRAT in an outer loop. A number of modifications have been proposed to circumvent some of these difficulties. Gundersen and Grossmann (1990) proposed a modified MELP transshipment model for step 2 that would favor selection of matches for vertical heat transfer. Floudas and Ciric (1989) proposed the application of Generalized Benders decomposition for step 3 by treating the flowrates as "complicating" variables to increase the likelihood of finding the global optimum. While these modifications were useful, it was also clear that a major underlying problem was the sequential decomposition of the synthesis problem, which by the way is also used in pinch technology. It was therefore clearly desirable to consider the development of *simultaneous* synthesis methods in which ideally the level of heat recovery, selection of matches, area and topology would all be optimized simultaneously so as to explicitly account for the trade-offs between energy, number of units and area.

Accomplishing such a goal was regarded as too difficult a task 10 years ago. The reason is that one of the elements required was the capability of solving mixed-integer nonlinear programming (MINLP) problems. That is, nonlinear optimization problems involving both discrete (mainly 0-1) and continuous variables. Despite the skepticism that was prevalent in the late 70's and early 80's for developing such a tool, research efforts that were initiated at Carnegie Mellon during the 80's (Duran and Grossmann, 1986; Kocis and Grossmann, 1987; Viswanathan and Grossmann, 1990) produced new MINLP optimization algorithms and codes (outer-approximation methods) that can solve typically problems with up to 50 0-1 variables and 1000 variables and 1000 constraints. This work also uncovered the seminal contribution by Geoffrion (1972) on Generalized Benders decomposition which had been overlooked by the chemical engineering community. For a review of these methods and discussion of relative advantages and disadvantages see Grossmann (1989).

As will be discussed in the next section, recent developments in MINLP optimization and the emergence of simulated annealing have started to produce automated synthesis tools that can perform simultaneous optimization.

Automated simultaneous synthesis

Three major efforts have that been done in developing methods for simultaneous optimization for synthesis of networks are the following.

At VPI, Dolan et al. (1989) developed a simultaneous synthesis method using simulated annealing (Aarts and van Laarhoven, 1985). The authors were able to optimize the selection of matches, areas and heat recovery level without relying on the sequential decomposition. Furthermore, they did not have to assume fixed values of the temperature approaches. While their work was a significant development it has two limitations. Firstly, the application of simulated annealing to this problem requires the definition of "moves" which are generated randomly for both discrete and continuous variables, and for which there is not a clear systematic method for doing this. Secondly, while this technique can often overcome the problem of getting trapped into local solutions, it is computationally very intensive. Nevertheless, simulated annealing is a viable synthesis method that has produced interesting results.

At Princeton, Floudas and Ciric (1989) expanded the superstructure by Floudas et al (1986) so as to consider the possible selection of all matches, thus eliminating step 2 from the previous section. However, the minimum utility target was still enforced in this method. The integration of steps 2 and 3 led to an MINLP problem in which 0-1 variables are used to denote the potential existence of units. The authors used Generalized Benders decomposition method and incorporated the MILP transshipment model in its master problem to reduce the number of iterations and the number of infeasible configurations that are commonly generated by this method. While the contribution of Ciric and Floudas (1989) was an important step to move away from the sequential synthesis strategy, it did not optimize the energy cost simultaneously with the area and number of units.

Yee and Grossmann (1990) proposed and MINLP optimization method in which the selection of matches, areas and heat recovery are optimized simultaneously. Also, no temperature approaches need to be specified. The basic idea of this method relies on the superstructure representation shown in Fig. 9. The basic idea here is to consider a sequence of stages in which hot and cold streams are successively split and remixed. The number of stages is commonly chosen as the larger of the number of hot and number of cold streams, although other choices are also possible. While this superstructure has the limitation that it does not embed all possible options for stream splitting (e.g. branches with two or more sequential matches), it has two major advantages. Firstly, it is very easy to impose constraints for no stream splitting with the 0-1 variables as one only has to specify that not more than one match can take place for any given stream in each stage. Secondly, if one assumes isothermal mixing no variables for the flowrates are required, and more importantly, all the constraints become linear which greatly simplifies the solution of the MINLP which is solved with the computer code DICOPT ++ (Viswanathan and Grossmann, 1990). In the case when stream splits are obtained, the mixing temperatures can be refined by an NLP optimization of that structure. As will be shown later in the results, this method has the tendency of producing networks with simple structures. Thus, the significance of this method is that it provides an efficient and practical tool for automated synthesis in which constraints on stream splitting can be imposed and where no fixed values for minimum temperature approaches (HRAT, EMAT) need to be specified. Also the inlet and outlet temperatures can be specified as inequalities. As with the other methods, however, global optimum solutions cannot be guaranteed.

Computer tools and examples

A number of the mathematical methods discussed in the previous sections have been implemented in various software packages. For instance, the LP, MILP transshipment models and the NLP superstructure optimization have been implemented in MAGNETS

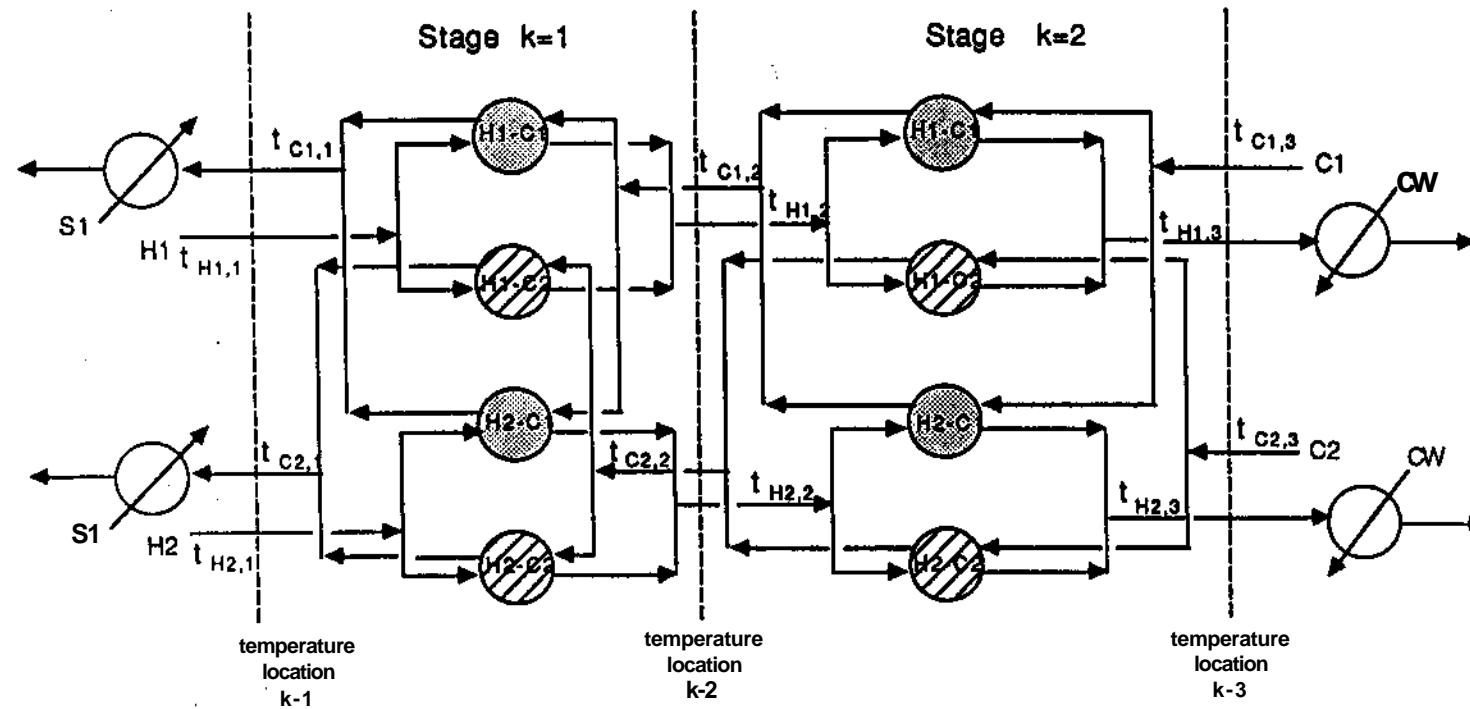
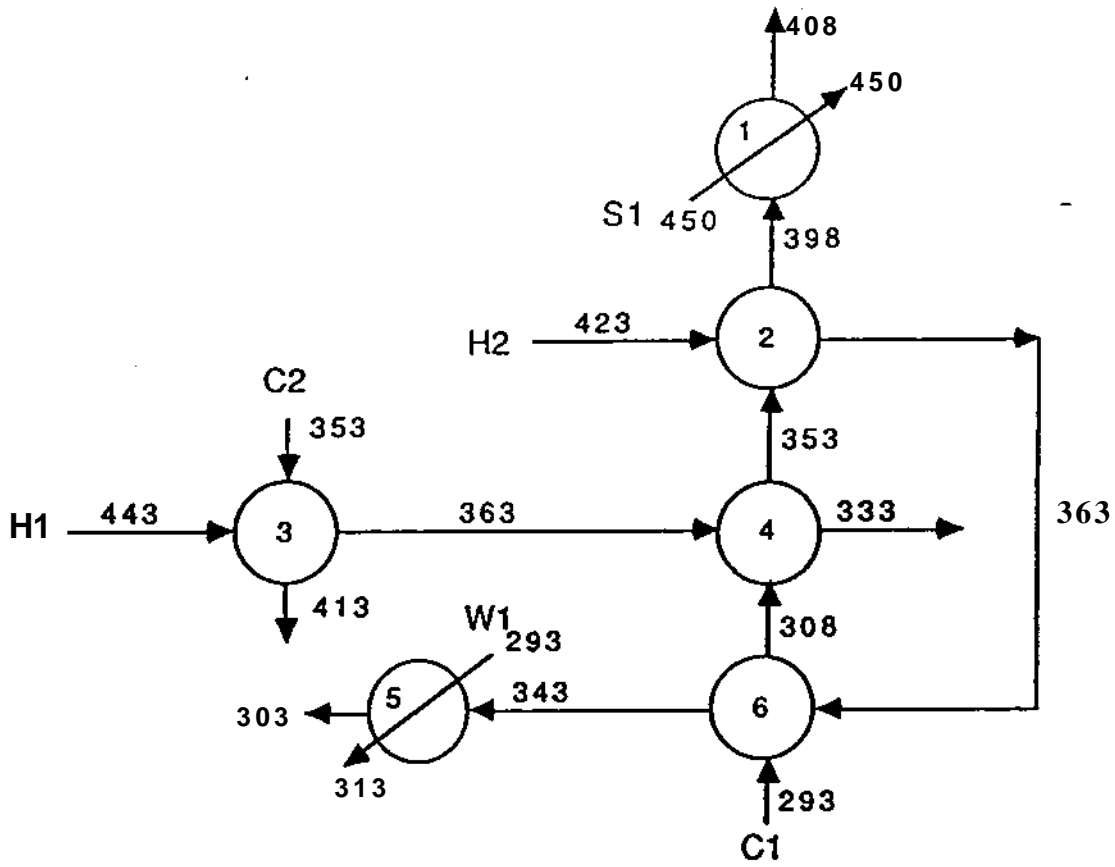


Figure 9. Two-stage superstructure by Yee and Grossmann (1990)



Annual Utility Cost = \$28,000
 Annual Capital Cost = \$61,832
 Total Annual Cost = \$89,832

Exch.	Heat Load (kVO)	Area(m ²)
1	200	3.6
2	900	68.7
3	2400	164.8
4	900	68.7
5	600	41.2
6	300	7.1

Figure 10. Network structure synthesized with pinch technology and MAGNETS

(Floudas et al, 1986). The LP and MELP transshipment models have been implemented in RESHEX (Saboo et al, 1986). The MINLP method by Yee and Grossmann (1990) has been implemented in SYNHEAT. At this time reasonable computer times with these packages (few minutes) are still typically restricted to smaller problems (e.g. 5 hot, 5 cold streams).

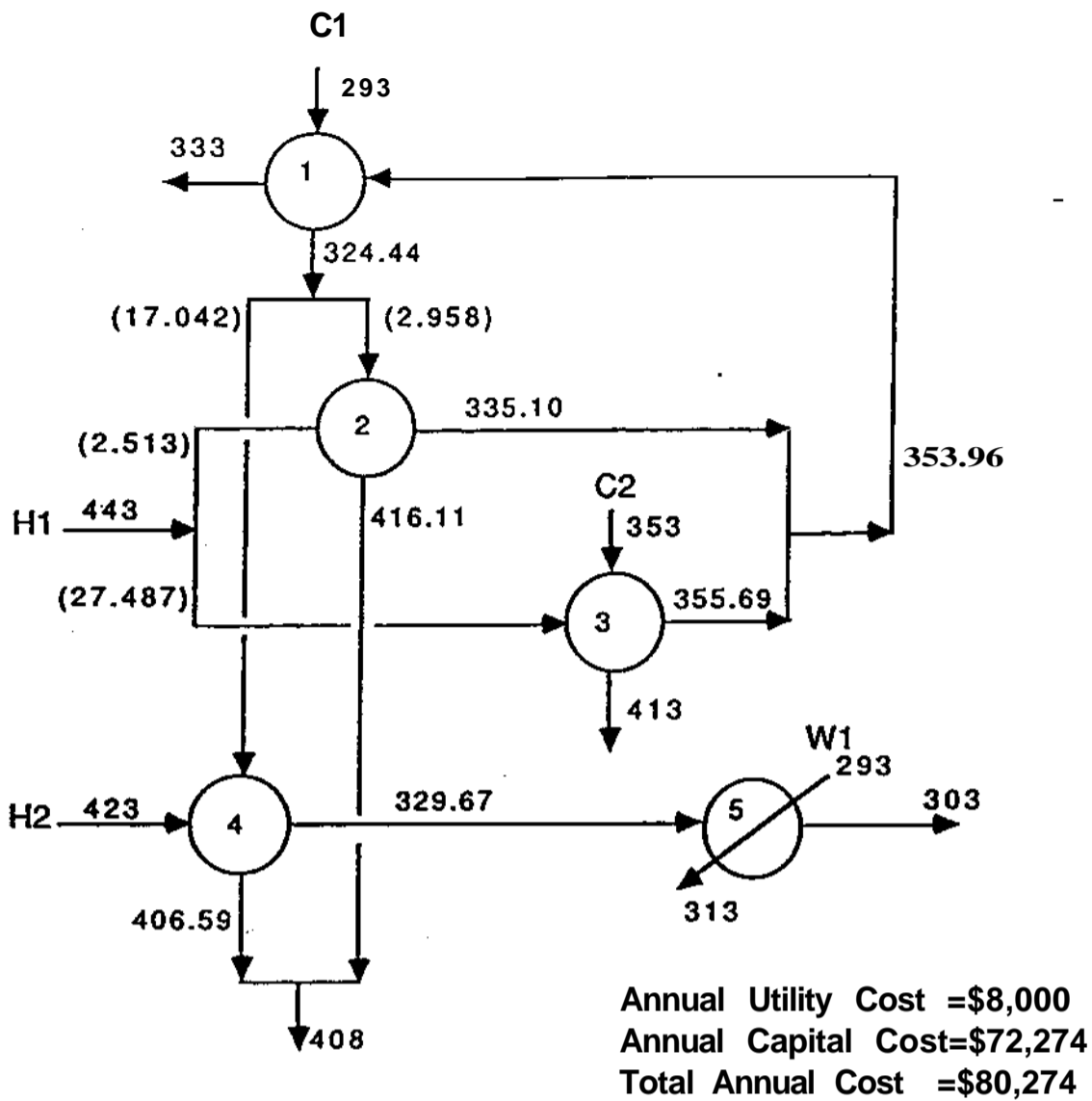
MAGNETS, RESHEX and SYNHEAT are interactive programs that do not require the user to be an expert in mathematical programming since they automatically generate the superstructures and equations. Also, in terms of robustness these packages have performed reasonably well. There are no difficulties with the LP models; MHP models are also robust but they can become expensive for larger problems; the NLP models may occasionally experience difficulties of convergence. The main point however, is that what these implementations have shown is that they have dispelled the myth that mathematical methods are hard to use. On the other hand there is still clearly scope for improving these methods especially in terms of the size of problems that can be handled.

To illustrate the scope of these tools consider first the network structure in Fig. 10 which was synthesized manually as reported in Linnhoff et al (1982). Maintaining the same temperature approach of 10K, the program MAGNETS was able to synthesize exactly the same structure. If the simultaneous synthesis strategy in SYNHEAT is used, the network that is obtained is shown in Fig. 11. Note that by not specifying a minimum temperature approach a substantial reduction in the cost is obtained (from \$89,832/yr down to \$80,274/yr). Also, this network in fact eliminates the use of steam. This network structure, however, exhibits two stream splits which could make the network unattractive for operation. With SYNHEAT, however, one can easily impose constraints for no stream splits. Doing this the network that is automatically synthesized is shown in Fig. 12, which has only a slightly higher cost: \$80,909/yr. This network from a practical standpoint would be most likely the preferred choice. Thus, as seen in this example, using this a tool such as SYNHEAT one can explore several alternatives through the specification of various constraints (e.g. no stream splits, forbidden matches, etc.). One is not necessarily tied to one single solution.

A final example is given in Figs. 13 and 14 for a problem which involves 1 cold and 5 hot streams. The network in Fig. 13 was automatically synthesized by MAGNETS for a fixed HRAT = 5K, while the network in Fig. 14 was synthesized by SYNHEAT. Note that the solution by MAGNETS, which follows the pinch approach, produces a network that is slightly cheaper (\$575,595/yr vs. \$576,640/yr). However, the network in Fig. 14 is remarkably simpler. It involves 2 fewer units and only 1 less splitting point. Also, note that in this network the choice of HRAT, the heat recovery approach temperature, with a value of 13.1K was determined as part of the optimization. Closer examination of this network reveals that in fact exchanger 2, 3 and 4 exchange heat across the pinch, thereby reducing the number of units. In contrast, the guideline of no heat flow across the pinch point was strictly enforced in the MAGNETS solution which therefore led to a larger number of units and stream splits. What this example then shows is that by relying too heavily on design guidelines such as the ones given by pinch technology, one may in fact overlook interesting design alternatives. The example also shows that automated synthesis tools have started to achieve a quite respectable design capability that can enhance the productivity of design engineers. It should be noted that the above problems required no more than two minutes of CPU-time on a conventional mainframe computer (VAX-6320).

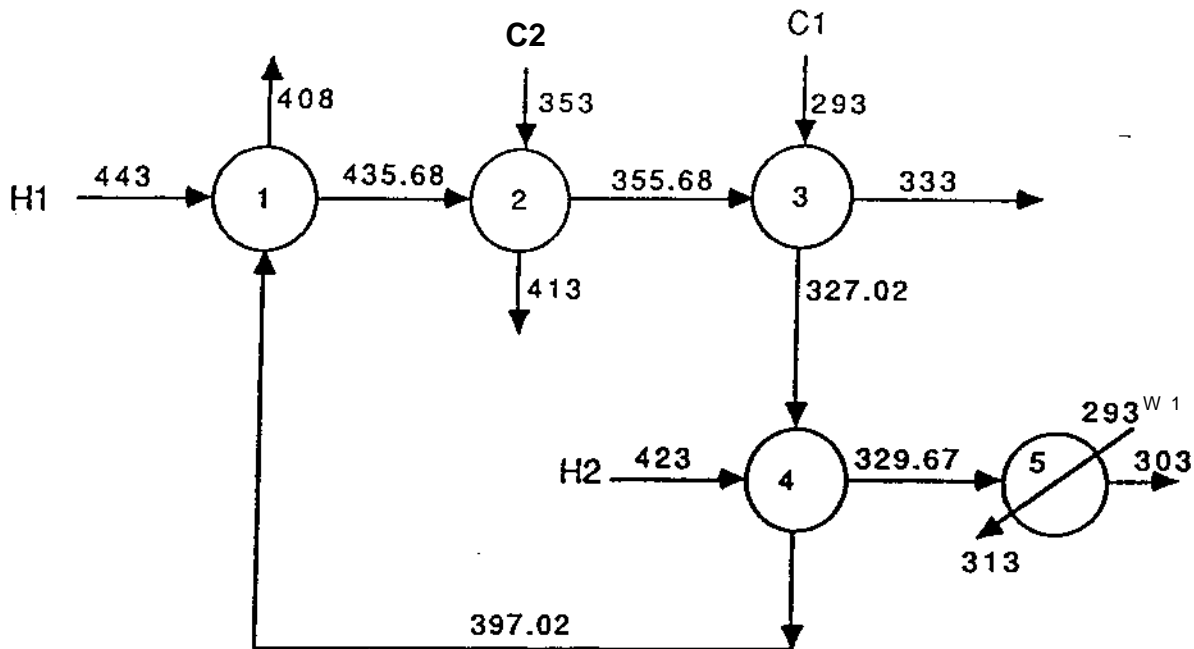
Beyond HEN's

One of the important aspects of mathematical models is that a number of them can be extended so as to *simultaneously* optimize process flowsheets and heat exchanger networks. The key requirement here is that the flows and temperatures be treated as variables for both the process and the HEN. Papoulias and Grossmann (1983) were the



Exch.	Heat Load (kW)	Area(m ²)
1	628.8	22.8
2	271.2	19.3
3	2400	265.1
4	1400	179.0
5	400	38.3

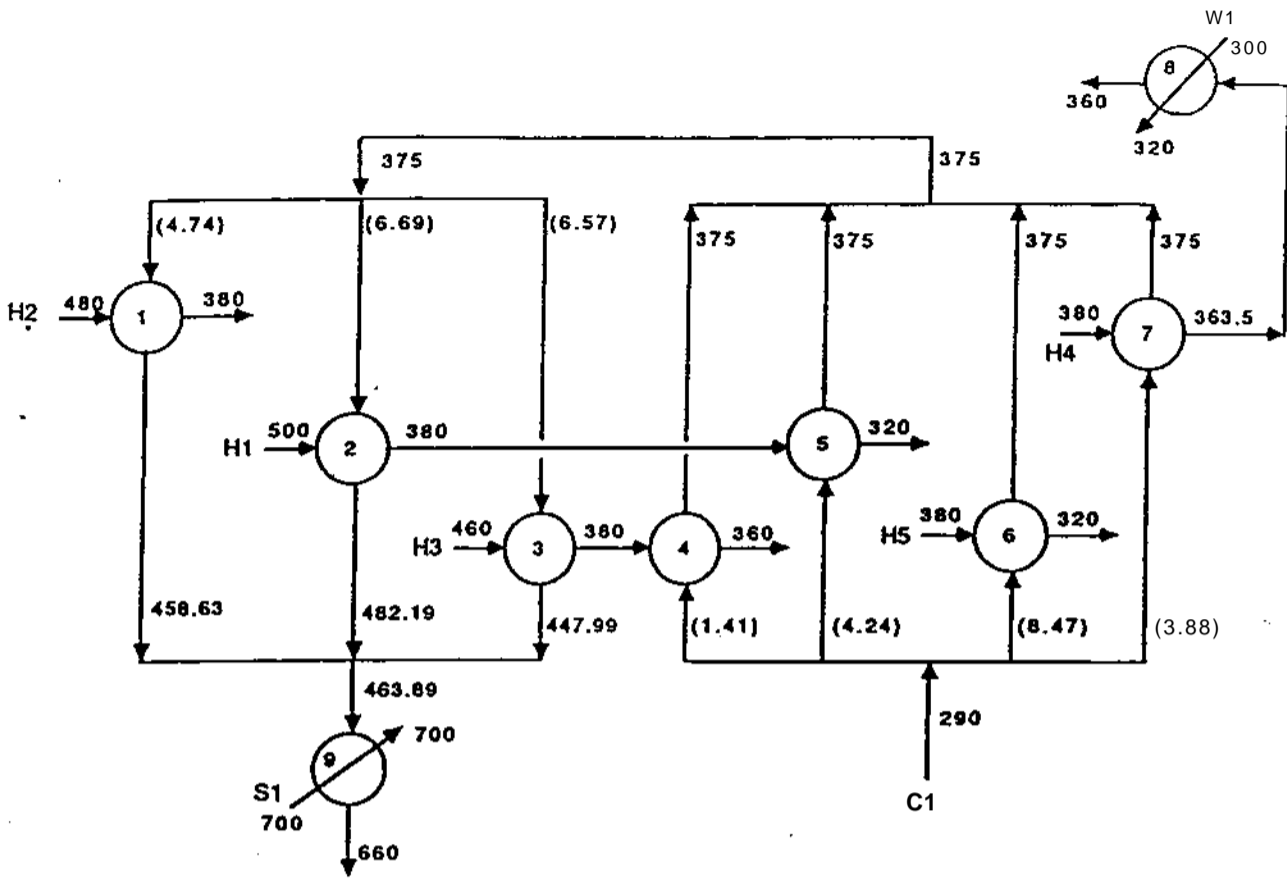
Figure 11. Network structure synthesized by SYNHEAT



Annual Utility Cost = \$8000
 Annual Capital Cost » \$72,909
 Total Annual Cost = \$80,909

Exch.	Heat Load (kW)	Area(m ²)
1	219.6	7.5
2	2400	320.3
3	680.4	25.0
4	1400	171.3
5	400	38.3

Figure 12. Network structure synthesized by SYNHEAT with no split constraints

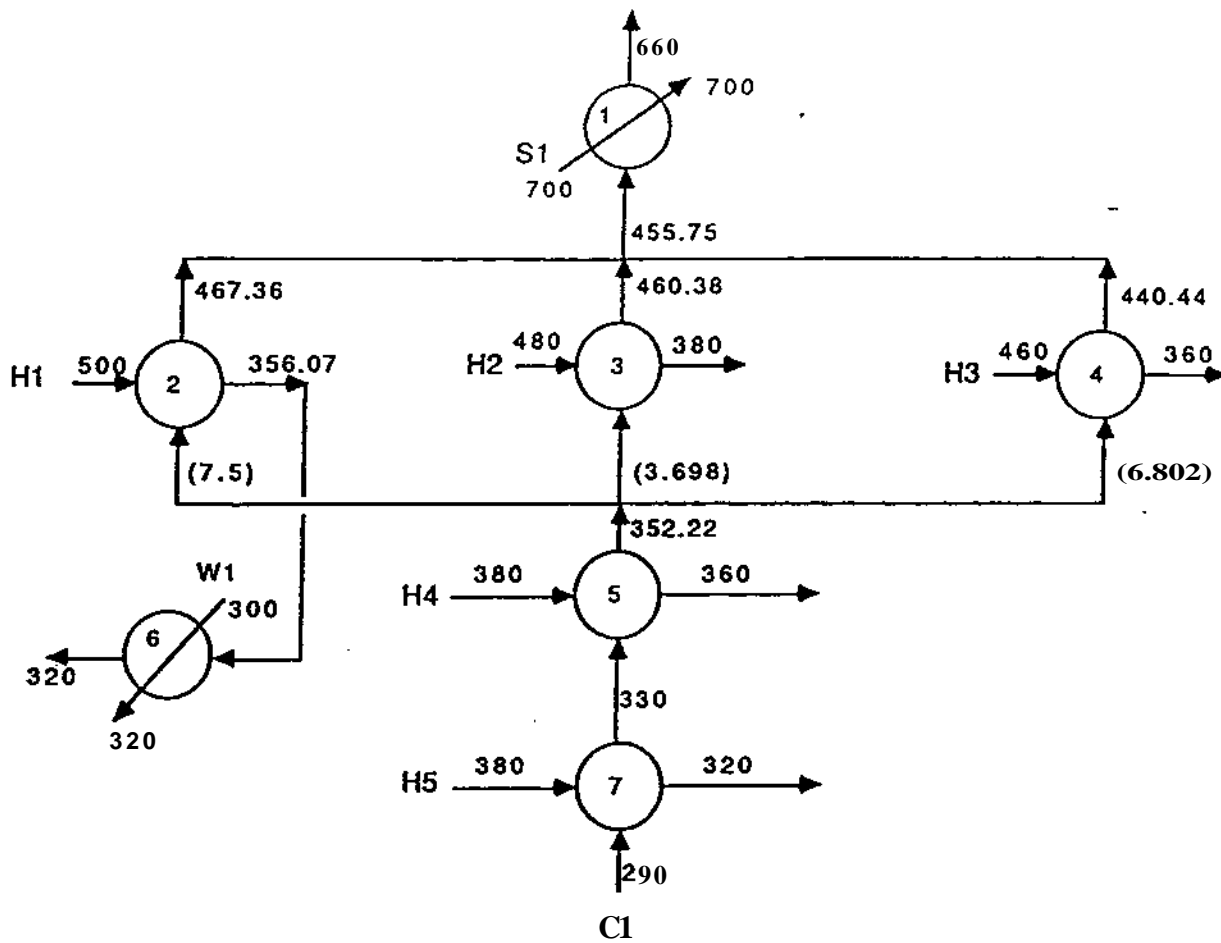


Exch.	Heat Load (kW)	Area(m ²)
1	400	35.5
2	720	71.4
3	480	60.0
4	120	4.9
5	360	25.8
6	720	51.6
7	330	12.9
8	70	1.4
9	3530	32.0

Pinch location: 380-375K
 Annual Utility Cost « \$494,900
 Annual Capital Cost = \$80,695

Total Cost = \$575,595
 Total Area = 295.5 m²

Figure 13. Network synthesized by MAGNETS



Exch.	Heat Load (kAM)	Area (m ²)
1	3676.4	32.6
2	863.6	64.1
3	400	17.1
4	600	47.0
5	400	13.8
6	216.4	7.9
7	720	18.4

Pinch Location: 380-366.9K
 Annual Utility Cost = \$516,860
 Annual Capital Cost = \$59,780
 Total Annual Cost = \$576,640
 Total Area = 200.9 m²

Figure 14. Network synthesized by SYNHEAT

first to apply this strategy by embedding the LP transshipment model within an MHJP model for a superstructure of a process flowsheet. In this case temperature levels were discretized and flowrates of the streams were treated as variables. Subsequently Duran and Grossmann (1986) developed a nonlinear heat integration model in which both flowrates and temperatures can be treated as variables. Another recent development is the extension of the model of Yee et al (1990) in which not only the utility cost but the network structure can be simultaneously optimized with the process flowsheet

An interesting result that has emerged from a number of examples, including ammonia and methanol processes, is the fact that simultaneous optimization and heat integration tends to produce large economic savings. Interestingly, not necessarily by reducing the energy cost, but by reducing the amount of raw materials required (e.g. see Duran and Grossmann, 1986; Lang et al, 1988). Qualitatively the explanation is that by performing efficient energy management, flows and operating conditions can be adjusted appropriately to increase the overall conversion. Here again case studies have demonstrated that the sequential approach of optimizing the process first, followed by heat integration for fixed flows and temperatures tends to produce significantly inferior solutions.

Concluding remarks

This paper has given an overview of the evolution of mathematical methods for HEN synthesis, and emphasized the state of the art of the current methods. While there is clearly scope for future advances, a number of points that are worth noting in terms of the lessons that have been learned are the following.

1. Optimization models are greatly influenced by the type of representations and assumptions being used. The initial work suffered from a lack of understanding of the pinch point. On the other hand, the capability of handling 0-1 variables in MINLP, and the development of general superstructures has removed many of the initial limitations. Future work will have to concentrate on issues related to global optimality and capability for handling larger sized problems. Also, a number of simplifying assumptions must be removed.
2. Physical insights can greatly help to simplify mathematical models as was clearly the case with the LP and MILP targeting models. There is the danger, however, of placing too much faith in some of these insights and oversimplify the solution with simple decompositions. Recent progress in mathematical methods has been possible by ignoring some of these heuristic guidelines. In fact we have the ironic situation that several recent simultaneous optimization methods (e.g. Dolan et al, 1989; Yee and Grossmann, 1990) do not make explicit use of pinch concepts. They are only used for an a-posteriori analysis.
3. Recent optimization methods have promoted and supported the concept of simultaneous optimization which is clearly the correct conceptual framework, and the one that can yield large economic payoffs. This has been illustrated not only in HEN synthesis applications, but also in the optimization of process flowsheets.
4. The debate of physical insights versus mathematical models is an essence a non-issue. We need both and they, clearly complement each other. Furthermore, design engineers can always remain in control of the decisions by using automated methods that can accommodate a variety of constraints and specifications, and are implemented within an interactive environment.

Finally, given the significant changes that have taken place in computational power over the last few years, there is certainly reason to believe that mathematical based methods will play an increasing role in commercial software for HEN synthesis. These could expand significantly the capabilities of current industrial tools for heat integration.

References

- Aarts, E.H.L. and van Laarhoven, P.J.M. Statistical Cooling: A General Approach to Combinatorial Optimization Problems. *Phillips J. Res*, 40,193 (1985)
- Cerda J. and A.W. Westerberg. Synthesizing Heat Exchanger Networks Having Restricted Stream/Stream Match Using Transportation Problem Formulations. *Chem. Engng. Sci.* 38, 1723-1740 (1983)
- Cerda J., A. W. Westerberg, D. Mason and B. Linnhoff. Minimum Utility Usage in Heat Exchanger Network Synthesis - a transportation problem. *Chem. Engng Sci.* 38, 373-387 (1983).
- Dolan, W.B., Cummings P.T. and LeVan M.D. Process Optimization via Simulated Annealing: Application to Network Design. *AIChE J.*, 35, 5,725-736, (May 1989).
- Duran M.A. and Grossmann I.E. An Outer-Approximation Algorithm for a Class of Mixed-Integer Non-Linear Programs. *Math. Progr.*, 36, 307-339, (1986a).
- Duran M.A. and Grossmann US. Simultaneous Optimization and Heat Integration of Chemical Processes. *AIChE J.*, 32, 123-138 (1986).
- Floudas C.A., A.R. Ciric and I.E. Grossmann. Automatic Synthesis of Optimum Heat Exchanger Network Configurations. *AIChE J.*, 32, 276-290 (1986).
- Floudas C.A. and Ciric A.R. Strategies for Overcoming Uncertainties in Heat Exchanger Network Synthesis. *Comp and Chem Engng*, 13, 10, 1117-1132, (1989).
- Grossmann, I.E., "Problems in the Optimum Design of Chemical Plants", Ph.D. thesis, Imperial College, University of London (1977).
- Grossmann I.E. MINLP Optimization Strategies and Algorithms for Process Synthesis. In Siirola J.J., Grossmann I.E. and Stephanopoulos G. "Foundations for Computer Aided Process Design", Proc. of 3rd Int. Conf. on FOCCAPD, Snowmass Village, Colorado, July 1989, Elsevier, pp. 105-132, (1990a).
- Grossmann, I.E. and R.W.H. Sargent, Optimum Design of Chemical Plants with Uncertain Parameters. *AIChE J.*, 24,1021-1028 (1978b).
- Gundersen T. and Grossmann I.E. Improved Optimization Strategies for Automated Heat Exchanger Network Synthesis through Physical Insights. *Comp. and Chem. Engng.* 14, 9, 925-944 (1990).
- Gundersen T. and Naess L. The Synthesis of Cost Optimal Heat Exchanger Networks. An Industrial Review of the State of the Art. *Comp. and Chem. Engng.* 12, 6, 503-530 (1988).
- Hwa C.S. Mathematical Formulation and Optimization of Heat Exchanger Networks using Separable Programming. *AIChE J. Chem E. Symp. Ser.* 4, 101-106 (1965).
- Jones, S.A. and D.W. T. Rippin. The Generation of Heat Load Distributions in Heat Exchanger Network Synthesis. *Proc. Int. Conf. Process Systems Engng (PSE-85)*, 157-177, Cambridge (1985).

Kesler M.G. and R.O. Parker. Optimal Networks of Heat Exchange. *Chem. Engng Prog. Symp Ser.* 65, 111-120 (1969).

Kocis G.R. and Grossmann I.E. Relaxation Strategy for the Structural Optimization of Process Flowsheets. *Ind. Engng. Chem. Res.* 26, 9, 1407-1421, (1988).

Lang, Y.-D., Biegler L.T. and Grossmann I.E. Simultaneous Optimization and Heat Integration with Process Simulators. *Comp. and Chem. Engng.* 12, 4, 311-327 (1988).

Lee K.F., A.M. Masso and D.F. Rudd. Branch and Bound Synthesis of Integrated Process Designs. *Ind. Engng Chem. Fundam.* 9, 48-58 (1970).

Linnhoff, B. and J.R. Flower, "Synthesis of Heat Exchanger Networks. I. Systematic Generation of Energy Optimal Networks", *AIChE J.*, 24, 633-642 (1978).

Linnhoff B. and D.R. Vredeveld. Pinch Technology has Come of Age. *Chem. Engng. Prog.* 80, 33-40 (1984).

Linnhoff et al. User Guide on Process Integration for the Efficient Use of Energy. *ICHEME*, (1982).

Papoulias S.A. and Grossmann I.E. A Structural Optimization Approach to Process Synthesis - I. Utility Systems. *Comp. and Chem. Engng.* 7, 695-706 (1983).

Papoulias S.A. and Grossmann I.E. A Structural Optimization Approach to Process Synthesis - II. Heat Recovery Networks. *Comp. and Chem. Engng.* 7, 707-721 (1983).

Papoulias S.A. and Grossmann I.E. A Structural Optimization Approach to Process Synthesis - m. Total Processing Systems. *Comp. and Chem. Engng.* 7, 723-734 (1983).

Rathore R.N.S. and G.J. Powers. A Forward Branching Scheme for the Synthesis of Energy Recovery Systems. *Ind. Engng Chem. Process Des. Dev.* 14, 175-181 (1975).

Saboo A.K., M. Morari and R.D. Colberg. RESHEX - and Interactive Software Package for the Synthesis and Analysis of Resilient Heat Exchanger Networks - 1. Program Description and Application. *Comput. chem. Engng.* 10, 577-589 (1986).

Saboo A.K., M. Morari and R.D. Colberg. RESHEX - and Interactive Software Package for the Synthesis and Analysis of Resilient Heat Exchanger Networks - n. Discussion of Area Targeting and Network Synthesis Algorithms. *Comput. chem. Engng.* 10, 591-599 (1986).

Townsend D.W. and B. Linnhoff. Surface Area Targets for Heat Exchanger Networks. *ICHEME Annl Res. Mtg. Bath* (1984).

Umeda T., Itoh J. and Shiroko K. Heat Exchange System Synthesis. *CEP*, 74, 7, 70-76 (1978).

Viswanathan J. and Grossmann I.E.. "A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization", *Comp. and Chem. Eng.*, 14, 769-782 (1990).

Viswanathan J. and Grossmann I.E. DICOPT++ a Program for Mixed Integer Non-Linear Optimization. A User's Guide, EDRC, Carnegie Mellon University, Pittsburgh, PA (April 1990).

Yee T.F. and Grossmann I.E. Simultaneous Optimization Models for Heat Integration -1. Area and Energy Targeting and Modeling of Multistream Exchangers. *Comp. and Chem. Engng.* 14, 10, 1165-1184 (1990).

Yee T.F. and Grossmann I.E. Simultaneous Optimization Models for Heat Integration - H Heat Exchanger Network Synthesis. *Comp. and Chem. Engng.* 14, 10, 1165-1184 (1990).

Yee T.F., Grossmann I.E. and Kravanja Z. Simultaneous Optimization Models for Heat Integration - in. Process and Heat Exchanger Network Optimization. *Comp and Chem Engng.* 14, 11, 1185-1200(1990).