

# Integrated Synthesis of Optimal Separation and Heat Exchanger Networks Involving Separations Based on Various Properties

I. HECKL and F. FRIEDLER

Department of Computer Science, University of Veszprém, Veszprém, Hungary

L. T. FAN

Department of Chemical Engineering, Kansas State University, Manhattan, KS, USA

*The current effort aims at contributing to the algorithmic synthesis of a heat-integrated separation network system involving separations based on various properties, such as volatility, solubility, and permeability. This is unlike any of the previous works on heat-integrated network synthesis involving separation based only on a single property, such as volatility. The network under consideration consists of mixers, dividers, separators, utilities, and heat exchangers. The network system produces pure or multicomponent product streams from a single or multiple feed streams. Meanwhile, it satisfies the heat requirements not only between reboilers and condensers but also between hot and cold streams throughout the entire network of a production plant with the lowest possible annualized cost. The costs of the mixers and dividers are regarded as negligible: the cost of a separator, a linear function of the flowrate of its input stream without an additive constant parameter, and the cost of a utility, proportional to the heat provided or extracted. The cost of a heat exchanger is calculated based on logarithmic-mean temperature difference (LMTD).*

## INTRODUCTION

Both separation network synthesis (SNS) and heat exchanger network synthesis (HENS) are among the most important sub-disciplines of process synthesis. Their significance is obvious: separation and heat exchanger networks are ubiquitous throughout the chemical and allied industries. The separation network can account for more than half of the total capital cost of a typical chemical plant. The energy demands of separation tasks are usually inordinately high, and the consumption of utilities to satisfy these demands constitutes a major part of the operating outlay. Thus, the optimal syntheses of separation and heat exchanger networks would substantially reduce the cost of production.

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Address correspondence to F. Friedler, Department of Computer Science, University of Veszprém, Veszprém, Hungary. E-mail: friedler@dcs.vein.hu

A separation network comprises dividers, mixers, and separators through which multi-component streams flow while being processed. A multitude of networks can be constructed from these operating units, with the resultant networks differing from one another according to their intended purposes. The aim of SNS is to identify a separation network performing the intended separation with the lowest possible cost. Various methods are available for SNS that can be categorized in terms of the quality and quantity of the feed streams (multicomponent; single or multiple streams) as well as product streams (pure or multicomponent), the search techniques for solution (heuristic, stochastic, algorithmic), the mathematical programming models adopted (linear, convex, non-convex), and the types of the separators (sharp, simple, non-sharp, complex).

Two conventional SNS models involving sharp separators based on composition and component flowrate have been introduced [1]. Moreover, a novel approach that incorporates the linear constraints from both models as well as a functional relationship between the composition and component flowrate has been also proposed. This model gives rise to a lower bound

for the globally optimal solution. The globally optimal network was determined by resorting to a branch and bound algorithm on the basis of this model. Conceptual programming that develops the design targets of separators and reactor-separator networks have also been introduced [2]. Conceptual programming involves heuristic rules, a shortcut method, and mathematical programming to provide a reliable result with modest computational effort. A mixed integer nonlinear programming model to synthesize the optimal separation network featuring non-sharp separators has been presented [3]. In that model, the recovery ratios of the light and heavy key components are treated as optimization variables. The cost functions of the separators were determined with shortcut simulation and regression. A decomposition algorithm was also introduced to solve the mathematical model efficiently. A unique policy for purifying an intermediate boiling component via batch distillation with side withdrawal has also been introduced [4]. Two operational modes are executed sequentially to carry out the separation. In the closed operational mode, the columns are operated with total reflux to fully separate A and C. At the end of the closed operational mode, the slump vessel will contain B and C while the distillate vessel will contain A and B. In the open operational mode, component B is withdrawn.

A HEN is composed of heat exchangers and hot and cold utilities for both subtracting heat from a set of hot process streams that are to be cooled and supplying heat to a set of cold process streams that are to be heated. In HENS, the input and output temperatures, flowrates, and specific heats of the streams are given in advance. The optimal heat exchanger network layout is to be identified along with the operating and annualized capital cost.

At the very early stage of research on HENS, the major concern was the determination of the minimum utility load in conjunction with the minimum number of heat exchangers. The well-known composite diagram to identify the utility load and pinch points has been introduced elsewhere [5]. Eventually, the algorithmic methods have gained popularity. Different versions of the trans-shipment model to determine networks corresponding to the minimum number of heat exchangers and the minimum utility load have been proposed [6]. The algorithmic methods rendered it possible to address HENS problems of increasing complexity, such as multiperiod HENS and HENS containing uncertainties. A simultaneous approach for systematically determining the optimal heat exchanger network design has also been introduced [7]. Their method is suitable for both strict-pinch and pseudo-pinch design problems. A comprehensive review of the synthesis of cost-optimal heat exchanger networks can be found elsewhere [8].

Traditionally, the design of a process plant has been carried out sequentially, starting with the flowsheeting of the process system, followed by the design of a set of the subsystems, such as the separation network (SN), the heat exchanger network (HEN), and the utility network. The design of each of these subsystems is a major challenge by itself; moreover, it usually

depends on previous decisions regarding other subsystems. For example, the process streams of the HEN are defined only after the process flowsheet is composed and the SN is designed. Nevertheless, the subsystems should be designed simultaneously to account for the interactions among them: the greater the interactions between the subsystems, the greater the possible gain by designing them simultaneously. As stated previously, both SN and HEN are costly, and their performances are intimately coupled: the latent heat released from a separation unit inevitably emerges in the HEN. If the interactions between the SN and HEN are neglected, the SN can be designed without regard to the heat integration. While the cost of the SN can be minimized as such, the cost of the HEN based on this network, as well as the combined cost of the SN and HEN, will be higher than those resulting from the simultaneous approach.

A method for assessing a thermally coupled, side-column system has been presented previously [9]. This method resorts to the Underwood technique for shortcut design, thereby providing the initial estimates for rigorous process simulation. A thermodynamic approach to the heat integration of processes involving the separation of multicomponent mixtures has recently been introduced [10]. This approach defines an integrability criterion for rapid screening of process alternatives. It yields the most promising sequences of heat-integrated distillation columns; nevertheless, these sequences should be explored further.

A method has been demonstrated [11] to generate the optimal heat-integrated separation network comprising nonsharp separators. The method determines the cost models of the separators with a shortcut method followed by rigorous simulation, constructs a super-structure, generates a mixed-integer nonlinear programming (MINLP) model based on such a superstructure, and devises the solution strategy based on the resultant mathematical model. The adoption of nonsharp separators is the advantage of the method; nevertheless, the model is strongly non-continuous and non-convex, thus rendering the attainment of the global optimum extremely difficult if not impossible.

Such a hybrid optimization method has been proposed [12] that is sufficiently robust to handle nonlinear, non-convex objective functions that are not smooth. This hybrid method consists of a local search method to initially identify a feasible sequencing and a genetic algorithm to finally determine the optimal HEN corresponding to the actual sequencing. A simple yet effective filtering procedure has also been devised to handle the nonlinearity of the objective function.

Note that all these works consider only distillation columns as separation units; however, separators based on separation methods effected by properties other than the relative volatility are steadily gaining popularity. For instance, if the separation, solely by distillation, of components A and B is expensive due to the minute difference in their relative volatilities, incorporating extraction by adding a third component as the solvent would reduce the cost of the network. Theoretically, any physical or chemical properties of the components to be separated can be exploited to effect their separation. If various types of separators based on

different separation methods are involved, the available methods are incapable of identifying the optimal heat-integrated separation network.

In general, the conventional algorithmic methods for the heat-integrated separation network synthesis give rise to MINLP models. The incorporation of realistic models of separators naturally leads to non-convexities, thereby rendering their solutions almost always only locally optimal. Even if the most simple separator model is used, the resulting mathematical model is always nonlinear unless it is based on the current superstructure.

The method proposed herein involves simple and sharp separators based on different separation methods effected by various physical or chemical properties; each separator is described with a simple model. The temperatures of the inlet, top, and bottom streams; the number and nature of the latent heats of the separator; the amount of heat released at each latent heat source or absorbed at each latent heat sink to process one unit of the inlet stream; the type of the separator with a set of components in the inlet, top, and bottom streams; and the overall cost coefficient are all given. Suppose that the separator is a distillation column; then, its condenser is a hot source and its reboiler a cold source of the latent heat. The only variable of the separator's model is the flowrate at its inlet. The latent heat loads and the separator's cost are linear functions of the inlet flowrate. The dividers and mixers are simple devices to direct the streams. For both, the material balances hold, and the compositions of all branches issuing from each divider are identical. The costs of the mixers and dividers are regarded as negligible. The cost of a utility is proportional to the heat provided by or extracted from it, and the cost of a heat exchanger is calculated in terms of logarithmic mean temperature difference (LMTD).

The current work aims at creating, or synthesizing, the optimal heat-integrated separation network producing the desired pure or multicomponent products from the given feed or feeds. The resultant network comprises various types of separators based on different separation methods. The proposed method for accomplishing the synthesis allows the inclusion of the sources of sensible as well as latent heats in the entire plant.

### SUPERSTRUCTURE OF THE SNS PART

Given briefly in this section is the generation of the separation part of the superstructure. In the proposed method, separators are considered simple and sharp. In other words, each separator has exactly one input and two outputs, and each component of the input stream appears only in one of the output streams. An algorithm is available to generate a superstructure of the separation network with such separators (see [13]). Some modification renders it possible for this algorithm to take into account separators based on different separation methods effected by various physical and chemical properties (e.g., volatilities, permeabilities, and solubilities).

It has been proved [13] that if the separator's cost is regarded as a linear function of its mass load and the cost of the separator

network is the sum of the individual separator's costs, then every SNS problem of the given class has a loopless optimal network. Moreover, each instance of the class of SNS problems of interest gives rise to such a loopless optimal network in which mixers are attached only to the product streams.

The superstructure explicitly includes all such solution structures in which mixers are attached only to products. What follows is the procedure for generating the super structure:

- Step 1 creates one divider for each feed stream and links each divider to the corresponding feed stream
- Step 2 creates one mixer for each product stream and links each mixer to the corresponding product stream
- Step 3 selects an unexplored divider
- Step 4 creates a separator for each possible cut and a bypass to each mixer created in Step 2, both of which are connected to the divider selected in Step 3
- Step 5 generates a divider for each of the outlets from the separators created in Step 4.

Hereafter, Steps 3–5 are iterated until the complete superstructure is generated. The creation of a bypass between an outlet of any divider and the inlet of a mixer is possible only when every component in the former appears in the product stream from the latter.

It is worth noting that if separators are based on separation methods effected by different phenomena or properties of the components involved, two or more separators may yield identical top and bottom product streams. Nevertheless, both separators must be included in the superstructure, unless, apart from the overall cost coefficient, all the properties of the separators are the same.

The algorithm is finite: after every separation step, the number of components in the top stream is at least one less than that in the inlet stream; this is also the case for the bottom stream. The streams resulting after at most (component number  $-1$ ) separations are of pure products; consequently, no further separation can be effected. After all the dividers are selected, the algorithm halts at Step 3.

The algorithm is demonstrated with an example. Its input data can be found in Table 1 and Figure 1. Steps 3–5 are iterated after the initiating steps, Steps 1 and 2. Figure 2 shows the result after the first iteration, and Figure 3 is the complete super structure.

It is noteworthy that the mathematical models derived from the previously known superstructures for SNS are inevitably nonlinear, even if the cost function of the separators are strictly

**Table 1** Data pertaining to the components and utilities for the first example

Name	Components		Utilities	
	Specific heat (kJ/(kg°C))	Type	Temperature (°C)	Cost (\$/(kW s))
A	2	High-pressure steam	250	11
B	3	Cooling water	20	1.6
C	1			

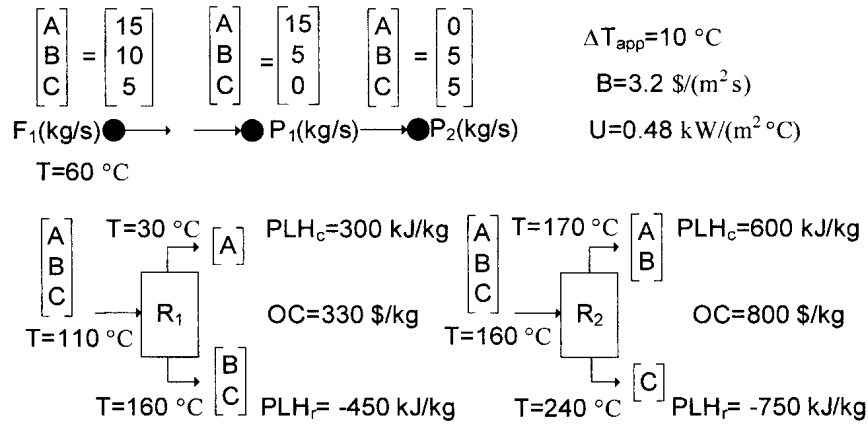


Figure 1 Input data for the first example.

linear. In contrast, the current superstructure gives rise to a linear mathematical model without fail, although the number of variables increases exponentially. Most important of all, the current superstructure can also accommodate separators based on different separation methods effected by various physical or chemical properties. This is especially advantageous in biochemical separation and purification.

**IDENTIFICATION OF THE SOURCES OF SENSIBLE AND LATENT HEATS**

With the superstructure of the separation network constructed, the proposed method focuses on the identification of the sources of sensible and latent heats that can possibly be included in the solution structures. The proposed method resorts to the combi-

natorial approach to HENS based on hP-graphs, adapted from the P-graphs, in conjunction with the appropriate selection of temperature intervals (see [14]).

To execute the HENS based on hP-graphs, the sources of sensible and latent heats must be identified at the outset. A stream in the superstructure is one of the sources of sensible heat, while the condenser and reboiler of a distillation column are two of the sources of latent heat. In reality, utilities can also be the sources of either latent or sensible heat, although the latent heat predominates.

The properties of any stream pertinent to HENS are the inlet temperature,  $T_{in}$ , the outlet temperature,  $T_{out}$ , the total flowrate,  $f_{ij}$ , and the specific heat,  $CS_{ij}$ . For convenience, the heat content of the stream,  $qns_e$ , is defined as

$$qns_e = CS_{ij} f_{ij} (T_{in} - T_{out}) \tag{1}$$

The magnitude of  $qns_e$  is positive when  $T_{in} > T_{out}$ , thus indicating the release of heat from the stream that is absorbed by other parts of the system. When  $T_{in} < T_{out}$ ,  $qns_e$  is negative, thus indicating the absorption of heat by the stream from other parts of the system. In the superstructure, streams span between the feeds and dividers, dividers and separators, dividers and mixers, separators and dividers, and mixers and products. In general, these streams are interdependent of each other. For instance, a divider itself does not induce temperature variations; thus, the elevation of the temperature of a stream at the inlet of a divider will accordingly increase the temperatures at its outlets to the same extent. To execute the HENS, it suffices to take into account only any stream spanning a divider and a separator or a divider and a mixer. Figure 4, constructed in connection with the first example to be elaborated later, illustrates a hot stream and a cold stream that can possibly be the sources of sensible heat (i.e., candidate streams). Obviously, if the inlet and outlet temperatures of any of them are identical, this stream's heat content is zero, and the stream is ignored. The temperatures in the superstructure are defined by the input parameters, including the temperatures of the feed; inlet, top, and bottom product streams of separators; and the temperatures of the sources of latent heat of each separator.

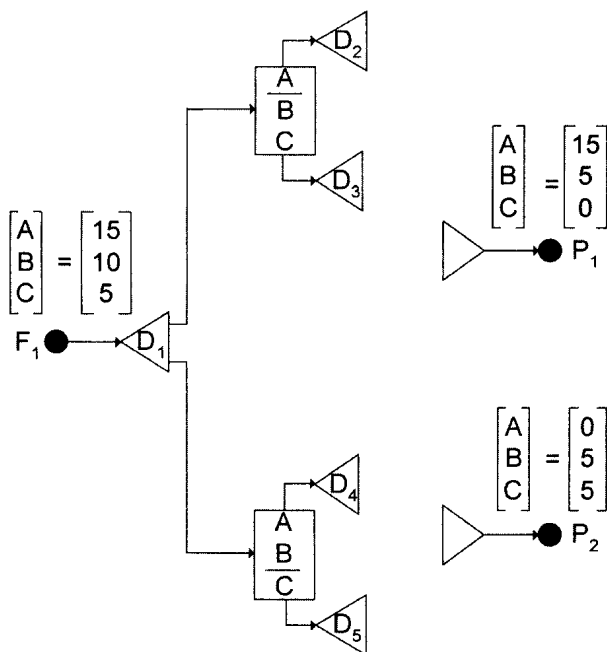


Figure 2 Generation of the superstructure for the first example: Steps 3-5; iteration 1.

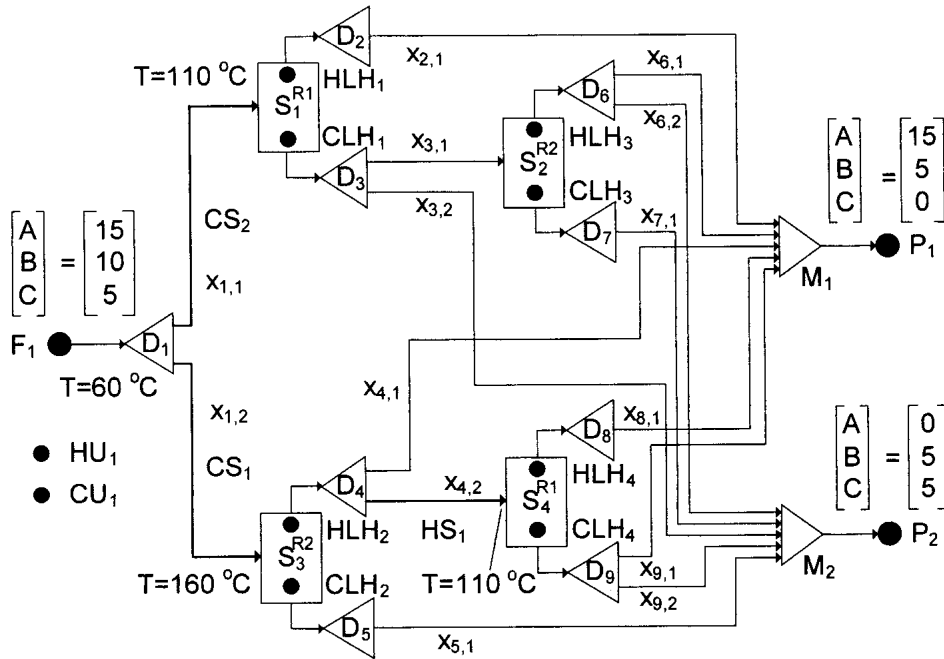


Figure 3 Superstructure and the sources of sensible and latent heats for the first example.

The temperature of a product stream is calculated from the temperatures and flowrates of the bypass streams subsequent to the determination of the optimal structure. A bypass stream is defined as a stream that terminates at a mixer. The entering temperature of a bypass stream is defined by the product temperature of a separator or by the temperature of a feed stream, while the terminating temperature of a bypass stream can vary between its entering and ambient temperatures, both of which are input parameters. The regular stream differs from a bypass stream in that the former must reach its terminating temperature while the latter may remain invariant. The heat content of a bypass stream should be exploited whenever appropriate. For instance, if the heat content of a hot-bypass stream can be transferred to a cold stream, this bypass stream will be involved in the HEN; otherwise, it will only change the temperature of the prod-

uct. Obviously, matching two bypass streams would invariably increase the cost.

Note that not all the candidate streams are generally included in the optimal structure. If the flowrate of a candidate stream in the resultant optimal structure is zero, so is its heat content, according to Eq. (1). As such, no stream can be matched with this candidate stream.

A latent heat source releases or absorbs heat without temperature change. The heat contents of the sources of latent heat are the consequences of phase change (e.g., boiling, condensation, or chemical reactions). In contrast, the heat contents of the sources of sensible heat (e.g., streams) are due to their temperature changes. A source of latent heat can be regarded as a stream with identical entering and terminating temperatures. The sources of latent heat are common in distillation columns.

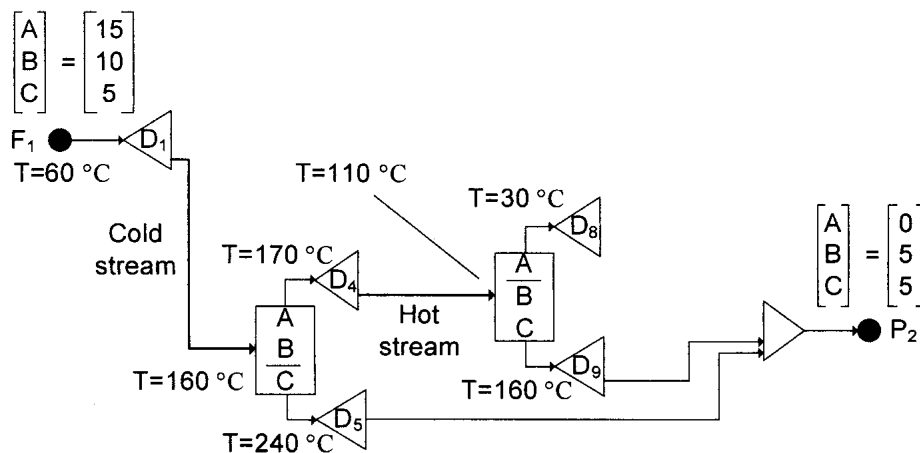


Figure 4 Illustration of the identification of candidate streams for the first example.

The reboiler of a distillation column is a negative source (i.e., sink) of the latent heat and vice versa for the condenser of a distillation column. Naturally, the reboiler and condenser within the same distillation column can not be integrated: the reboiler needs the heat at a higher temperature than that supplied by the condenser. In general, a separator can contain any number of latent heat sources; for example, a distillation column with a side column accommodates an additional condenser, while a flash unit has only a single hot latent heat source. The rate of heat release or absorption per unit time, or simply the heat content,  $q_{lh_g}$ , of a given latent heat source, can be calculated from the load of the separator,  $f_{ij}$ , containing the latent heat source and the heat parameter of this latent heat source,  $PLH_g$ . The latter corresponds to the heat content of the latent heat source if the load of the separator is unity. The heat parameter is positive for a heat source and negative for a heat sink.  $f_{ij}$  is the flowrate of the stream entering into the separator.  $q_{lh_g}$  can be calculated as

$$q_{lh_g} = PLH_g f_{ij} \quad (2)$$

The types and heat parameters of the latent-heat sources of a separator are given as part of the input for the separator. The superstructure of the problem contains the candidate separators explicitly; therefore, the candidate sources of latent heat can be readily enumerated. If the inlet flowrate of a separator is determined to be negligible, the separator is inevitably excluded from the optimal structure; as a result, its latent heat sources do not come into play in heat integration.

Although the heat integration of a separation network in itself is of utmost importance, it should not be neglected for other sectors of a process plant where heat exchanges occur. The proposed method is capable of taking into account the sources of both sensible and latent heats that are external to the superstructure. This renders it possible to perform the HENS for the entire plant. These sources of sensible and latent heats must be listed in the input along with their characteristics.

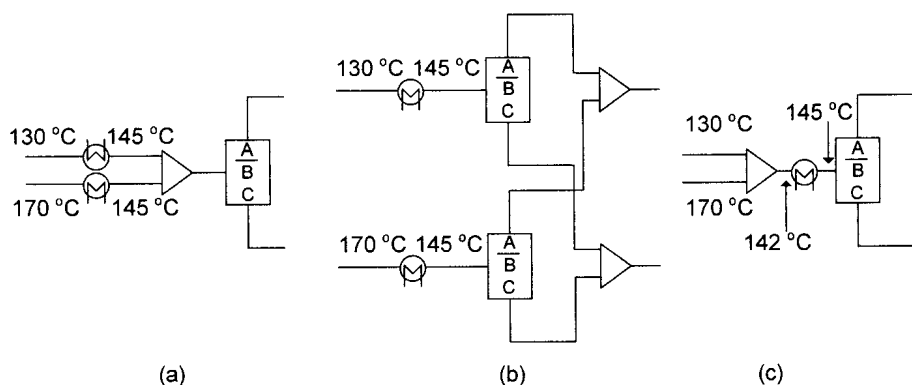
Utilities are generally regarded as sources of latent heat in this work. The hot utilities supply the extra heat to the system, and the cold utilities extract the surplus heat from it. The proposed method can accommodate a multitude of hot and cold utilities. The available utilities are also listed in the input along with their

pertinent information, including the type, cost coefficient, and temperature.

The majority of conventional methods considers only the sources of latent heat and ignores the sources of sensible heat in integrated syntheses of SN and HEN (see, e.g., [1, 3]). Naturally, ignoring the sensible heat sources would lower the thermal efficiency and increase the cost of the resultant network. Moreover, the separators are almost always regarded as simple distillation columns in the conventional SNS. Each simple distillation column contains one condenser and one reboiler; only the condensers and reboilers of the distillation columns in the SN are to be involved in the integrated syntheses. Disregarding the hot and cold streams, however, drastically simplifies the problem: it reduces the number of the heat transfer variables because of the drastic reduction in the numbers of the heat sources and sinks that need to be taken into account. The LMTDs can be simply calculated as the differences of the fixed temperatures of the reboilers and the condensers, thereby eliminating the sources of nonlinearity.

The proposed method implicitly invokes an assumption that only isothermal mixing is allowed except in the final mixers. This assumption is the consequence of the statement in the preceding section, "Each instance of the class of SNS problems of interest gives rise to such a loopless optimal network, in which mixers are attached only to the output streams." The proof of the statement contains a step that transforms the configuration depicted in Figure 5a into that in Figure 5b. This transformation does not alter the cost of the network if the cost of a separator is linear and only isothermal mixing is allowed; as such, the heat loads of the heat exchangers remain invariant. If non-isothermal mixing is allowed and one of the input streams to the mixer is hot and the other is cold, as illustrated in Figure 5c, then the temperatures of the two streams vary in the mixer without a heat exchanger, thereby lowering the cost below those in Figures 5a and 5b. Nevertheless, the assumption might not be unduly restrictive; the examples in the literature are largely void of non-isothermal mixing in the resultant optimal structures.

With all the candidate sources of sensible and latent heats selected (see Figure 3 constructed in connection with the first example to be elaborated later), the possible heat exchanges must



**Figure 5** Illustration of the possible heat transfers in the presence or absence of a mixer prior to separation: (a) isothermal mixing; (b) no mixer; (c) non-isothermal mixing.

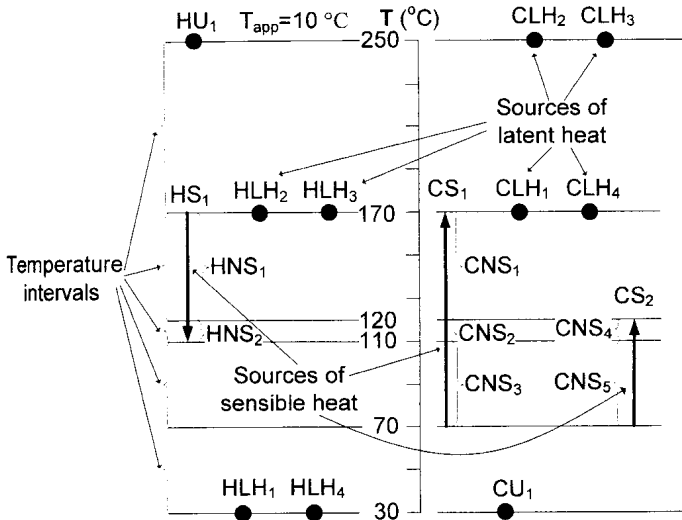


Figure 6 Component streams in the temperature interval diagram for the first example.

be exhaustively identified. First, a temperature interval diagram is constructed. It contains all the streams and sources of latent heat. The cold streams are shifted upward with the minimum approach temperature,  $\Delta T_{app}$ ; this value is selected to be 10°C throughout the current work. The inlet and outlet temperatures of the streams and the temperatures of the latent heat sources are sorted in the increasing order. Every pair of two adjacent temperatures from the resulting list defines a temperature interval.

The temperature intervals divide the streams into the component streams; see Figure 6 constructed in connection with the first example to be elaborated later. If a pair of hot and cold component streams is to be matched and the heat content of the hot component stream is less than that required by the cold component stream, the latter must be split into two. The first part is matched with the given hot component stream, and the second part is matched with another hot source (see Figure 7).

The cost of the heat exchanger between hot component stream  $e$  and cold component stream  $g$  is calculated as

$$Cost = \frac{B_{eg}}{U_{eg} (LMTD_{eg})} q_{eg} \quad (3)$$

where  $B_{eg}$  denotes the cost of unit heat transfer area;  $U_{eg}$ , the heat transfer coefficient;  $q_{eg}$ , the rate of heat transferred between  $e$  and  $g$ ; and  $LMTD_{eg}$ , the logarithmic mean temperature difference. The heat transfer coefficient,  $U_{eg}$ , depends on the nature of the two materials passing through the heat exchanger.

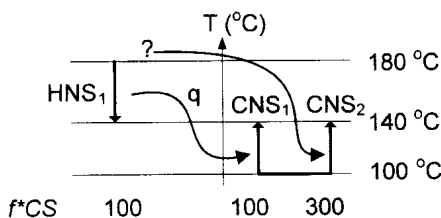


Figure 7 Illustration of the split component stream in the temperature interval diagram.

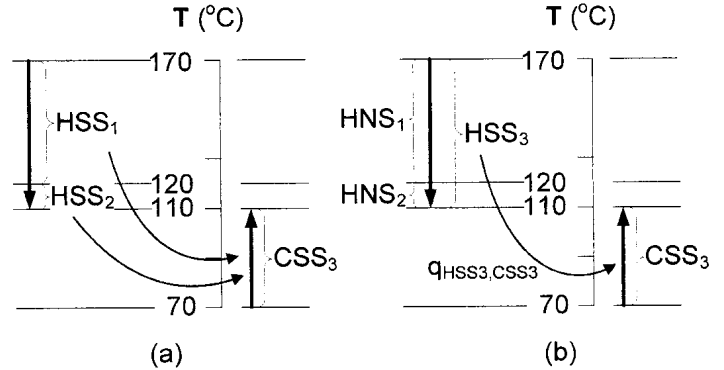


Figure 8 Illustration of the heat transfers from a stream: (a) with two heat exchangers; (b) with one heat exchanger.

the flowrates of these materials through the heat exchanger, and the geometry of the heat exchanger. It is possible to estimate uniquely  $U_{eg}$  for each heat exchange subsequent to the construction of the superstructure.

$LMTD_{eg}$  is calculated as

$$LMTD_{eg} = \begin{cases} \frac{x-y}{\ln(\frac{x}{y})} & \text{if } x \neq y \\ x & \text{otherwise} \end{cases} \quad (4)$$

where

$$x = T_{e,in} - T_{g,out}$$

$$y = T_{e,out} - T_{g,in}$$

This equation is nonlinear, and thus the cost of two adjacent heat exchangers on the same stream will differ from the cost of a merged heat exchanger (see Figure 8, constructed for the first example to be elaborated later). This leads to the notion of composite streams in Figure 9. A composite stream comprises adjacent component streams, all on a single stream. Figure 10, constructed for the first example to be elaborated later, illustrates the definition of six composite streams on cold stream 1 ( $CS_1$ ), which is divided into three component streams initially. Upon the generation of the composite streams, the heat transfer variables

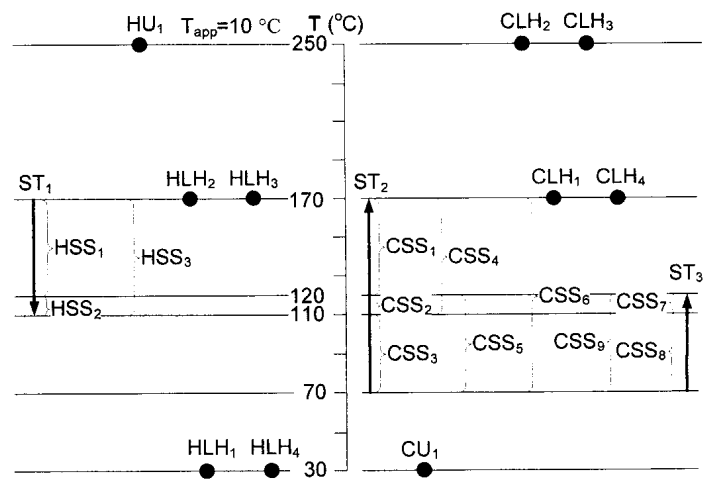


Figure 9 Composite streams in the temperature interval diagram for the first example.

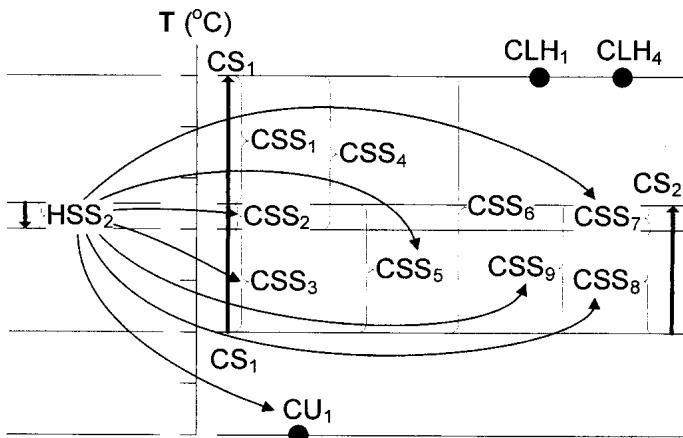


Figure 10 Feasible heat transfers from hot composite stream 2 for the first example.

are assigned to every feasible match of a heat source and heat sink except that between hot and cold utilities.

A match is feasible if it obeys the second law of thermodynamics; accordingly, heat can be transferred only from a hotter spot to a colder one. Hence, the inlet temperature of the heat source must be greater than or equal to the sum of the outlet temperature of the heat source and the minimum approach temperature,  $\Delta T_{ap}$ . This is also the case between the outlet temperature of the heat source and the inlet temperature of the heat sink (see Figure 10). Nevertheless, the inlet and outlet temperatures are equal for each source of latent heat and every utility.

Obviously, the number of composite streams and heat transfer variables is far greater than the number of component streams. The definition of composite streams, however, renders it possible to estimate the cost of the optimal network with increasing accuracy. The main advantage of the proposed method is that the LMTDs can be evaluated prior to generating the mathematical model. As a result, non-linearity is eliminated from the formalism.

## MATHEMATICAL MODEL

Even when all the cost functions are linear, any of the conventional methods of the integrated SN and HEN syntheses results in nonlinear mathematical models; moreover, they mostly contain binary or integer variables. The solutions of such models tend to be highly cumbersome. In fact, finding an initial feasible structure is already a challenging task. The convergence of the solution procedure is usually slow; furthermore, it is difficult to ascertain if the optimal solution has been reached when the procedure terminates or how far the point of termination is from the optimal solution. It is therefore desirable to devise a linear mathematical model that gives rise to a linear programming model (LP). For optimization, various robust and efficient solvers are available for executing LPs; such solvers are capable of solving LPs with a large number variables exceeding tens or even hundreds of thousands, and the average solution time is a polynomial function of the number of variables. Naturally, a

trade-off exists between the size and complexity of the mathematical model. The current model gives rise to an exceedingly large number of variables as the consequences of the large size of the superstructure as well as the large number of composite streams.

The current model is formulated in terms of the feed allocation ratio,  $x_{ij}$ , and the heat transfer rate,  $q_{ef}$ . The feed allocation ratio,  $x_{ij}$ , represents the fraction of the flowrate of the feed stream in the network in outlet  $j$  from divider  $i$ . For the divider of the feed stream to the network, the feed allocation ratio and the corresponding splitting ratio are identical. In general, however, the former differs from the latter: for any given divider, the sum of the splitting ratios of its outlets is unity; in contrast, the sum of the feed allocation ratios of its outlets is equal to the feed allocation ratio of its inlet. The heat transfer rate,  $q_{ef}$ , is the rate of heat exchange between heat source  $e$  and heat sink  $f$ .

The mathematical model is constructed based on the superstructure and the feasible matches identified. This entails the definition of the following basic sets:  $C$ , the set of components;  $FS$ , the set of feeds;  $P$ , the set of products;  $D$ , the set of dividers;  $M$ , the set of mixers;  $S$ , the set of separators;  $AR$ , the set of arcs of the superstructure;  $HNS$ , the set of hot component streams;  $HBS$ , the set of hot component streams of the bypass streams;  $HSS$ , the set of hot composite streams;  $HLH$ , the set of hot latent heats;  $HU$ , the set of hot utilities;  $CNS$ , the set of cold component streams;  $CBS$ , the set of cold component streams of the bypass streams;  $CSS$ , the set of cold composite streams;  $CLH$ , the set of cold latent heats; and  $CU$ , the set of cold utilities. In addition, the following sets must be defined:  $HSLU = HSS \cup HLH \cup HU$ ;  $CSLU = CSS \cup CLH \cup CU$ ;  $FM_e = \{f \in CSLU \mid \text{heat transfer is feasible between } e \text{ and } f\}$  for each  $e \in HSLU$ ; and  $FM_f = \{e \in HSLU \mid \text{heat transfer is feasible between } e \text{ and } f\}$  for each  $f \in CSLU$ . The superstructure can be described unambiguously as

$$\delta(k, i, c) = \begin{cases} 1 & \text{when a path exists between nodes } k \text{ and } i \\ & \text{which contains } c \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

where

$$\begin{aligned} k &\in FS \\ i &\in D \\ c &\in C. \end{aligned}$$

The flowrate of stream  $(i, j)$ ,  $f_{ij}$ , can be calculated as

$$f_{ij} = x_{ij} \sum_{\{(k,c) \in FE \times C : \delta(k,i,c)=1\}} FE_{kc} \quad \forall i \in D, \quad \forall j \in M \cup S \quad (6)$$

where  $FE_{kc}$  is the flowrate of component  $c$  in feed stream  $k$ . It is worth noting that a path exists from only one feed stream to stream  $(i, j)$ ; the summation operates only on this feed stream. One or more separators reside between the selected feed stream and stream  $(i, j)$ ; the summation operates only on those  $FE_{kc}$  for which  $c$  is present in  $(i, j)$ . Multiplying the sum of the selected  $FE_{kc}$  values with  $x_{ij}$  yields  $f_{ij}$ , appearing in Eqs. (1) and (2).

The aforementioned definition of the sets and variables renders it possible to formulate the mathematical model of the problem as follows:



Minimize

$$\sum_{\{s \in S: \exists i(i.s) \in AR\}} \left( OC_s x_{is} + \sum_{\{(k,c): k \in F, c \in C, \delta(k,i,c)=1\}} FE_{kc} \right) + \sum_{\substack{e \in HSLU \\ g \in FM_e}} \frac{B_{eg}}{U_{eg} LMTD_{eg}} q_{eg} + \left( \sum_{\substack{e \in HTU \\ g \in FM_e}} CCU_e q_{eg} + \sum_{\substack{g \in CU \\ e \in FM_g}} CCU_g q_{eg} \right) \quad (7)$$

subject to

$$\sum_{\{j:(i,j) \in AR\}} x_{ij} = 1 \quad \forall i \in D \quad (8)$$

where

$$\exists k \in FS$$

such that  $(k, i) \in AR$

$$\sum_{\{j:(i,j) \in AR\}} x_{ij} = x_{si} \quad \forall i \in D \quad (9)$$

where

$$\exists k \in FS$$

such that  $(k, i) \notin AR$

$$\sum_{\{(i,m) \in A: (m,q) \in A, \exists k(\delta(k,i,c)=1)\}} (x_{im} FE_{kc}) = PR_{qc} \quad \forall q \in P \text{ and } \forall c \in C \quad (10)$$

$$0 = qns_n - \sum_{\{\forall e \in HSS: n \subseteq e\}} \left( R_{ne} \left( \sum_{g \in FM_e} q_{eg} \right) \right) \quad \forall n \in HNS \quad (11)$$

$$0 = qns_n + \sum_{\{\forall e \in HSS: n \subseteq g\}} \left( R_{ng} \left( \sum_{e \in FM_g} q_{eg} \right) \right) \quad \forall n \in CNS \quad (12)$$

$$0 \leq qns_n - \sum_{\{\forall e \in HSS: n \subseteq e\}} \left( R_{ne} \left( \sum_{g \in FM_e} q_{eg} \right) \right) \quad \forall n \in HBS \quad (13)$$

$$0 \geq qns_n + \sum_{\{\forall e \in HSS: n \subseteq g\}} \left( R_{ng} \left( \sum_{e \in FM_e} q_{eg} \right) \right) \quad \forall n \in CBS \quad (14)$$

$$0 = qlh_e - \sum_{g \in FM_e} q_{eg} \quad \forall e \in HLH \quad (15)$$

$$0 = qlh_g + \sum_{e \in FM_g} q_{eg} \quad \forall g \in CLH \quad (16)$$

$$0 \leq x_{ij} \quad \forall (i, j) \in AR, \text{ where } i \in D \quad (17)$$

$$0 \leq q_{eg} \quad e \in HSLU, g \in CSLU \quad (18)$$

The model comprises four parts, including the objective function (Eq. [7]), material balances (Eqs. [7–10]), heat balances (Eqs. [11–16]) and non-negativity constraints, (Eqs. [17] and [18]). The objective function consists of three terms. The first term signifies the costs of separators. The cost of an individual separator is considered to be proportional to the flowrate of the stream to be separated; thus, it can be calculated by multiplying the flowrate of the inlet stream of the separator with the overall cost coefficient of the separator. The overall cost coefficient depends on the degree of difficulty of separation and the cost coefficient. The second term represents the cost of the heat transfer, which corresponds to the annualized capital costs of the heat exchangers. The cost of any heat exchanger is given by Eq. (3), in which only  $q_{eg}$  is a variable. The third term accounts for the utility cost. The costs of utilities depend on the temperature of the heat they supply or withdraw. The cost coefficients of the utilities,  $CCU$ , are input parameters.

Equations (8) and (9) are the material balances around dividers. These equations for material balances are originally expressed in terms of component flowrates; subsequently, they are simplified via Eq. (6). Equation (8) is for the divider linked to the feed stream, and Eq. (9) is for any of the remaining divider. Figure 11 illustrates two dividers and the corresponding material balance equations. Equation (10) expresses the material balance for component  $c$  of product  $q$ . Note that the required component flowrate, which is an input parameter, is on the right-hand side, and the component flowrates of those streams, which are fed into the mixer yielding product  $q$  and containing component  $c$ , are on the left-hand side. Figure 12 illustrates the material balance of mixer 1 for component B. Note that it is not always necessary to define the products in terms of their exact compositions; instead, we can specify the products by various constraints imposed on their components (e.g., the sum of the components and the ratios of the components). Material balances are not explicitly required for separators because the feed allocation ratios at the inlet and outlets of the separator remain invariant.

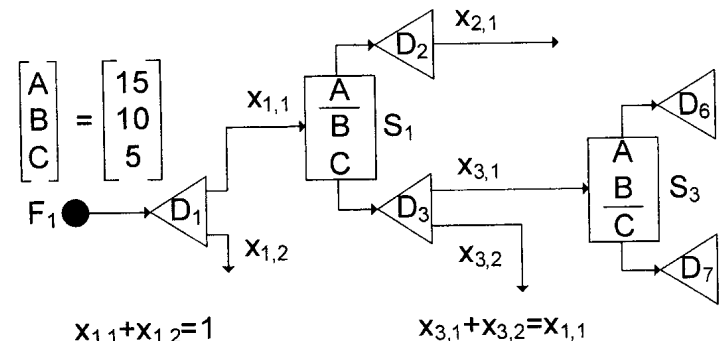


Figure 11 Illustration for the material balances.

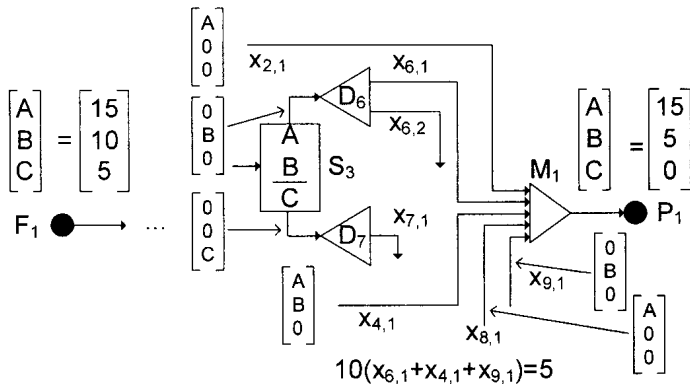


Figure 12 Illustration for the product constraint.

Equations (11) and (12) signify heat balances for the hot and cold component streams, respectively. The fulfillment of heat requirements by all the component streams implies the same by the streams comprising these component streams. Equation (11) and (12) express that the heat content of a component stream must be equal to the heat provided or withdrawn by the heat exchangers. The term  $q_{ns}$  denotes the heat content of component stream  $n$ , which can be calculated from Eq. (1). As indicated earlier, the specific heat of any stream can be calculated as the weighted average of the specific heats of the components based on their concentrations under the assumption that the stream is an ideal mixture of its components (see Figure 13). Otherwise, they are estimated individually after the generation of the superstructure. The term,  $n \subseteq e$ , implies that composite stream  $e$  contains component stream  $n$ . A heat exchanger can span over several component streams, but only the heat content of component stream  $n$  is accounted in each instance of Eqs. (11) and (12). In these equations,  $R_{ne}$  expresses the portion of  $q_{ef}$  contributed by component stream  $n$ . Its value can be readily calculated as the ratio of the heat contents of component stream  $n$  and composite stream  $e$ . The ratio of the heat contents can be simplified so that  $R_{ne}$  is equal to the ratio of the temperature range of component stream  $n$  and composite stream  $e$ , as in  $R_{HS2,HS3} = (120-110)/(170-110)$  in Figure 8.

Equations (13) and (14) represent the heat balances for the component streams of the bypass streams. They are expressed as inequalities: bypass streams (not always but potentially) can be involved in heat transfer.

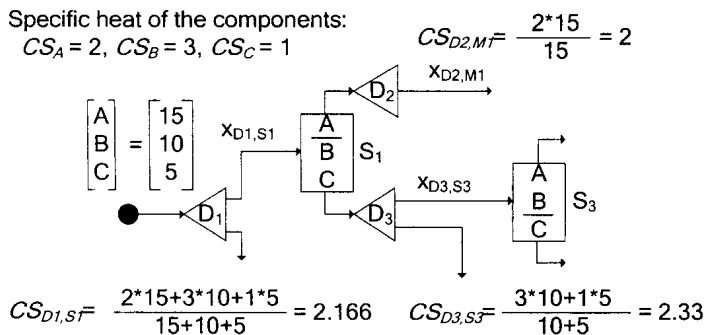


Figure 13 Calculation of the specific heats of streams.

Table 2 Cost coefficients of the heat transfer for the first example

	$HSS_1$	$HSS_2$	$HSS_3$	$HLH_2,$ $HLH_3$	$HLH_1,$ $HLH_4$	$HU_1$
$CSS_1$	0.6667			0.2389		0.0589
$CSS_2$	0.1831	0.6667	0.2389	0.1028		0.0460
$CSS_3$	0.1028	0.2036	0.1122	0.0753		0.0394
$CSS_4$	0.4621		0.6667	0.2162		0.0568
$CSS_5$	0.1111	0.2682	0.1215	0.0808		0.0407
$CSS_6$	0.2389		0.2682	0.1599		0.0498
$CSS_7$	0.1831	0.6667	0.2389	0.1028		0.0460
$CSS_8$	0.1028	0.2036	0.1122	0.0753		0.0394
$CSS_9$	0.1111	0.2682	0.1215	0.0808		0.0407
$CLH_2, CLH_3$						0.6667
$CLH_1, CLH_4$				0.6667		0.0741
$CU_1$	0.0541	0.0702	0.0568	0.0444	0.6667	0.0290

Equations (15) and (16) signify heat balances for the hot and cold latent heats, respectively. The term  $qlh_e$  denotes the heat content of latent heat  $e$ ; it can be calculated from Eq. (2).

Lastly, Eqs. (17) and (18) impose non-negativity constraints on all model variables—obviously, neither the flowrates nor the heat transfer rates can be negative.

EXAMPLES

The first example illustrates the procedure and demonstrates the efficacy of the proposed method. This simple example involves one feed and two product streams, three components, one hot and one cold utility and two separators of the same type. Table 1 lists the data pertinent to the example. Some of

Table 3 Data pertaining to the components, streams, utilities, and heat exchangers for the second example

Component and stream					
Name	$F_1$ (kg/s)	$P_1$ (kg/s)	$P_2$ (kg/s)	$P_3$ (kg/s)	Specific heat (kJ/[kg°C])
A	10	8	2	0	2
B	12	0	5	7	3
C	30	15	5	10	5
D	20	10	5	5	4
E	18	6	6	6	3
Utility					
Type	T (°C)		Cost (\$/[kW s])		
High-pressure steam	250		0.8		
Medium-pressure steam	200		0.2		
Cooling water	20		0.085		
Heat exchanger					
$\Delta T_{app}$					10°C
B					0.9 \$/(m <sup>2</sup> s)
U					0.1 kW/(m <sup>2</sup> °C)

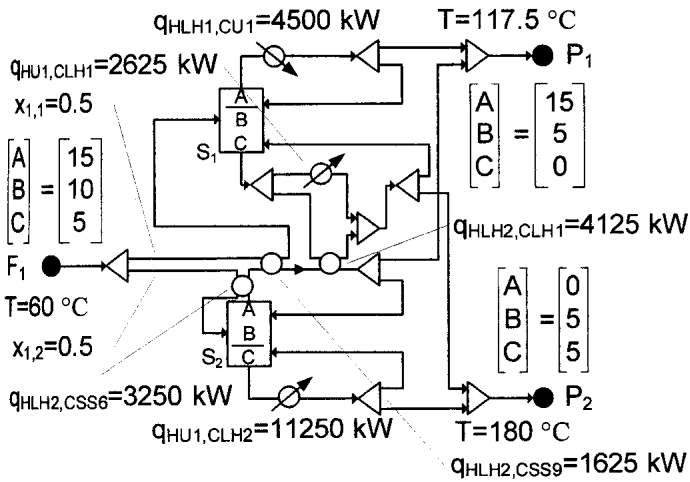


Figure 14 Optimal solution structure for the first example.

the pertinent data are also indicated on Figure 1. The first step of the procedure constructs the superstructure according to the proposed algorithm. The second step identifies the sources of sensible and latent heats. For simplicity, the heat contents of the bypass streams are disregarded. Figure 3 exhibits the superstructure along with the streams, sources of latent heat, and utilities, which are identified. Altogether, the dividers in the superstructure have fourteen outputs, thereby entailing the specification of fourteen feed allocation ratios. Each stream is regarded as an ideal mixture of components. This renders it possible to calculate its specific heat as the weighted average of the components' specific heats based on their mass concentrations. Three hot and nine cold composite streams are defined based on the temper-

ature intervals and the one hot and two cold streams. Four hot and four cold latent heat sources are contained in the superstructure. Altogether, 111 feasible matches are identified between the heat sources and sinks; therefore, the same number of variables representing the heat transfer rates is defined, and the corresponding values of LMTDs and cost coefficient for the heat transfer area,  $CH_{eg}$ , are calculated (see Table 2). The third step formulates the mathematical model. The resultant model consists of thirty constraints along with the objective function. The fourth step solves the resultant LP model on a PC (AMD-XP 2GHz); it has yielded the optimal objective function value of 190,871 in 0.9s. Figure 14 illustrates the optimal structure and the value of the non-zero variables; it also indicates the calculated temperatures of the product streams. Moreover, the figure shows that the condenser of  $S_2$  preheats the streams fed to the separators and provides part of the heat required by the reboiler of  $S_1$ ; meanwhile, the remaining part is provided by the hot utility.

The integration of the SN and HEN syntheses with a sequential method (see [13]) results in a structure costing 25% more than that obtained by the proposed method. The sequential method proceeds as follows:

1. The SN is synthesized initially
2. This is followed by the identification of the sources of sensible and latent heats in the resultant SN
3. Finally, the HEN is synthesized.

Note that the sequential method differs obviously from the proposed method: in the former, two distinct models are solved sequentially; in contrast, a single comprehensive model is solved in

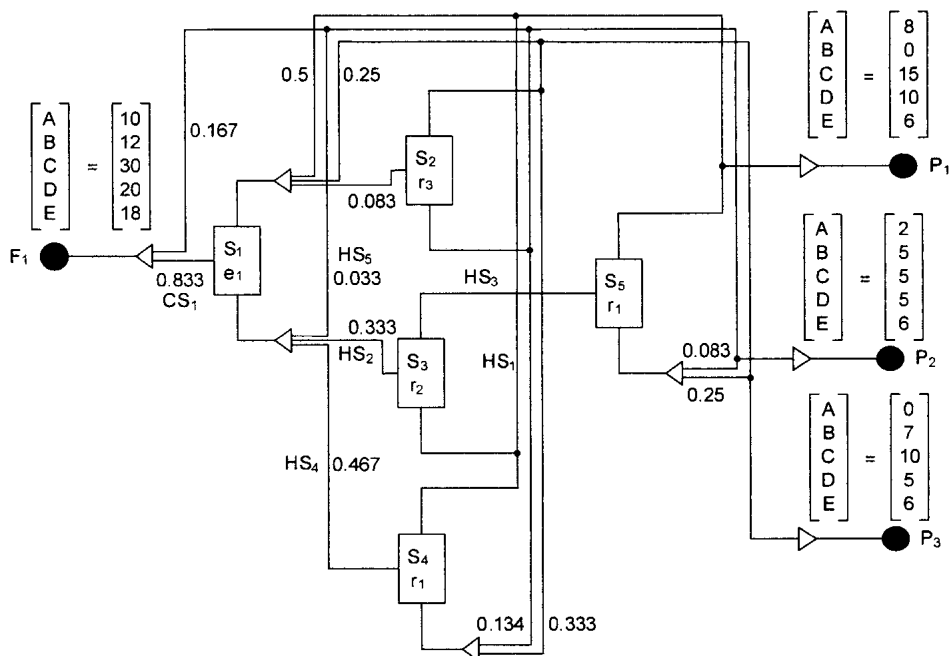


Figure 15 Optimal solution structure for the second example.

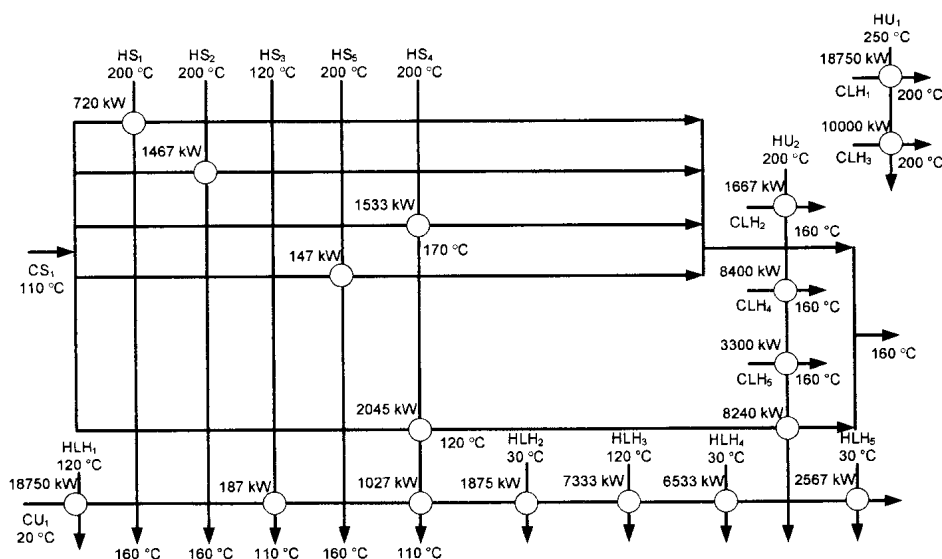


Figure 16 Grid diagram for the second example.

the latter. Both methods require the identification of the sources of sensible and latent heats; however, while the proposed method identifies the possible (i.e., candidate), sources, of which existence depends on the flowrates of streams, the sequential method identifies the sources, which are predestined to exist.

The second example features one feed and three product streams, five components, two hot and one cold utility, and five separators. Four of the separators are based on distillation, and the remaining one is based on extraction. Table 3 lists the data pertaining to the components, streams, heat-exchangers, and utilities; Table 4 contains the data pertaining to the available separators. Executing Steps 1 through 4 of the procedure for implementing the proposed method has yielded the optimal structure illustrated in Figure 15. The grid diagram in Figure 16 shows the heat exchanges occurring in the optimal structure. The solution time is sixteen minutes on a PC (AMD-XP 2 GHz), giving rise to 85,186 as the objective function. Solving the problem with the sequential method increases the cost 18%; in contrast, the solution time decreases to 15 s.

The details for solving the first example are provided in the Appendix. Moreover, the solver and the two examples are available at <http://www.des.vein.hu/capo/demo/sns/HTE-2004>.

## CONCLUSIONS

The current work addresses for the first time the integrated syntheses of SN and HEN, in which separators based on different separation methods effected by various physical or chemical properties are involved. A systematic procedure is proposed for constructing the superstructure. The resultant superstructure renders it possible to identify the candidate sources of sensible and latent heats. The variables in terms of the feed allocation ratios are assigned to the outputs of the dividers in the superstructure and those in terms of the heat transfer rates to the feasible matches for heat exchangers. Subsequently, a single, comprehensive mathematical programming model is formulated; its solution determines the optimally integrated SN and HEN.

Unlike any available method for the heat integrated synthesis of SN, the proposed method takes into account the sources of both sensible and latent heats. The mathematical model of the proposed method is linear, thereby assuming the attainment of the global optimum.

## NOMENCLATURE

### Basic Sets

AR	arcs
C	components
CBS	cold component streams of the bypass streams
CLH	cold latent heats
CNS	cold component streams
CS	cold streams
CSS	cold composite streams
CU	cold utilities
D	dividers
FS	feeds

Table 4 Data pertaining to the available separators for the second example

Separator	Component		$T_{in}$ (°C)	$PLH_c$ (kJ/kg)	$T_c$ (°C)	$PLH_r$ (kJ/kg)	$T_r$ (°C)	OC (\$/kg)
	Top	Bottom						
S1	A	B, C, D, E	110	350	30	-450	160	850
S2	A, B	C, D, E	160	550	120	-750	200	120
S3	A, B, C	D, E	120	450	30	-400	160	1150
S4	A, B, C, D	E	120	400	30	-600	200	290
E1	C, D	A, B, E	160	250	120	-250	200	40

<i>HBS</i>	hot component streams of the bypass streams
<i>HLH</i>	hot latent heats
<i>HNS</i>	hot component streams
<i>HS</i>	hot streams
<i>HSS</i>	hot composite streams
<i>HU</i>	hot utilities
<i>M</i>	mixers
<i>P</i>	products
<i>S</i>	separators

**Other Sets**

<i>CSLU</i>	$CSS \cup CLH \cup CU$
$FM_e$	set of those $g \in CSLU$ for which heat transfer is feasible between $e$ and $g$ , $e \in HSLU$
$FM_g$	set of those $e \in HSLU$ for which heat transfer is feasible between $e$ and $g$ , $g \in CSLU$
<i>HSLU</i>	$HSS \cup HLH \cup HU$

**Parameters**

$B_{eg}$	unit cost of heat transfer area, $e \in HSLU$ , $g \in CSLU$ , $\$/(\text{m}^2 \text{ s})$
$CCU_e$	cost coefficient of utility $e$ , $\$/(\text{kW s})$
$CH_{eg}$	cost coefficient of heat transfer $q_{eg}$ , $e \in HSLU$ , $g \in CSLU$ , $\$/(\text{kJ})$
$CS_c$	specific heat of component $c$ , $\text{kJ}/(\text{kg } ^\circ\text{C})$
$CS_{ij}$	specific heat of stream, $(i, j) \in D \times (M \cup S)$ , $\text{kJ}/(\text{kg } ^\circ\text{C})$
$\Delta T_{ap}$	approach temperature, $^\circ\text{C}$
$FE_{kc}$	flowrate of component $c$ in feed stream $k$ , $\text{kg}/\text{s}$
$LMTD_{eg}$	logarithmic mean temperature difference, $e \in HSLU$ , $g \in CSLU$ , $^\circ\text{C}$
$OC_s$	overall cost coefficient for separator $s$ , $\$/\text{kg}$
$PLH_g$	heat parameter of the source of latent heat $g$ , $\text{kJ}/\text{kg}$
$PR_{qc}$	flowrate of component $c$ in product stream $k$ , $\text{kg}/\text{s}$
$R_{ne}$	ratio of component stream $n$ and composite stream $e$
$T$	temperature, $^\circ\text{C}$
$U_{eg}$	heat transfer coefficient, $e \in HSLU$ , $g \in CSLU$ , $\text{kW}/(\text{m}^2\text{ } ^\circ\text{C})$

**Variables**

$f_{ij}$	total flowrate of stream, $(i, j) \in D \times (M \cup S)$ , $\text{kg}/\text{s}$
$q_{eg}$	heat transfer variable, $e \in HSLU$ , $g \in CSLU$ , $\text{kW}$
$qlh_g$	heat content of source of latent heat $g$ , $\text{kW}$
$qns_e$	heat content of component stream $e$ , $\text{kW}$
$x_{ij}$	feed allocation ratio, $i \in D$ , $j \in M \cup S$

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**APPENDIX****Details of the First Example**

The superstructure has been constructed from the operating units given in Figure 1, according to the procedure described in Steps 1 through 5 of Section 2 of the text. Figure 3 depicts the resultant superstructure. This superstructure makes it possible to identify the sources of sensible and latent heats. Each feed allocation ratios,  $x_{ij}$ , is indexed by two subscripts. The first subscript,  $i$ , indicates that it belongs to divider  $i$  on the superstructure, and the second subscript,  $j$ , signifies that it is the  $j$ th outlet from the top of this divider. For example,  $x_{3,2}$  is assigned

to the second outlet of divider 3, as shown in Figure 3. The same figure indicates that

$$FS = \{F_1\}$$

$$P = \{P_1, P_2\}$$

$$D = \{D_1, D_2, D_3, D_4, D_5, D_6, D_7, D_8, D_9\}$$

$$M = \{M_1, M_2\}$$

$$S = \{S_1, S_2, S_3, S_4\}$$

$$AR = \{(F_1, D_1), (D_1, S_1), (D_1, S_3), (S_1, D_2), (S_1, D_3), \\ (S_3, D_4), (S_3, D_5), (D_3, M_2), (D_3, S_2), (D_3, M_2), \\ (D_2, M_1), (D_9, M_1), (D_9, M_2), (D_6, M_1), (D_6, M_2), \\ (S_2, D_6), (S_2, D_7), (S_4, D_8), (S_4, D_9), (D_5, M_2), (D_4, M_1), \\ (D_4, S_4), (D_8, M_1), (D_7, M_2), (M_1, P_1), (M_2, P_2)\}$$

Subsequently, the component and composite streams are created from the sources of sensible heat (see Figures 6 and 9). For simplicity, the heat contents of the bypass streams are disregarded in this example, thus reducing the size of the problem. The feasible matches of the sources and sinks are determined based on the second law of thermodynamics, requiring that heat transfer occurs only if the temperature of the source is at least the temperature of the sink plus  $\Delta T_{ap}$ . The resultant matches are:

$$FM_{HSS1} = \{CSS_1, CSS_2, CSS_3, CSS_4, CSS_5, \\ CSS_6, CSS_7, CSS_8, CSS_9, CU_1\}$$

$$FM_{HSS2} = \{CSS_2, CSS_3, CSS_5, CSS_7, CSS_8, CSS_9, CU_1\}$$

$$FM_{HSS3} = \{CSS_2, CSS_3, CSS_4, CSS_5, CSS_6, \\ CSS_7, CSS_8, CSS_9, CU_1\}$$

$$FM_{HLH1} = \{CU_1\}$$

$$FM_{HLH2} = \{CSS_1, CSS_2, CSS_3, CSS_4, CSS_5, \\ CSS_6, CSS_7, CSS_8, CSS_9, CLH_1, \\ CLH_4, CU_1\}$$

$$FM_{HLH3} = \{CSS_1, CSS_2, CSS_3, CSS_4, CSS_5, CSS_6, \\ CSS_7, CSS_8, CSS_9, CLH_1, CLH_4, CU_1\}$$

$$FM_{HLH4} = \{CU_1\}$$

$$FM_{HU1} = \{CSS_1, CSS_2, CSS_3, CSS_4, CSS_5, CSS_6, \\ CSS_7, CSS_8, CSS_9, CU_1\}$$

$$FM_{CSS1} = \{HSS_1, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS2} = \{HSS_1, HSS_2, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS3} = \{HSS_1, HSS_2, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS4} = \{HSS_1, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS5} = \{HSS_1, HSS_2, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS6} = \{HSS_1, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS7} = \{HSS_1, HSS_2, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS8} = \{HSS_1, HSS_2, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CSS9} = \{HSS_1, HSS_2, HSS_3, HLH_2, HLH_3, HU_1\}$$

$$FM_{CLH1} = \{HLH_2, HLH_3, HU_1\}$$

$$FM_{CLH2} = \{HU_1\}$$

$$FM_{CLH3} = \{HU_1\}$$

$$FM_{CLH4} = \{HLH_2, HLH_3, HU_1\}$$

$$FM_{CU1} = \{HSS_1, HSS_2, HSS_3, HLH_1, HLH_2, HLH_3, \\ HLH_4, HU_1\}$$

The terms calculated in what follows appear in the mathematical model. For instance,  $qns_{HNS1}$  and  $R_{HNS1,HSS3}$  are in Eq. A6.1, and  $qlh_{CLH1}$  is in Eq. A9.1.

$$CS_{D4,S4} = CS_{HNS1} = CS_{HNS2} = (15*2 + 3*10)/(15 + 10) \\ = 2.4$$

$$CS_{D1,S3} = CS_{CNS1} = CS_{CNS2} = CS_{CNS3} = (15*2 + 3*10 \\ + 1*5)/(15 + 10 + 5) = 2.166$$

$$CS_{D1,S1} = CS_{CNS4} = CS_{HNS5} = (15*2 + 3*10 + 1*5)/ \\ (15 + 10 + 5) = 2.166$$

$$qns_{HNS1} = 2.4(x_{4,2}(15 + 10))(170 - 120) = 3000x_{4,2}$$

$$qns_{HNS2} = 2.4(x_{4,2}(15 + 10))(120 - 110) = 600x_{4,2}$$

$$\begin{aligned} qns_{CNS1} &= 2.166(x_{1,2}(15 + 10 + 5))(110 - 160) \\ &= -3250x_{1,2} \end{aligned}$$

$$\begin{aligned} qns_{CNS2} &= 2.166(x_{1,2}(15 + 10 + 5))(100 - 110) \\ &= -650x_{1,2} \end{aligned}$$

$$\begin{aligned} qns_{CNS3} &= 2.166(x_{1,2}(15 + 10 + 5))(60 - 100) \\ &= -2600x_{1,2} \end{aligned}$$

$$\begin{aligned} qns_{CNS1} &= 2.166(x_{1,1}(15 + 10 + 5))(100 - 110) \\ &= -650x_{1,1} \end{aligned}$$

$$\begin{aligned} qns_{CNS2} &= 2.166(x_{1,1}(15 + 10 + 5))(60 - 100) \\ &= -2600x_{1,1} \end{aligned}$$

$$qlh_{HLH1} = 300(x_{1,1}(15 + 10 + 5)) = 9000x_{1,1}$$

$$qlh_{HLH2} = 600(x_{3,1}(10 + 5)) = 9000x_{3,1}$$

$$qlh_{HLH3} = 600(x_{1,2}(15 + 10 + 5)) = 18000x_{1,2}$$

$$qlh_{HLH4} = 300(x_{4,2}(15 + 10)) = 7500x_{4,2}$$

$$qlh_{CLH1} = -450(x_{1,1}(15 + 10 + 5)) = -13500x_{1,1}$$

$$qlh_{CLH2} = -750(x_{3,1}(10 + 5)) = -11250x_{3,1}$$

$$qlh_{CLH3} = -750(x_{1,2}(15 + 10 + 5)) = -22500x_{1,2}$$

$$qlh_{CLH4} = -450(x_{4,2}(15 + 10)) = -11250x_{4,2}$$

$$R_{HNS1.HSS1} = (170 - 120)/(170 - 120) = 1$$

$$R_{HNS1.HSS3} = (170 - 120)/(170 - 110) = 0.833$$

$$R_{HNS2.HSS2} = (120 - 110)/(120 - 110) = 1$$

$$R_{HNS2.HSS3} = (120 - 110)/(170 - 110) = 0.166$$

$$R_{CNS1.CSS1} = (160 - 110)/(160 - 110) = 1$$

$$R_{CNS1.CSS4} = (160 - 110)/(160 - 100) = 0.833$$

$$R_{CNS1.CSS6} = (160 - 110)/(160 - 60) = 0.5$$

$$R_{CNS2.CSS2} = (110 - 100)/(110 - 100) = 1$$

$$R_{CNS2.CSS4} = (110 - 100)/(160 - 100) = 0.166$$

$$R_{CNS2.CSS5} = (110 - 100)/(110 - 60) = 0.2$$

$$R_{CNS2.CSS6} = (110 - 100)/(160 - 60) = 0.1$$

$$R_{CNS3.CSS3} = (100 - 60)/(100 - 60) = 1$$

$$R_{CNS3.CSS5} = (100 - 60)/(110 - 60) = 0.8$$

$$R_{CNS3.CSS6} = (100 - 60)/(160 - 60) = 0.4$$

$$R_{CNS4.CSS7} = (110 - 100)/(110 - 100) = 1$$

$$R_{CNS4.CSS9} = (110 - 100)/(110 - 60) = 0.2$$

$$R_{CNS5.CSS8} = (100 - 60)/(100 - 60) = 1$$

$$R_{CNS5.SS9} = (100 - 60)/(110 - 60) = 0.8$$

The values of the cost coefficient for the heat transfer area,  $CH_{eg}$ , are given in Table 2. They are calculated by substituting  $B_{eg}$ ,  $U_{eg}$ , and  $LMTD_{eg}$  into Eq. (3); the empty cell means that the corresponding heat transfer is infeasible. The superstructure, together with the calculated data, such as  $CS_{ij}$ ,  $qns_e$ ,  $qlh_g$ , and  $R_{ne}$ , and with the data indicated in Figure 1 and listed in Table 1, makes it possible to formulate a linear programming model according to expressions (7) through (18) in the text. The resultant linear programming model is in the following.

Minimize:

$$\begin{aligned} &330(15 + 10 + 5)x_{1,1} + 800(10 + 5)x_{3,1} \\ &+ 800(15 + 10 + 5)x_{1,2} + 330(15 + 10)x_{4,2} + \sum_{\substack{e \in HSLU \\ e \in FMe}} CH_{eg}q_{eg} \\ &+ 11 \sum_{g \in FM_{HU1}} q_{HU1,g} + 1.6 \sum_{e \in FM_{CU1}} q_{e,CU1} \end{aligned} \quad (A1)$$

subject to

$$x_{i,j} \geq 0 \quad \text{for all feed-allocation ratios,}$$

$$q_{eq} \geq 0 \quad \text{for all heat-transfer rates (A2)}$$

$$x_{1,1} + x_{1,2} = 1 \quad (A3)$$

$$x_{2,1} = x_{1,1} \quad (A4.2)$$

$$x_{3,1} + x_{3,2} = x_{1,1} \quad (A4.3)$$

$$x_{4,1} + x_{4,2} = x_{1,2} \quad (\text{A4.4})$$

$$x_{5,1} = x_{1,2} \quad (\text{A4.5})$$

$$x_{6,1} + x_{6,2} = x_{3,1} \quad (\text{A4.6})$$

$$x_{7,1} = x_{3,1} \quad (\text{A4.7})$$

$$x_{8,1} = x_{4,2} \quad (\text{A4.8})$$

$$x_{9,1} + x_{9,2} = x_{4,2} \quad (\text{A4.9})$$

$$15(x_{2,1} + x_{4,1} + x_{8,1}) = 15 \quad (\text{A5.1.1})$$

$$10(x_{6,1} + x_{4,1} + x_{9,1}) = 5 \quad (\text{A5.1.2})$$

$$10(x_{6,2} + x_{3,2} + x_{9,2}) = 5 \quad (\text{A5.2.2})$$

$$5(x_{7,1} + x_{3,2} + x_{5,1}) = 5 \quad (\text{A5.2.3})$$

$$0 = 3000x_{4,2} - 1 \left( \sum_{g \in FM_{HSS1}} q_{HSS1,g} \right) - 0.833 \left( \sum_{g \in FM_{HSS3}} q_{HSS3,g} \right) \quad (\text{A6.1})$$

$$0 = 600x_{4,2} - 1 \left( \sum_{g \in FM_{HSS2}} q_{HSS2,g} \right) - 0.166 \left( \sum_{g \in FM_{HSS3}} q_{HSS3,g} \right) \quad (\text{A6.2})$$

$$0 = -3250x_{1,2} + 1 \left( \sum_{e \in FM_{CSS1}} q_{e,CSS1} \right) + 0.833 \left( \sum_{e \in FM_{CSS4}} q_{e,CSS4} \right) + 0.5 \left( \sum_{e \in FM_{CSS6}} q_{e,CSS6} \right) \quad (\text{A7.1})$$

$$0 = -650x_{1,2} + 1 \left( \sum_{e \in FM_{CSS2}} q_{e,CSS2} \right)$$

$$+ 0.166 \left( \sum_{e \in FM_{CSS4}} q_{e,CSS4} \right) + 0.2 \left( \sum_{e \in FM_{CSS5}} q_{e,CSS5} \right) + 0.1 \left( \sum_{e \in FM_{CSS6}} q_{e,CSS6} \right) \quad (\text{A7.2})$$

$$0 = -2600x_{1,2} + 1 \left( \sum_{e \in FM_{CSS3}} q_{e,CSS3} \right) + 0.8 \left( \sum_{e \in FM_{CSS5}} q_{e,CSS5} \right) + 0.4 \left( \sum_{e \in FM_{CSS6}} q_{e,CSS6} \right) \quad (\text{A7.3})$$

$$0 = -650x_{1,1} + 1 \left( \sum_{e \in FM_{CSS7}} q_{e,CSS7} \right) + 0.2 \left( \sum_{e \in FM_{CSS9}} q_{e,CSS9} \right) \quad (\text{A7.4})$$

$$0 = -650x_{1,1} + 1 \left( \sum_{e \in FM_{CSS8}} q_{e,CSS8} \right) + 0.8 \left( \sum_{e \in FM_{CSS9}} q_{e,CSS9} \right) \quad (\text{A7.5})$$

$$0 = 9000x_{1,1} - \sum_{g \in FM_{HLH1}} q_{HLH1,g} \quad (\text{A8.1})$$

$$0 = 9000x_{3,1} - \sum_{g \in FM_{HLH2}} q_{HLH2,g} \quad (\text{A8.2})$$

$$0 = 18000x_{1,2} - \sum_{g \in FM_{HLH3}} q_{HLH3,g} \quad (\text{A8.3})$$

$$0 = 7500x_{4,2} - \sum_{g \in FM_{HLH4}} q_{HLH4,g} \quad (\text{A8.4})$$

$$0 = -13500x_{1,1} + \sum_{e \in FM_{CLH1}} q_{e,CLH1} \quad (\text{A9.1})$$

$$0 = -11250x_{3,1} + \sum_{e \in FM_{CLH2}} q_{e,CLH2} \quad (\text{A9.2})$$



$$0 = -22500x_{1,2} + \sum_{e \in FMCLH3} q_{e,CLH3} \quad (\text{A9.3})$$

$$0 = -11250x_{4,2} - \sum_{e \in FMCLH4} q_{e,CLH4} \quad (\text{A9.4})$$

Note in the above equations that Eq. A1 is the cost function; Eq. A2, the non-negativity constraints; Eq. A3, the mass-balance equation for the initial divider in terms of the feed allocation ratios; Eq. A4. $i$ ,  $i = 2, 3, \dots, 9$ , the mass-balance equation around divider  $i$ ; Eq. A5. $i, j$ ,  $i = 1, 2$ ;  $j = 1, 2, 3$ , the mass-balance equation for component  $j$ , which is one of components A, B, and C in product  $i$  (i.e., product  $P_1$  or  $P_2$ ); Eq. A6. $e$ ,  $e = 1, 2$ , the heat balance equations for hot component stream  $e$ ; Eq. A7. $g$ ,  $g = 1, 2, \dots, 5$ , the heat balance equations for cold component stream  $g$ ; Eq. A8. $e$ ,  $e = 1, 2, 3, 4$ , the heat balance equations for the hot latent heat source  $e$ ; and Eq. A9. $g$ ,  $g = 1, 2, 3, 4$ , the heat balance equations for the cold latent heat source  $g$ .

The optimal solution of the linear programming model is:

$$x_{1,1} = x_{1,2} = x_{2,1} = x_{3,2} = x_{4,1} = x_{5,1} = 0.5$$

$$q_{HU1,CLH1} = 2625$$

$$q_{HLH1,CU1} = 4500$$

$$q_{HLH2,CLH1} = 4125$$

$$q_{HLH2,CSS6} = 3250$$

$$q_{HU1,CLH2} = 11250$$

$$q_{HLH2,CSS9} = 1625.$$

The values of all other variables are 0, and the corresponding value of the overall cost function is 190,871. The optimal structure obtained is given in Figure 14 in the text.



**Istvan Heckl** was born in Budapest, Hungary, in 1976. He received his M.S. in Information Technology in 2000 from the University of Veszprem, Veszprem, Hungary. His research area is in process network synthesis and integration. He is currently pursuing his doctoral degree at the Department Computer Science of the University of Veszprem.



**Professor F. Friedler** ([www.dcs.vein.hu/friedler](http://www.dcs.vein.hu/friedler)) is the Dean of Faculty of Information Technology, the Head of the Department of Computer Science, and the Chair of Information Technology (IT) Ph.D. program at the University of Veszprem, Hungary. He received his MS equivalent diploma in Mathematics, Ph.D. and Doctor of Science degrees in chemical engineering, and Habilitation in IT. His research interests include process systems engineering and operations research. He is one of

the founders of the P-graph framework for process design and synthesis. Dr. Friedler is Hungary's representative in the Computer Aided Process Engineering Working Party of the European Federation of Chemical Engineers and Chair of the Electronics and IT Jury of the Hungarian Scientific Research Fund. He has been served as chair and co-chair of international conferences.



**L. T. Fan** ([www.engg.ksu.edu/CHEDEPT/fan.htm](http://www.engg.ksu.edu/CHEDEPT/fan.htm)) is a University Distinguished Professor, holds the Mark H. and Margaret H. Hulings Chair in Engineering, and is the Director of Institute of Systems Design and Optimization at Kansas State University. He served as Department Head of Chemical Engineering between 1968 and 1998. He received a B.S. from National Taiwan University, an M.S. from Kansas State University, and a Ph.D. from West Virginia University, all in chemical

engineering, in addition to an M.S. in mathematics from West Virginia University. An honorary doctorate was bestowed on him by the University of Veszprem, Hungary, in 1990. His research interests include process systems engineering, environmental pollution control, biochemical engineering, chemical reaction engineering, transport phenomena, and material processing. Dr. Fan has published over 800 publications, including books, journal articles and reports; he has been granted fourteen patents.