ϵ = molar extinction coefficient, length^{-1}
ϵ_0 = radius of the diffusing sphere, length
η = indice of refraction of the liquid
η_0 = indice of refraction of the fiber
θ = cylindrical coordinate
λ = wavelength of radiation, length
μ = absorption coefficient, length
ν = natural optical density of the filter
ρ = cylindrical coordinate, length
σ = standard deviation defined in Figure 10b
φ = spherical coordinate
Ω = solid angle

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R & D NOTES

Process Synthesis Using Structural Parameters: Further Discussion of Inequality Constraints

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As a result of their study on the synthesis of a small heat exchanger network, Shah and Westerberg (1977) have shown that "if the structural parameters are to be used for a synthesis problem, and if inequality constraints are involved, the problem has to be formulated very carefully, if indeed it can be, to make it a continuous one." The purpose of this note is to show how structural parameters (Umeda et al., 1972; Ichikawa and Fan, 1973) can be used to formulate their problem in such a way as to have a continuous objective function; however, this is not to suggest that the

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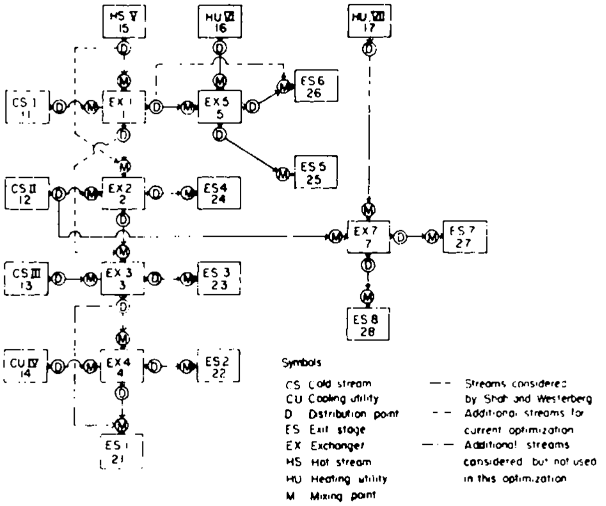


Figure 1. Structural parameter representation of the flowsheet.

structural parameter method is always all powerful in synthesizing heat exchanger networks.

In Figure 1, the synthesis problem presented by Shah and Westerberg (1977) is cast in the formalism of the structural parameter method. Each stage except an inlet is preceded by a mixing point (M) and each stage except an exit is followed by a distribution point (D). To guarantee that the optimal structure is included in the flowsheet, all possible subsystems must be imbedded in it. This could be accomplished by having a stream connecting each distribution point to each mixing point. However, this approach is not practical because the resultant optimization problem would be both difficult and inefficient due to the large number of independent variables introduced as stream-splitting parameters. To reduce the dimensionality, heuristics can be employed to eliminate some of the streams but care must be taken not to eliminate the optimal system nor to create any discontinuities in the objective function.

The structure considered by Shah and Westerberg (1977) is indicated by the solid lines in Figure 1. As they stated, heat exchangers 2, 4, and 5 are potentially redundant, and thus in this study, by-pass streams which are indicated by the two types of dashed lines are provided so that the flow through these exchangers

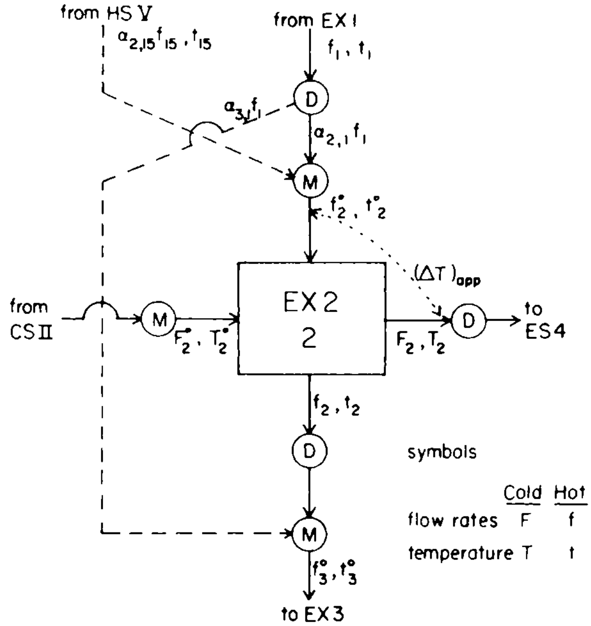
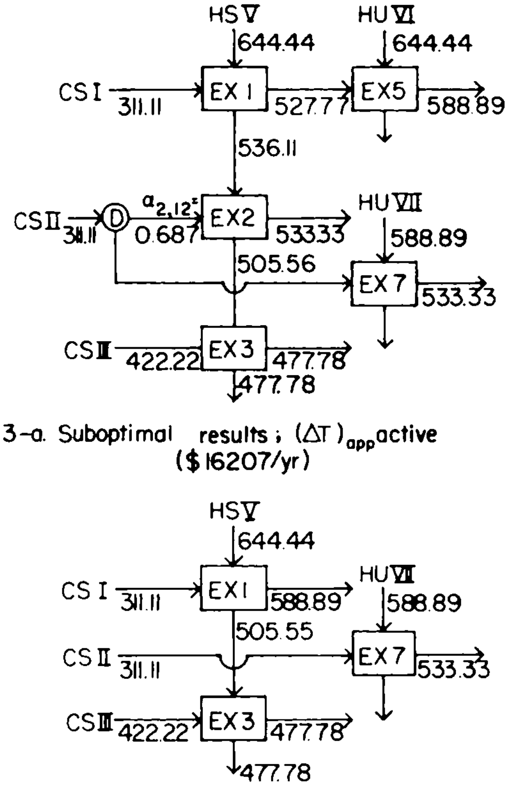


Figure 2. Heat exchanger 2 showing the effect of (ΔT)app.



3-a. Suboptimal results ; $(\Delta T)_{app}$ active ($16207/yr)

3-b. Optimal results ; $(\Delta T)_{app}$ not active ($ 6268/yr)

Figure 3. Results of Shah and Westerberg (1977).

can go to zero. To see why these streams are needed to preserve a continuous objective function in the presence of inequality constraints, the detail of the network around exchanger 2 shown in Figure 2 is examined. The approach temperature requirement is given by:

$$t_2^0 - T_2 \geq (\Delta T)_{app} \tag{1}$$

If the heat capacity is constant, the temperature of the hot stream at the inlet of exchanger 2 is:

$$t_2^0 = \frac{\alpha_{2,1} f_1 t_1 + \alpha_{2,15} f_{15} t_{15}}{\alpha_{2,1} f_1 + \alpha_{2,15} f_{15}} \tag{2}$$

For the structure considered by Shah and Westerberg (1977), $\alpha_{2,1} = 1$ and $\alpha_{2,15} = 0$; thus,

$$t_1 = t_2^0 \geq T_2 + (\Delta T)_{app} \tag{3}$$

unless A_2 was identically zero. If A_2 was zero, a discontinuity arose since t_1 no longer had to satisfy the inequality given by Eq. 3.

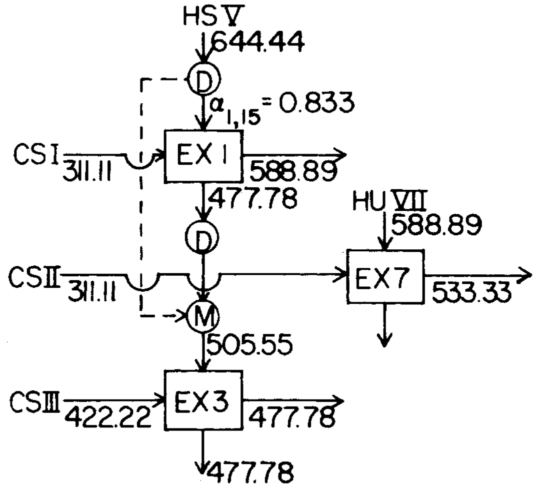
When the by-pass streams (dashed lines) are added, the mixing of a fraction of hot stream V with the exit from exchanger 1 allows t_2^0 to satisfy the approach temperature requirement in cases when t_1 does not. As the fraction of the exit from exchanger 1 going to exchanger 2 approaches zero ($\alpha_{2,1} \rightarrow 0$), the fraction of hot stream passing directly to exchanger 2 can also approach zero ($\alpha_{2,15} \rightarrow 0$) without violating Eq. 1. Thus, the temperature of the exit from exchanger 1 can be decreased in a continuous manner even though the inequality constraint is still active.

The by-pass streams represented by the dashed lines in Figure 2 were not considered by Shah and Westerberg (1977) either because stream-splitting was not allowed or because of the thermodynamic argument that it is inefficient to mix streams of different temperatures. While the latter reasoning suggests that such mixing should not occur at the optimal solution, the inclusion of the by-pass streams in the formulation of the optimization problem results in a continuous objective function. The addition of by-pass streams increases the number of independent variables, and thus the

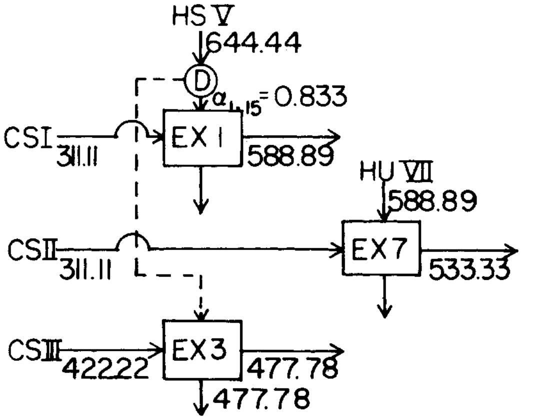
TABLE 1. STREAM SPECIFICATIONS AND COST DATA (SHAH AND WESTBERG, 1977)

	Stream I	II	III	IV	V	VI	VII
Flow, kg/s	1.26	0.504	1.26	—	2.52	—	—
Inlet temperature, °K	311.11	311.11	422.22	311.11	644.44	644.44	588.89
Outlet temperature, °K	588.88	533.33	477.78	355.56	477.78	644.44	588.89
Boiling Point, °K	755.56	755.56	755.56	373.33	755.56	644.44	588.89
Liquid heat capacity, kJ/kg°K	4.19	4.19	4.19	4.19	4.19	4.19	4.19
Film heat transfer coefficient, kW/m^2 °K	1.70	1.70	1.70	1.70	1.70	8.52	8.52
Cost, \$/kg	0	0	0	1.10×10^{-4}	0	2.21×10^{-3}	5.20×10^{-4}
Heat of vaporization, kJ/kg	698	698	698	1786	698	1628	1396
Inlet vapor fraction	0.0	0.0	0.0	0.0	0.0	1.0	1.0
Outlet vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Minimum approach temperature: 2.78°K
Heat exchanger cost equation (A in m^2): $0.1(1456\,A^{0.6})$
Equipment down time: 280 h/yr
Cost per year: utilities + heat exchangers, \$/yr



4-a. Suboptimal results
(\$ 6296/yr)



4-b. Optimum results with additional split
(\$ 5948/yr)

Figure 4. Results of this study.

streams by-passing exchangers 4 and 5 are not considered in this study in an effort to keep the dimensionality low.

The suboptimal structure obtained by Shah and Westerberg (1977) when the approach temperature was constrained is shown in Figure 3-a while their optimal results when the constraint was not active is shown in Figure 3-b. The costs using the data in Table 1 are slightly different from those in the original article (probably due to conversion of units) but have no effect on the structures. The annual cost without exchanger 2 represents a 61% improvement over the sub-optimal case. In this study, a four dimensional search was performed using a random-to-pattern minimization procedure (Heydweiller and Fan, 1979). With the two additional by-pass streams included in the objective function, the search has led to the sub-optimal structure shown in Figure 4-a. Note that this structure is not the same as the optimal structure obtained by Shah and Westerberg. Since their example was made up simply to demonstrate that a discontinuity could result from an inequality constraint, they had not considered the globally optimum solution which could be obtained if stream-splitting were allowed. The mixing of the exit stream from heat exchanger 1 at 477.78°K (which is the desired final temperature) with the uncooled portion of hot stream 5 at 644.44°K before exchanger 3 indicates that the structure in Figure 4-a is definitely not optimal. In order to obtain the global optimum shown in Figure 4-b, a stream would have to be included to connect the exit from exchanger 1 directly to the mixing point before the outlet of the system (ES1). One is again reminded to be careful to weigh the consequences before removing any stream from the structure.

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