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A Thermodynamic Approach to Multicomponent Distillation System Synthesis

This paper shows a synthesis method of multicomponent distillation systems with heat integration based on the available energy concept. With this method, the problem of synthesizing the heat integrated distillation systems in which there are heat source and sink streams supplied from other processes can be solved so as to minimize the process utilities. Moreover, since the system synthesis is executed in the $(1 - T_o/T)$ vs. Q diagram, it is possible to visibly represent the physical meanings of the computing process.

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SCOPE

Distillation systems are widely employed as the main separation process because such systems have the ability to separate various kinds of mixtures into their components and are easy to operate. However, the associated energy consumption is much larger than that of other separation systems (Fitzmorris and Mah, 1980) and it is consequently very important and necessary to carry out the synthesis of distillation systems paying particular attention to saving energy.

Considering the synthesis problem of a heat-integrated distillation system, we are facing two subproblems: (1) the selection of a separation sequence, and (2) the determination of a heat exchanger network around the distillation system (Rathore et al., 1974a). The proposed approach methods are classified into two techniques: a mathematical approach and a thermodynamic approach. Rathore et al. (1974) presented a synthesis method for determining the optimal sequence and operating conditions; first investigate all possibilities of condenser-reboiler matches for every subsystem and then combine the suitable subproblems by using dynamic programming in order to minimize the total cost. But as there is the feedback information for the relationship between two synthesis subproblems, the dynamic programming generates an infeasible solution. Also, this method forces users to spend an excessive amount of computation time for all the possible heat matches of subproblems. On the other hand, Umeda et al. (1979) presented an evolutionary approach method for heat-integrated system design based on the available energy concept. This method can advance the heat recovery around distillation systems using heat pumps and multi-effect as well as intermediate-boilers and coolers. But it cannot systematically generate a distillation sequence.

When saving energy in chemical processes, engineers analyze energy flows of units in the systems and then synthesize or modify the systems using the information from the analysis. So, engineers need a method to treat both of the analysis and design problems iteratively. From this point of view, since distillation systems are parts of the whole process systems, engineers may reconsider the design conditions for heat integration from the total system. For example, a mathematical method can derive the optimal distillation sequence, but advancing the heat recovery for preheating feed streams and cooling product streams needs a very different method.

The available energy concept is very powerful in the analysis of energy flows and thermodynamic efficiencies for chemical units. Many researchers have thermodynamically analyzed various kinds of distillation systems, multi-effect systems and distillation systems with heat pumps, intermediate-boilers and coolers (Freshwater, 1951; Null, 1976; Mah, 1977, 1979; Naka, 1980). But, there is a few studies for the application of the concept to the synthesis problems such as heat exchanger networks

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(Umeda et al., 1977) and steam supply systems with condensate recovery and reuse (Naka et al., 1979). In general, though a thermodynamic approach cannot explicitly evaluate the capital cost, it has the remarkable advantage; simple calculation of the minimum heat energy requirement and representation of synthesizing or modifying process in the $(1 - T_o/T)$ vs. Q diagram. So, engineers can easily understand the physical meanings of computational strategy and synthesize the heat-integrated systems, communicating with computer.

This paper proposes to apply the available energy concept to the synthesis problem for a multicomponent distillation system with heat integration. Specifically, this method treats distillation systems in which there are heat sources and sink sources with fixed heat loads from the other processes as well as process utilities. Two examples are shown in illustration of application.

CONCLUSIONS AND SIGNIFICANCE

A thermodynamic synthesis method for the design of a heat-integrated multicomponent distillation system has been developed. This method can easily obtain the optimal sequence as arranging the available energy losses of distillation subproblems closely with branch and bound method so as to minimize the available energy loss of utilities required. Specifically, this method can be effectively applied to distillation systems in which there are several heat sources and sink sources inclusive of sources with fixed heat load such as waste heat from other systems. This result means that in advancing the heat recovery from the viewpoint of the whole system this approach can be used with a thermodynamic design method for heat exchanger systems.

SYNTHESIS PROBLEM FOR MULTICOMPONENT DISTILLATION SYSTEMS

Consider the following synthesis problem:

Synthesize a distillation system, using conventional columns, to separate a C-component mixture into pure component products, so as to minimize the demand for process utilities, assuming that the upper and lower bounds of operating pressure and heat and sink source streams are given. This operating pressure range could be specified from the physical properties of mixtures and components such as the critical point, freezing point and so on. Distillation system can be realized theoretically in the pressure range.

(1) *Heat Source Streams*

(H1) Process heat utilities at fixed temperatures

(H2) Heat source streams available from other processes (The temperature and heat load of each source stream are given.)

(H3) Heat sources represented by heat removed by condensers in the system (The temperature and heat load depend on the operating pressure and reflux ratio of each column relating to the condenser.)

(2) *Heat Sink Streams*

(C1) Process cold utilities at fixed temperatures

(C2) Heat sink streams available from other processes (The temperature and heat load of each heat sink stream are given.)

(C3) Heat demands by reboilers (The temperature and heat load of each column depend on the operating pressure and reflux ratio.)

EVALUATION OF AVAILABLE ENERGY LOSS OF A DISTILLATION SYSTEM

The dead state of available energy is defined as the temperature, T_o, pressure, P_o, and composition $x_o = (x_{o1}, \ldots, x_{oc})^T$ of the surroundings or the dead state. The total available energy loss for the j-th distillation sequence with a system input of a flow rate F and composition x_F at T_o and P_o and with system outputs of products at T_o and P_o (as in Figure 1) is as follows (where, key components are separated into nearly pure components):

$$\Delta E_R(j) = \sum_{k=1}^{N} [\Delta e^k_{\mathrm{COL}}(j) + \Delta e^k_{\mathrm{EX}}(j) + W^k_p(j)] \tag{1}$$

where $W^k_P(j)$ is the mechanical work required to transport the process stream and to adjust the stream pressures in the k-th column of the j-th sequence. In general, the mechanical work is very much less than the other available energy losses in usual distillation systems. The first term is the available energy loss for the k-th column without considering the heat exchangers at the condenser and reboiler.

$$\mathrm{qc}\Delta e^k_{\mathrm{COL}}(j) = (e^k_r - e^k_c) + (e^k_F - e^k_D - e^k_W) \tag{2}$$

$$= T_o\left\{\left(\frac{Q_c}{T_D} - \frac{Q_r}{T_W}\right) - Fc_F\ell n\frac{T_F}{T_o} + DC_D\ell n\frac{T_D}{T_o} + Wc_W\ell n\frac{T_W}{T_o}\right\}\Bigg|_j^k + \text{const.}\Bigg|_j^k \tag{3}$$

where

$$\text{const.}\Bigg|_j^k = \tilde{R}T_o\left[D\sum_{i=i_D}^{ik} X_{Di}\ell n\frac{X_{Di}}{X_{Fi}} + W\sum_{i=i'_{k+1}}^{iw} X_{Wi}\ell n\frac{X_{Wi}}{X_{Fi}}\right]\Bigg|_j^k \tag{4}$$

The value of const. $|_j^k$ is the minimum available energy required for the separation of components into two products at T_o, and is independent of the operating conditions of the k-th column. Accordingly, the avoidable available energy loss of the k-th column, depending on the operating conditions, is as follows;

$$\Delta\bar{e}^k_{\mathrm{COL}}(j) = \Delta e^k_{\mathrm{COL}}(j) - \text{const.}|_j^k \tag{5}$$

The second term in Eq. 1 is the sum of available energy loss generated by a condenser and reboiler attached to the k-th column.

$$\Delta e^k_{\mathrm{EX}}(j) = \Delta e^k_{\mathrm{EX}c}(j) + \Delta e^k_{\mathrm{EX}r}(j) \tag{6}$$

where,

$$\Delta e^k_{\mathrm{EX}c}(j) = T_o\left(\frac{1}{T_C} - \frac{1}{T_o}\right)Q_c\Bigg|_j^k \tag{7}$$

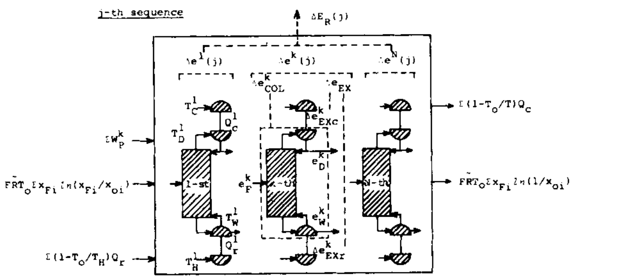


Figure 1. Available energy flow.

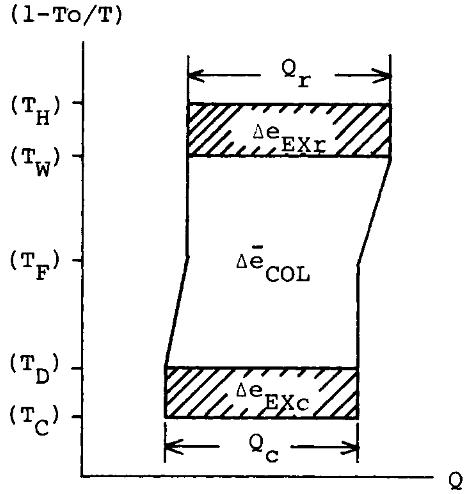


Figure 2. Available energy loss of $\Delta\bar{e}_{COL}$ and Δe_{EX}.

$$\Delta e^k_{EXr}(j) = T_o\left(\frac{1}{T_W} - \frac{1}{T_H}\right)Q_r\bigg|^k_j \tag{8}$$

The available energy losses, $\Delta\bar{e}^k_{COL}(j)$, $\Delta e^k_{EXc}(j)$ and $\Delta e^k_{EXr}(j)$ are shown in Figure 2. Substituting Eqs. 3, 4, 7 and 8, and the overall heat balance equation of a column into Eq. 1, the following equation is obtained:

$$\begin{aligned}\Delta E_R(j) = \sum_{k=1}^{N}\left\{\left(1 - \frac{T_o}{T_H}\right)Q_r - \left(1 - \frac{T_o}{T_C}\right)Q_c\right\}\bigg|^k_j \\ - \sum_{k=1}^{N}{}'\left\{Fc_F\left(T_F - T_o - T_o\ell n\frac{T_F}{T_o}\right)\right. \\ - Dc_D\left(T_D - T_o - T_o\ell n\frac{T_D}{T_o}\right) \\ \left. - Wc_W\left(T_W - T_o - T_o\ell n\frac{T_W}{T_o}\right)\right\}\bigg|^k_j - F\tilde{R}T_o\sum_{i=1}^{C}X_{Fi}\ell nX_{Fi}\end{aligned} \tag{9}$$

The first term is the available energy loss of the heat source and sink streams. When considering isobaric operations, the second term is related to the sensible heat change depending on the state of the system input and output and has a very small value compared with the first term, in general. In other words, available energy loss in multicomponent distillation system tends to be dominated by the heat source and sink terms. The terminal temperatures and heat loads in each column depend on the operating conditions of the column, but the available energies, namely $(H2)$, $(H3)$, and $(C2)$, $(C3)$ are already calculated as the removal available energies to be transfered to or from other systems and units. For example, the waste heat from a reactor is calculated as the removable heat energy for the reactor which can be used as a heat source stream $(H2)$ for a distillation system.

Finally, the synthesis problem is equivalent to the problem of how to arrange the available energy loss of each distillation column closely in order to minimize the available energy loss of required process utilities by maximizing the use of $(H3)$ and $(C3)$.

$$\Delta E_R(j) \simeq \sum_s\left(1 - \frac{T_o}{T_{Hs}}\right)Q_{rs} - \sum_s\left(1 - \frac{T_o}{T_{Cs}}\right)Q_{cs} \tag{10}$$

where Q_{rs} and Q_{cs} are the heat loads supplied by $(H1)$ and $(C1)$ respectively. In this paper, the heat integration arising from the sensible heat is neglected at the stage of considering the distillation sequences, but it can be easily taken into account in a stage of the overall detailed design of the system.

SYNTHESIS METHOD

When considering the synthesis of multicomponent distillation systems with specific reference to heat-integrated systems, it should be appreciated that it is not possible to evaluate the design until all operating conditions in the sequence are specified. The number of sequences to separate a mixture using N columns ($N = C - 1$) is $(2N)!/((N+1)!N!)$ and the number of separation subproblems in all sequences is $(N-2)(N-1)N/6$ (Rathore et al., 1974a). So, exhaustive enumeration of all sequences may not be practically feasible. The procedure represented in this paper consists of three steps: (1) investigate the possibility of supplying $(H2)$ and $(C2)$ to each separation subproblem; (2) select a good initial sequence for calculation of the optimal sequence; and (3) find a strategy to decide on the optimal operating conditions of the sequence.

Bottom \ Top	1 A	2 B	3 C	4 D	5 A B	6 B C	7 C D	8 A B C	9 B C D	10 A B C D	Lowest temp. of the bottom
1 B	F										T_W(B)
2 C		F			F						T_W(C)
3 D			$H2_1$			$H2_1$		$H2_1$			T_W(D)
4 E				$H2_3$			$H2_3$		$H2_3$	$H2_2$	T_W(E)
5 BC	F										T_W(BC)
6 CD		$H2_3$			$H2_2$						T_W(CD)
7 DE			$H2_2$			$H2_2$		$H2_1$			T_W(DE)
8 BCD	F										T_W(BCD)
9 CDE		$H2_1$			$H2_1$						T_W(CDE)
10 BCDE	$H2_2$										T_W(BCDE)

$(T_{H2,1} < T_{H2,2} < T_{H2,3})$

Figure 3. Matrix for feasible separation subproblems and possible use of ($H2$) heat sources.

Utilization of Heat Source and Sink from Other Processes

In this step the possibility of utilizing the heat source and sink streams denoted by $(H2)$ and $(C2)$ is investigated. Let's define the matrix to represent feasible separation subproblems and possible utilization of $(H2)$ and $(C2)$. Figure 3 shows an example for a five-component separation system. The columns of the matrix correspond to the top products appearing in all sequences and the rows correspond to the bottom products. Each element of the matrix denotes whether a separation subproblem is feasible or not. If feasible, F is indicated and otherwise nil.

At the next, when considering the possibility of utilization of $(H2)$ streams, they are numbered in order of temperature as follows;

$$(H2_1), \ldots, (H2_m), \ldots, (H2_M), \qquad \text{where } T(H2_1) < \ldots < T(H2_M)$$

Let's consider the (i,j) separation subproblem posed by which it is assumed to be operated at the lowest pressure $\underline{P}$. It is assumed that each subproblem can be operated at a pressure between the lower limit, $\underline{P}$, and upper limit, $\overline{P}$, i.e.

$$\underline{P} \leqq P \leqq \overline{P} \tag{11}$$

If the bottom temperature, T_W, which is the bubble point at $\underline{P}$, is higher than $(T(H2_m) - \Delta T^{min}_a)$, it is impossible to use the streams $(H2_1)$ to $(H2_m)$, and the mark m is indicated at the (i,j) element. If a subproblem can utilize $(H2_M)$, F is left. The elements marked by F in Figure 3 can use any kind of given heat source streams. When the possibility of utilization of $(H2)$ streams is examined based on the lower limit of pressure $\underline{P}$, if the result interferes with the utilization of $(C1)$ and $(C2)$ streams, engineers should provide other heat sink streams in order to determine the operating pressure of subproblem (if $(C2)$ in the low temperature is very important, they should provide other heat source streams).

Evaluation of a Lower Bound of Heat-Integrated Distillation Sequences

In this step a lower bound of available energy loss, $\Delta E_H(j)$ of the j-th sequence is evaluated. The lower bound of the available energy

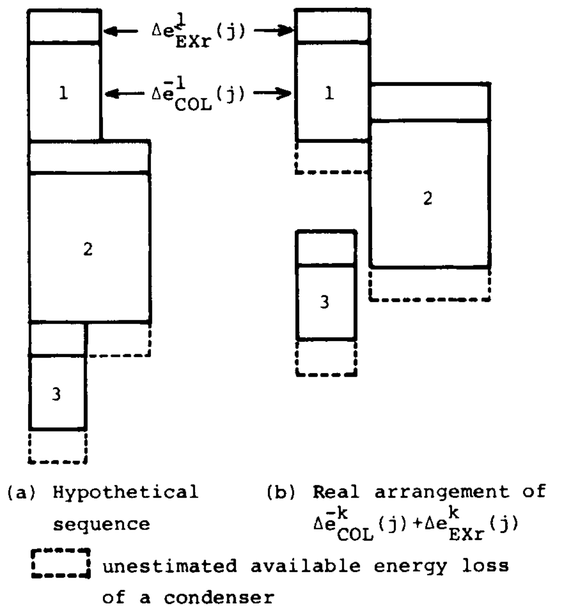


Figure 4. Schematic diagram of hypothetical sequence in $(1\text{-}T_o/T) - Q$ diagram.

loss means the loss of the j-th sequence with a kind of idealized and hypothetical heat integration. In other words, for a sequence with idealized and hypothetical heat integration, which has N columns with only N reboilers and one condenser each column in the sequence can be operated at any pressure $P(\underline{P} \leqq P \leqq \overline{P})$ independent of the operating conditions of the other columns. According to the assumption, even if the hypothetical j-th sequence is shown in Figure 4b, the hypothetical available energy loss, $\Delta E_H(j)$ is always evaluated based on the unit arrangement in Figure 4a, neglecting the temperature levels of each distillation. But when evaluating $\Delta E_H(j)$, though it is necessary to determine which column needs a condenser, it is nearly impossible to do so. The minimum available energy loss of the k-th separation subproblem with no condenser in the j-th sequence is defined as follows:

$$\Delta e^{\min,k}(j) = \underset{P_k,R_k}{\mathrm{Min}}[\Delta \bar{e}^{k}_{\mathrm{COL}}(j) + \Delta e^{k}_{\mathrm{EX}r}(j)] \tag{12}$$

where P_k and R_k are operating pressure and reflux ratio respectively. The total minimum avoidable available energy losses for the j-th hypothetical sequence with heat integration is

$$\Delta E^{\min}_{H}(j) = \sum_{k=1}^{N} \underset{P_k,R_k}{\mathrm{Min}}\,[\Delta \bar{e}^{k}_{\mathrm{COL}}(j) + \Delta e^{k}_{\mathrm{EX}r}(j)] + \Delta e^{\min,k'}_{\mathrm{EX}c}(j) \tag{13}$$

The second term at the right side, $\Delta e^{\min,k'}_{\mathrm{EX}c}(j)$ is the available energy loss in a condenser of the k'-th column which has the lowest column-top temperature in the sequence. But, $\Delta e^{\min,k'}_{\mathrm{EX}c}(j)$ is neglected so as to simplify the evaluation of avoidable available energy loss of this hypothetical sequence. Moreover, since the smaller a reflux ratio becomes, the smaller is the available energy of a column, and it may be expressed that the value of $\Delta \bar{e}^{k}_{\mathrm{COL}}(j)$ becomes the minimum value when $R = \theta R^{\min}$. When the value of θ is given, $\Delta \bar{e}^{k}_{\mathrm{COL}}(j)$ is the function of the operating pressure only. Accordingly, the hypothetical available energy loss of the j-th sequence can be treated as a function of the operating pressure only of each column in the sequence. If there are some heat source streams of $(H2)$, the hypothetical available energy loss should be modified using the information of the matrix in Step 1. The hypothetical available energy loss of the j-th sequence which has the possibility of using heat source streams of $(H2)$ should be reduced, as follows;

$$\Delta E_H(j) = \Delta E^{\min}_{H}(j) - \sum_{m=1}^{M'} \left(1 - \frac{T_o}{T_m}\right) Q_m \tag{14}$$

where, T_m and Q_m are the temperature and heat load of the m-th heat source stream in the M' possible source stream checked in Step 1. The operating pressure, P, should be in a feasible region given by Eq. 11, and furthermore, the temperatures of the top and bottoms should satisfy the following equations simultaneously,

$$T_W \leqq T^{\max}_{H} - \Delta T^{\min}_{a} \tag{15}$$

$$T_D \geqq T^{\min}_{C} + \Delta T^{\min}_{a} \tag{16}$$

where, $T^{\max}_{H}$ is the highest temperature of heat source streams, $(H1)$ and $(H2)$, $T^{\min}_{C}$ is the lowest temperature of heat sink streams, $(C1)$ and $(C2)$.

Here, another available energy loss is defined as follows; the minimum available energy loss for a real system, $\Delta E^{\min}_{R}(j)$, is the minimum available energy loss for the process utilities supplied to the heat-integrated j-th sequence with feasible operating conditions.

Though the calculation method will be presented in detail later on, the following equation should be noted:

$$\Delta E^{\min}_{R}(j) > \Delta E_H(j) \tag{17}$$

because $\Delta E^{\min}_{H}(j)$ does not include the available energy loss for any condenser and it may not be feasible to hold all operating pressure of $\Delta E^{\min}_{H}(j)$ when maximum heat integration is assumed. For the j'-th and j-th sequences, if the following relation holds;

$$\Delta E^{\min}_{H}(j') \geqq \Delta E^{\min}_{R}(j) \tag{18}$$

it is not necessary to evaluate $\Delta E^{\min}_{R}(j')$ of the j'-th sequence.

Calculation of Minimum Available Energy Loss, $\Delta E^{min}_{R}(j)$

This step determines the optimal feasible operating conditions and specifies the heat integrations system, using the $(1 - T_o/T)$ vs. Q diagram.

From the definition of $\Delta E^{\min}_{R}(j)$ it is clear that the optimal operating conditions can be obtained by locating the locus of $(\Delta \bar{e}^{k}_{\mathrm{COL}}(j) + \Delta e^{k}_{\mathrm{EX}}(j))$ on the $(1 - T_o/T)$ vs. Q diagram so as to minimize the total available energy loss of the process utilities required in the j-th sequence.

A method to determine the optimal operating pressure is as follows; When there are U process utilities and M heat source streams from other systems, the maximum number of possible utility temperatures which the first column in the j-th sequence can utilize is $(U + M)$. In general, as the k-th column has the possibility of using removable heat energy from the condensers from $k - 1$ columns, the maximum number of possible utility temperature is $(U + M + k - 1)$. For example, when there is one process utility $(H1)$ and one heat source stream $(H2)$, the possible temperatures of the second column are shown in Figure 5. The square with broken lines shows alternative positions at the same temperature of the second column. For a sequence with N columns, the number of the pressure combinations is, taking into account column arrangement,

$$(U + M)(U + M + 1) \ldots (U + M + N - 1)(N!)$$

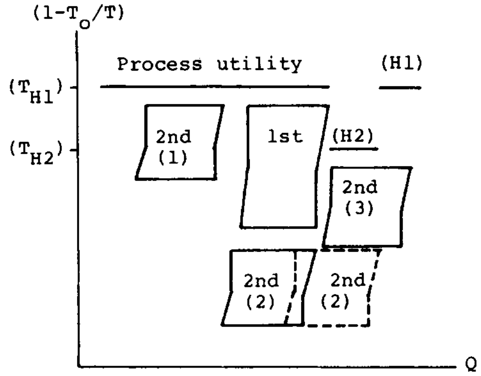
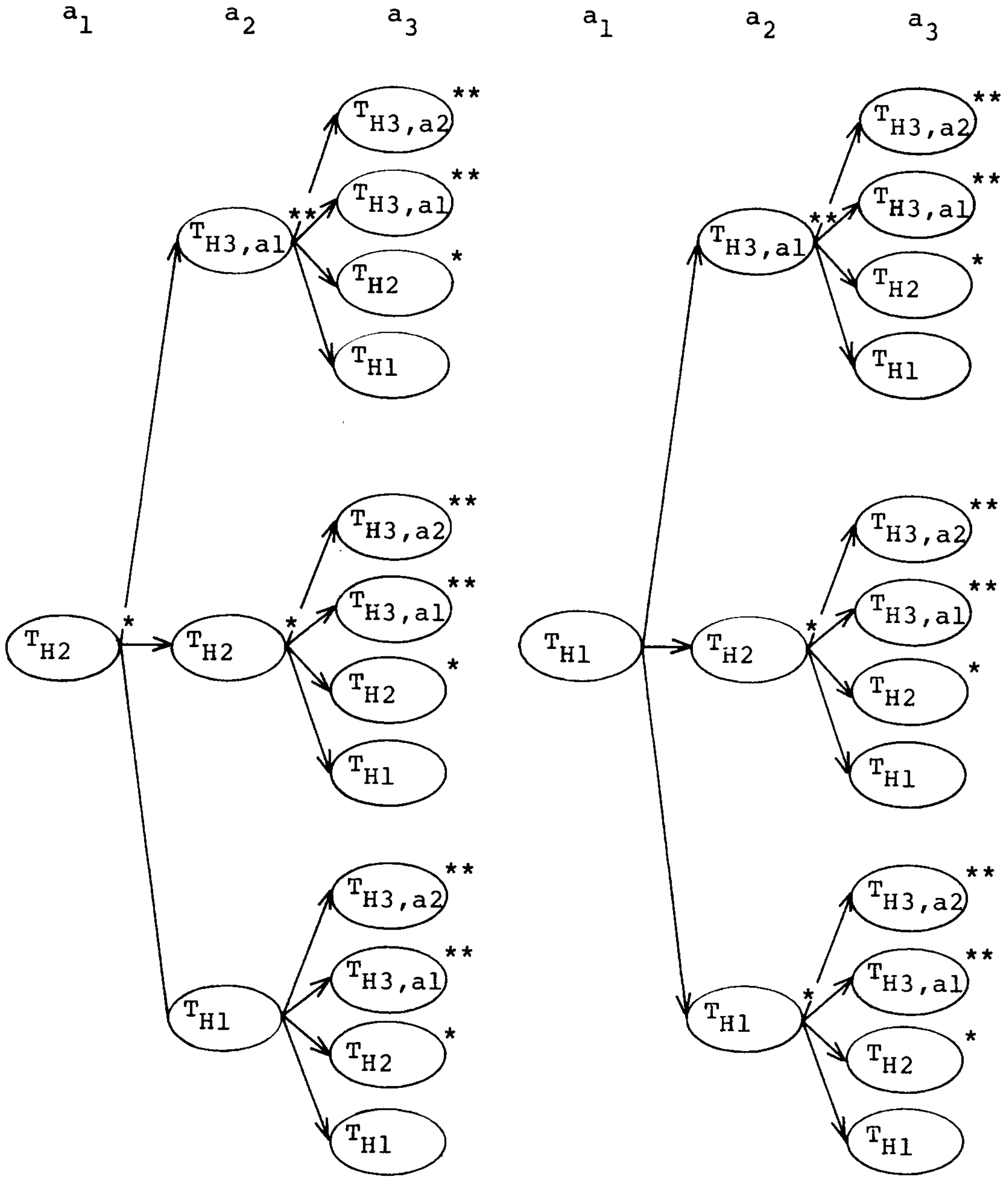


Figure 5. Possible temperature of 2nd column.



$(T_{H3,a2} \leq T_{H3,a1} \leq T_{H2} \leq T_{H1})$

* Check the residual heat load. If not enough, the additional heat sources should be supplied.

** Check the possibility of using the heat load and the residual heat load.

Figure 6. Possible utilization of heat sources.

To explore such a large number of pressure combinations would be very time-consuming so a tree searching method is employed (branch and bound method).

Another assumption is introduced here, namely that the operating pressure P is set equal to the pressure at the bubble point of the bottoms, T_W defined by

$$T_W = T_H(j) - \Delta T_a^{\min} \tag{19}$$

where, $T_H(j)$ is the temperature of heat source streams. The pressure of the k-th column is calculated by using the bubble point calculation at T_W. From the constraint on the operating pressure

$$\text{if } P \geqq \overline{P}, \qquad P = \overline{P} \tag{20}$$

or if

$$P \leqq \underline{P}, \qquad P = \underline{P} \tag{21}$$

Also, the temperature of the top product, T_D obtained from the dew point calculation should satisfy the following equation

$$T_D \geqq T_C^{\min} + \Delta T_a^{\min} \tag{22}$$

where, $T_C^{\min}$ is the minimum temperature of heat sink streams. The assumption mentioned above is acceptable because reducing the available energy loss of reboiler and making the temperature for heat removal from the condenser higher increases the possibility of reusing heat to the following columns.

The synthesis tree can thus evolve by adding further columns,

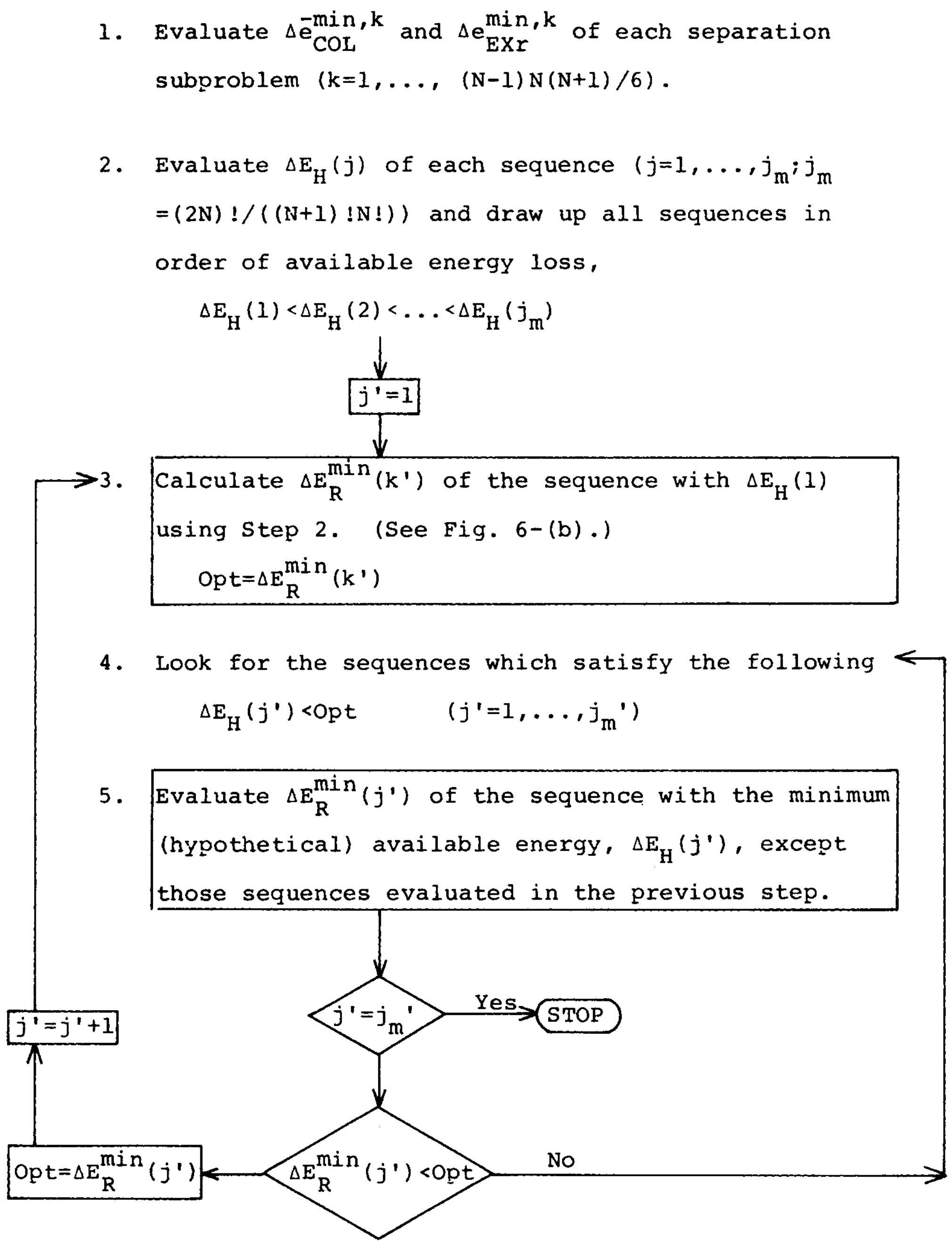


Figure 7a. Strategy of Step 2.

taking into account the heat integration as shown in Figure 3. For example, giving a process utility ($H1$) and heat source ($H2$) supplied to the three column system, the search tree for a column rearrangement is shown in Figure 6. Where, a_1, a_2, and a_3 are named corresponding to the subproblems in the j-th sequence respectively, and temperatures are those of the possible heat sources. The search is carried out on the outside nodes of the tree. When using a heat source stream of $H2$ or $H3$ at some node, the constraint for the heat load should be checked. If the whole heat load of such a stream is already supplied to reboilers of 1 to $k - 1$ columns, the branches with the node can be pruned. If satisfied, after checking the constraint of the pressure range, the search makes a comparison in the difference between the lower bound (LB) and the upper bound (UB) at every node. If $LB \geq UB$, the further branches at the node are pruned away and the search returns to the last node. When all possibilities have been examined, the feasible solution having UB is optimal.

If an initial value of UB is assumed near the optimal value, the computational time can obviously be reduced. For the sequence with the minimum value of $\Delta E_H(j)$ required in Step 2, the operating pressure for each column is selected which minimizes the available energy of the process utility requirement assuming an additional column. In other words, the position where the k-th column in an arrangement of the j-th sequence is identified on the $(1 - T_o/T)$ vs. Q diagram described previously. The operating pressure should satisfy Eqs. 19 to 22. Here, this available energy loss is denoted by ΔE_R^{*a} ($a = 1, \ldots, N$). The minimum value of ΔE_R^{*a} is then used as the initial value of UB.

$$\Delta E_R^{UB} = \min_a \Delta E_R^{*a}(j)$$

For example, assuming the separation sequence with four components shown in Figure 6 has the minimum hypothetical available energy loss, ΔE_R^{*a} is evaluated as follows: as the utilization of ($H2$) heat source to a_1 makes the available energy loss of consumed process utility small rather than that of ($H1$) heat source, the left search tree in Figure 6 is selected. Then, if ($H3$) heat source from the top of a_1 can be utilized to a_2, the path from (T_{H2}) to ($T_{H3,a1}$)

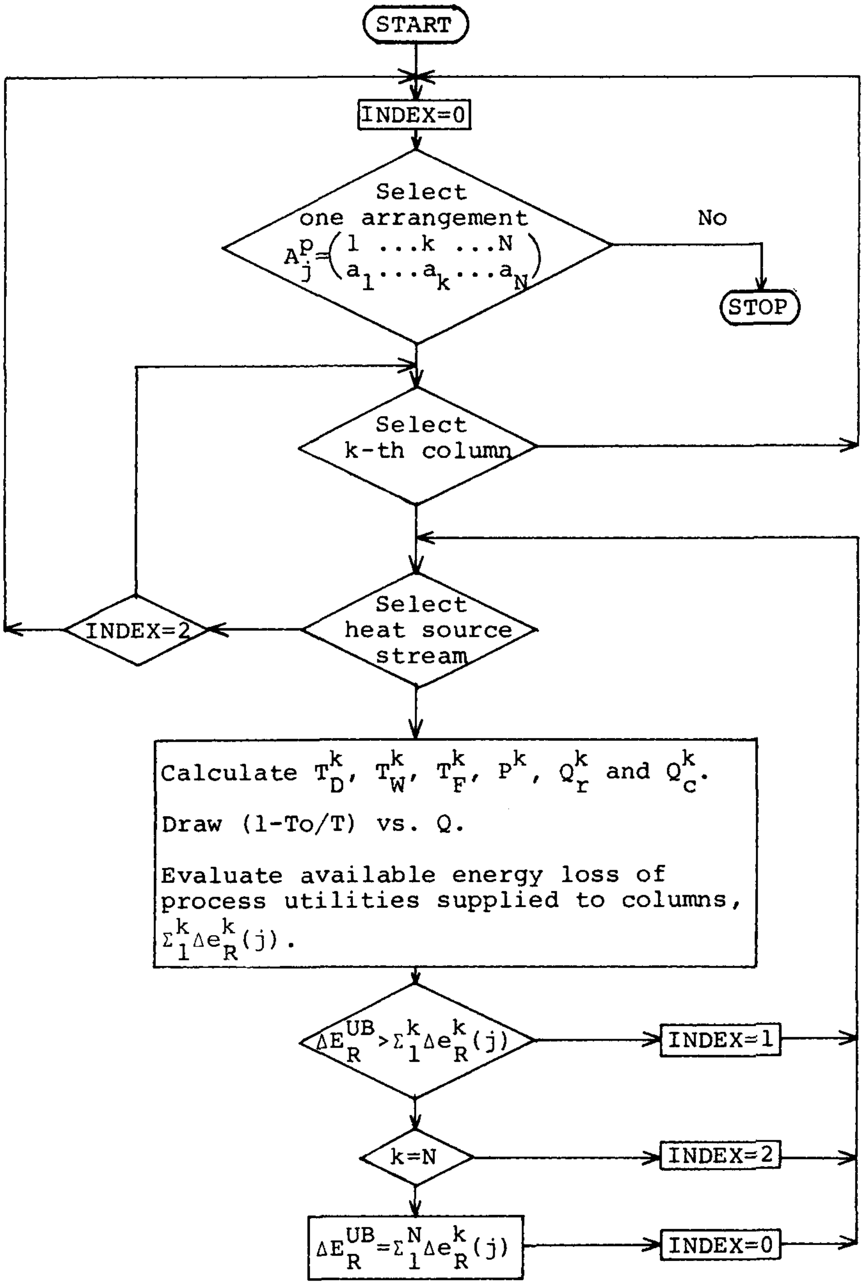


Figure 7b. Flow chart of Step 3.

is selected. Finally, if only $(H1)$ heat source is available for a_3, ΔE_R^{*a} is calculated at (T_{H1}) node.

The synthesis strategy is shown in Figure 7a and b.

EXAMPLES

Two examples of separation system synthesis are illustrated.

Example 1: This example is solved by Rathore et al. (1974b). The values of $\Delta E_H(j)$ and $\Delta E_R^{min}(j)$ and optimal separation sequence with heat integration are shown in Table 2 and Figure 8. A comparison of $\Delta E_H(j)$ and $\Delta E_{R(j)}^{min}$, shows that nine sequences can be neglected by using Eq. 18 in Step 2. The sequence with the minimum hypothetical available energy loss is the 8-th and is, in fact, the optimal sequence with minimum available energy loss. Figure 8 shows the heat integrated system of the 8-th sequence without the utilization of sensible heat. In this figure, S_k and D_k denote the heat load on the condenser of the k-th column and that supplied to the reboiler respectively. Also, the complete integrated system,

TABLE 1. DESIGN CONDITIONS FOR EXAMPLE 2

Feed Conditions			
Flow Rate [Kg-mol/h]			907.20
Comp.	Propane		0.05
	i-Butane		0.15
	n-Butane		0.25
	i-Pentane		0.20
	n-Pentane		0.35
$\theta = R/R^{min}$			1.00
Pressure			
Lower Limit		[Pa]	1.01×10^5
Upper Limit		[Pa]	26.34×10^5
Heat Source	$(H1)$	[K]	413.15
		[K]	393.15
	$(H2)$	[K]	343.15
		[J/h]	1.88×10^6
Heat Sink	$(C1)$	[K]	303.15
Min. Approach Temp.		[°C]	10.0
Surroundings		[K]	303.15
		[Pa]	1.01×10^5

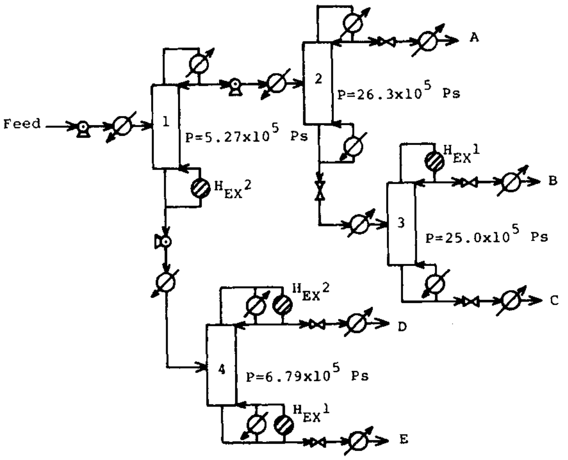


Figure 8. Optimal sequence of Example 1.

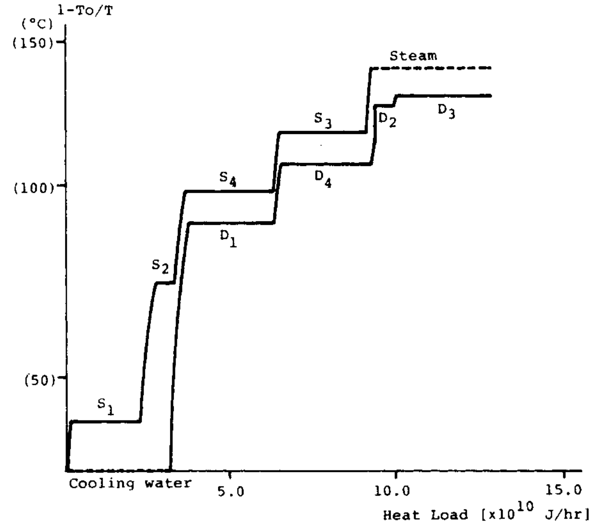


Figure 9. Heat Integration of Example 1.

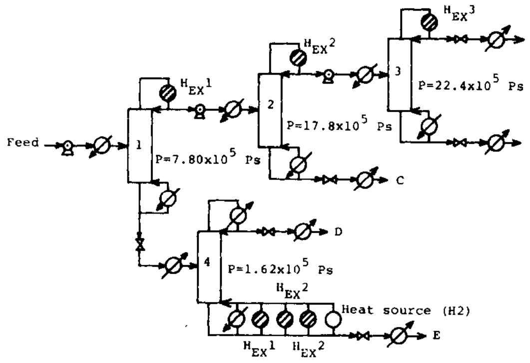


Figure 10. Optimal sequence of Example 2.

including sensible heat, is shown in Figure 9. Two heat exchangers, $H_{EX}1$ and $H_{EX}2$ are installed for heat integration.

Example 2: As shown in Table 1, two process utilities and one heat source stream as ($H2$) are available to the separation system, but only the lower temperature utility is employed and the heat source stream is utilized at the reboiler of the 4-th column. The optimal sequence using heat integration based on the latent heat is shown in Figure 10. Three heat exchangers, $H_{EX}1$ to $H_{EX}3$, are used for heat integration. The heat integration including sensible heat is shown in Figure 11.

TABLE 2. COMPARISON BETWEEN $\Delta E_H(J)$ AND $\Delta E_R^{\min}(j)$

Seq. No.	$\Delta E_H(j)$	$\Delta E_R^{\min}(j)$	Sequence
1	7.36	12.16	(10,1), (9,2), (7,3), (4,4)
2	9.03	—	(10,1), (9,2), (3,3), (4,7)
3	6.86	8.99	(10,1), (2,2), (4,4), (7,6)
4	10.66	—	(10,1), (6,2), (3,3), (4,9)
5	10.49	—	(10,1), (2,2), (3,6), (4,9)
6	8.15	11.54	(1,1), (7,3), (4,4), (9,5)
7	9.82	—	(1,1), (3,3), (9,5), (4,7)
8	7.19	8.65	(5,1), (2,2), (4,4), (7,8)
9	8.49	12.92	(1,1), (4,4), (2,5), (7,8)
10	11.62	—	(8,1), (6,2), (3,3), (4,10)
11	11.45	—	(8,1), (2,2), (3,6), (4,10)
12	12.58	—	(1,1), (3,3), (6,5), (4,10)
13	13.17	—	(1,1), (2,5), (3,8), (4,10)
14	11.87	—	(5,1), (2,2), (3,8), (4,10)

($\times 10^{10}$ J/h)

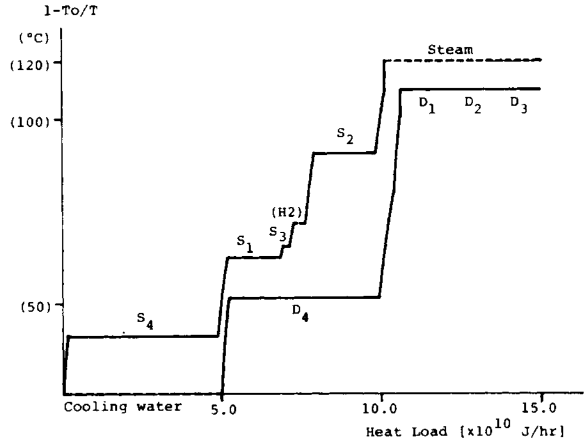


Figure 11. Heat Integration of Example 2.

NOTATION

C	= number of components
c_D, c_F, c_W	= heat capacity
D	= flow rate of the top product
ΔE_H	= available energy loss of a hypothetical system
ΔE_R	= available energy loss of a feasible system having heat integration
ΔE_R^*	= available energy loss of a feasible system with specified heat integration
e	= available energy
Δe_{COL}	= available energy loss of a column
$\Delta \bar{e}_{COL}$	= defined by Eq. 5
Δe_{EX}	= available energy loss of heat exchangers in a column $= \Delta e_{EXc} + \Delta e_{EXr}$
F	= flow rate of the feed
M	= number of ($H2$) heat sources
N	= number of columns
P	= pressure
$\underline{P}, \overline{P}$	= lower and upper pressure limits
Q_c, Q_r	= heat loads on condenser and reboiler
R	= reflux ratio
$\tilde{R}$	= gas constant
T	= temperature
$\Delta T_a^{\min}$	= approach temperature difference of heat exchangers
U	= number of process utilities
W	= flow rate of the bottoms
W_P	= mechanical work
x	= mole fraction vector $= (x_1, \ldots, x_c)T$
	= constant

Subscripts

a = index for arrangement
c = condenser
C, Cs = heat sink stream
D = top product
F = feed
H, Hs = heat source stream
i, i_D, i_k, i_W = component number
j = sequence number
k, k' = column number
r = reboiler
W = the bottoms
o = surroundings

Superscripts

max = maximum
min = minimum
UB = upper bound

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Solution of Recycle Problems in a Sequential Modular Approach

Recycle problems in a sequential modular approach are solved by adopting evolutionary models. When describing a process scheme by means of evolutionary models, a nonlinear algebraic system of equations is obtained. The resulting solution is utilized for updating the values of torn variables in the iterative solution of the scheme.

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SCOPE

The combination of a modular sequential approach, as a basic technique for the solution of process schemes, with an equation-oriented approach as convergence promoter for the solution of the recycle problems, has been successfully experimented by the authors. The basic idea is to define approximated, but evolutionary models associated to the rigorous ones adopted inside the process scheme. The evolutionary aspect is given by a set of internal, adaptive parameters, which are redefined after each iteration in order to fit the performance of the rigorous models.

The introduction of these new models adds a parallel simulation problem to the original one, that is the simulation of the same process scheme, where each unit is described by an evolutionary model. The solution is carried out according to an equation-oriented approach. The system of equations is properly decomposed and, then, solved by means of existing algorithms for the solution of nonlinear equations systems. As the evolutionary models give an approximated image, yet coincident with the corrected one at the convergence, the solution of the approximated scheme is seen as the prediction of the iteration variables in the original scheme.

As a consequence of the equation-oriented nature of the convergence promoter, all benefits intrinsic to the approach are present in the method: efficiency, stability and possibility of treating both simulation and design problems in the same manner.

CONCLUSIONS AND SIGNIFICANCE

The introduction of evolutionary models transforms the problem of promoting the convergence in a cyclical process scheme into the solution of an algebraic, nonlinear system of equations. The system is of a large scale but shows a sparse structure. Therefore, it may be easily decomposed following the results of the process scheme decomposition. A system with a

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