Utility Bounds for Nonconstant $Q\Delta T$ for Heat-Integrated Distillation Sequence Synthesis

In earlier work the authors presented a simple method to synthesize heat-integrated distillation sequences through the use of simple sketches on a diagram displaying temperature vs. enthalpy. Embedded in that work is the useful but incorrect assumption that the reboiler/condenser heat loads and the temperature difference across the column are independent of the temperature (pressure) level at which the column is operated. This assumption of constancy is removed here, and it is shown how to calculate the minimum utility target using a small linear programming formulation. It is also shown how to use the results of this calculation to synthesize distillation sequences that approach the bound discovered. For the example problems solved, the minimum utility target calculated increases about 25 to 60% over that calculated assuming constant $Q\Delta T$. The sequences synthesized based on this improved target are virtually the same as the constant $Q\Delta T$ method produces, suggesting that the earlier method is indeed a useful approach.

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SCOPE

This work is the third in a series of papers dicussing the synthesis of heat-integrated distillation sequences. In the first paper (Andrecovich and Westerberg, 1985a), we presented a method to synthesize the better heat-integrated sequences by a simple graphical method. This approach included an assumption that the column heat duty and the ΔT from the reboiler to the condenser are constant for a column vs. the pressure level at which the column operates. The second paper (Andrecovich and Westerberg, 1985b) presented a mixed integer linear programming (MILP) approach to select the better configurations, with the above assumption not needed. However, this approach is the equivalent of an extensive but efficient enumeration scheme to discover the better solutions. It does not permit one to see intuitively why the solutions are what they are. In this paper we focus back on relaxing the assumption of constant heat duty and ΔT, but with the intention of allowing one to use these ideas to construct solutions simply, again using essentially the same graphical ideas of the first paper.

CONCLUSIONS AND SIGNIFICANCE

We have presented a simple approach to permit the calculation of minimum utility use bounds for sequences of conventional and multieffected distillation columns. The results show that an approach presented earlier will significantly underestimate the bounds for the example problems included here. We have shown that the calculation given here also offers insight into how to structure heat-integrated solutions which approach the more correct bound. We have illustrated the ideas with two example problems used in the two previous papers.

A MODEL FOR NONCONSTANT $Q\Delta T$

In the method described in Andrecovich and Westerberg (1985a), $Q\Delta T$ is assumed to be independent of column operating conditions. However, as mentioned in this earlier paper, both Q and ΔT usually increase linearly with column operating temperature, and $Q\Delta T$ is weakly quadratic in the column operating temperature. The variation of $Q\Delta T$ with temperature for the separation of n-butane and i-pentane is shown in Figure 1. In this paper we present a method for estimating the minimum utility use of a distillation sequence which takes into account the variation of $Q\Delta T$ with column operating conditions.

$Q\Delta T$ can be evaluated at temperature T_0 from:

$$Q\Delta T(T_0) = Q_0[\Delta T_0 + \Delta T_{\min}] \qquad (1)$$

where Q_0 and ΔT_0 are the heat duty and column temperature

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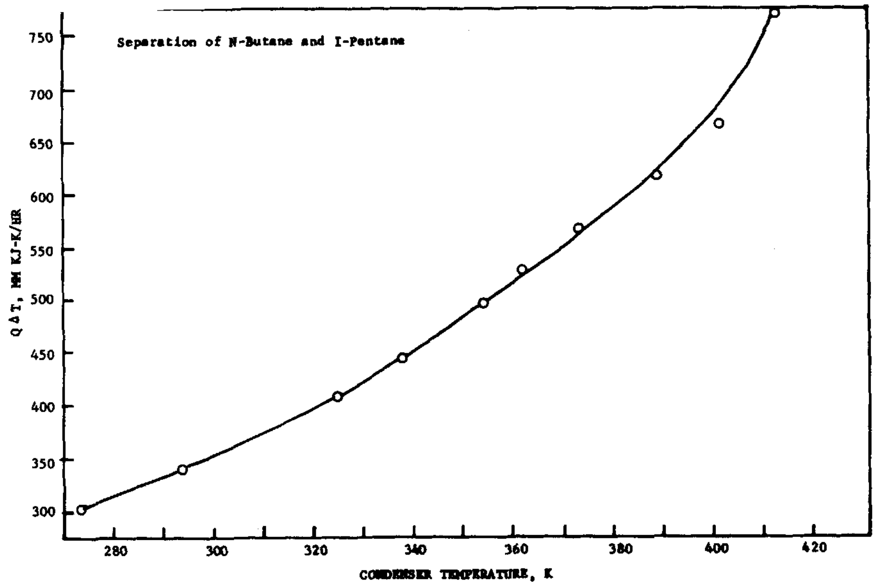

Figure 1. Variation of $Q\Delta T$ with condenser temperature.

difference at temperature T_0. We shall let T (i.e., T_0 and T^*) refer to the condenser temperature for a column in what follows here. In the constant $Q\Delta T$ method, $Q\Delta T$ is calculated at the lowest feasible operating conditions (temperature and pressure) for each distillation task and remains fixed. Assuming a linear variation for both Q and ΔT, the actual variation of Q, ΔT, and $Q\Delta T$ with temperature may be given by the following equations:

$$Q(T^*) = (1 + mT^*)Q_0 \tag{2}$$

$$\Delta T(T^*) = (1 + \mu T^*)\Delta T_0 \tag{3}$$

$$Q\Delta T(T^*) = (1 + mT^*)Q_0[(1 + \mu T^*)\Delta T_0 + \Delta T_{\min}] \tag{4}$$

where T^* is defined to be $T - T_0$ and the rates at which Q/Q_0 and $\Delta T/\Delta T_0$ increase with T^* are given by m and μ.

Consider the differential area, QdT^*, shown in Figure 2. At T^*, the temperature of this incremental bit of area, $Q\Delta T$ for a distillation task would be $Q\Delta T(T^*)$. The fraction ϕ, of this task which would be accomplished by this differential area is

$$\phi = \frac{QdT^*}{Q\Delta T(T^*)} \tag{5}$$

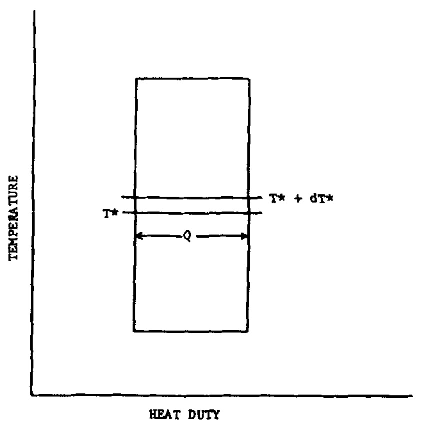

Figure 2. Differential area for a single task.

If the heat duty, Q, is held constant, the fraction of the distillation task performed in the interval from T_1^* to T_2^* is given by

$$\phi = Q \int_{T_1^*}^{T_2^*} \frac{dT^*}{Q\Delta T(T^*)} \tag{6}$$

Substituting Eq. 4 for $Q\Delta T(T^*)$ and integrating gives the following expressions for the fraction of the original distillation task performed by an area on the T-Q diagram with a width of Q units of heat duty and a height of $T_2^* - T_1^*$.

If $b^2 - 4ac > 0$

$$\phi = \frac{Q}{(b^2 - 4ac)^{0.5}} \ln \left\{ \frac{[2aT_2^* + b - (b^2 - 4ac)^{0.5}]}{[2aT_2^* + b + (b^2 - 4ac)^{0.5}]} \times \frac{[2aT_1^* + b + (b^2 - 4ac)^{0.5}]}{[2aT_1^* + b - (b^2 - 4ac)^{0.5}]} \right\} \tag{7}$$

if $b^2 - 4ac = 0$

$$\phi = \frac{2Q}{2aT_1^* + b} - \frac{2Q}{2aT_2^* + b} \tag{8}$$

if $b^2 - 4ac < 0$

$$\phi = \frac{2Q}{(4ac - b^2)^{0.5}} \left\{ \tan^{-1} \frac{2aT_2^* + b}{(4ac - b^2)^{0.5}} - \tan^{-1} \frac{2aT_1^* + b}{(4ac - b^2)^{0.5}} \right\} \tag{9}$$

where

$$a = Q_0 \Delta T_0 m \mu$$

$$b = Q_0 \Delta T_0 (m + \mu) + Q_0 \Delta T_{\min} m$$

$$c = Q_0 (\Delta T_0 + \Delta T_{\min})$$

If these expressions were used to evaluate the fraction of a distillation task performed by an area of width Q_0 and extending from $T_1^* = 0$ to $\Delta T_0 + \Delta T_{\min}$, the resultant value of ϕ should be one. The integrated expressions above, however, overcorrect for the effect of temperature so a normalization factor, η, is defined. The value of η is chosen such that the following equation is satisfied.

$$\eta Q_0 \int_0^{\Delta T_0 + \Delta T_{\min}} \frac{dT^*}{Q\Delta T(T^*)} = 1 \tag{10}$$

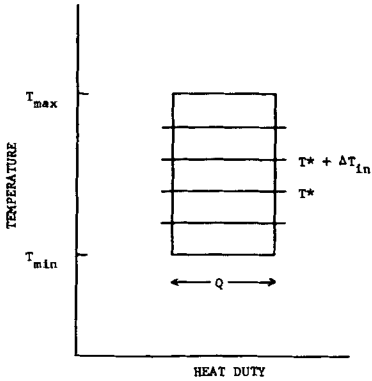

Figure 3. Area for a distillation sequence.

The factor η can be evaluated for any distillation task using this equation and the integrated expressions of Eqs. 7 to 9.

MINIMUM UTILITY CALCULATION

The expressions just developed can be used to calculate a minimum utility use bound for a single distillation task. Determine the maximum feasible reboiler temperature and minimum feasible condenser temperature for the distillation task and calculate T^*_{max}, T^*_{min}, and η. The minimum utility use for the distillation task can be obtained by solving Eq. 6 for Q with ϕ set equal to one. For the separation of n-butane and i-pentane the minimum utility use obtained using this method is 8.96 GJ/h.

The minimum utility use of a distillation sequence can also be calculated using $Q\Delta T$ corrected for temperature, but the procedure is more complex. Consider the area shown in Figure 3. This area has a height equal to ΔT_{avail}, a width of Q, and is divided into intervals of height ΔT_{int}. For a given distillation task i the fraction of the task which can be accomplished in a given interval j can be calculated from

$$\phi_{ij} = \eta_i Q \int_{T_1^*}^{T_2^*} \frac{dT^*}{Q\Delta T_i(T^*)} \tag{11}$$

where T_1^* and T_2^* are the temperatures at the ends of the interval. Equations 7 to 9 can be used in evaluating ϕ_{ij}.

Each of the sections of area in Figure 3 can be assigned to one or more distillation tasks. If all of section j is assigned to distillation task i, then that area will accomplish ϕ_{ij} of distillation task i. If portions of section j are assigned to several distillation tasks, the amount of each task i performed in interval j is $z_{ij}\phi_{ij}$ where z_{ij} is the fraction of interval j assigned to task i. If the width of the area is equal to the minimum utility use for the sequence, two conditions will be satisfied: the entire available temperature range will be used, and the sum of the ϕ_{ij} for each distillation task will be equal to one.

Calculating the minimum utility use for a distillation sequence involves assigning fractions of each interval of area to each distillation task such that the entire available temperature range is used and such that each distillation task is performed in full. An algorithm for performing this calculation is presented below.

1. Calculate the maximum and minimum feasible temperatures for the distillation sequence.
2. Divide this available temperature range into intervals. The intervals need not be evenly spaced. The number of intervals which span the available temperature range should be an integer, however. Also add one or two intervals above the maximum feasible temperature for the sequence.

TABLE 1. MINIMUM UTILITY USE FOR THE DISTILLATION SEQUENCES IN EXAMPLE PROBLEM 2 USING DIFFERENT METHODS

	Minimum Utility Use, MM kJ/h		
Sequence*	Multieffect Method	Constant $Q\Delta T$ Method	Corrected $Q\Delta T$ Method
1	86.48	49.56	62.21
2	102.72	61.84	86.46
3	74.52	41.98	52.09
4	101.9	64.32	98.38
5	97.24	61.97	93.46
6	74.62	49.00	62.02
7	90.86	61.29	86.39
8	70.38	40.11	51.76
9	67.52	42.36	54.10
10	122.6	69.60	114.19
11	118.0	67.24	110.10
12	122.6	70.85	107.92
13	122.2	67.79	102.47
14	119.34	70.02	106.11

* Sequence numbers refer to Figure 4 of Andrecovich and Westerberg (1985a).

3. For each distillation task in each interval calculate ϕ_{ij} from Eq. 11 assuming $Q = 1$.
4. Guess a value for the minimum heat duty for the entire sequence. Call this value Q_G.
5. Solve the following linear program:

$$\text{Min} \sum_{i=1}^{NT} \sum_{j=1}^{NI} z_{ij}$$

such that

$$Q_G \sum_{j=1}^{NI} \phi_{ij} z_{ij} = 1 \qquad i = 1,2\ldots, NT$$

$$\sum_{i=1}^{NT} z_{ij} \leq 1 \qquad j = 1,2,\ldots, NI$$

$$z_{ij} \geq 0 \qquad \text{for all } i \text{ and } j$$

6. If the value of the objective function of this linear program is equal to (within some specified tolerance) the number of intervals spanning the available temperature range for the sequence, stop. Q_{min} for this sequence is Q_G. If not, reguess Q_G and return to step 5.

The results for the sequences of example problem 2 in Andrecovich and Westerberg (1985a) obtained using this algorithm are shown in Table 1.

SYNTHESIS USING CORRECTED $Q\Delta T$

A better method for synthesizing minimum utility distillation systems can be obtained by using the corrected $Q\Delta T$ method for calculating the minimum utility use. The solution to the linear program in the corrected $Q\Delta T$ method provides not only a value for the minimum utility use but also an optimum set of values for z_{ij}, the fraction of temperature interval j assigned to distillation task i. This information can be used to guide the synthesis process since it suggests which distillation tasks should be assigned to which temperature intervals to obtain the minimum utility use. How this information is used can be illustrated using the sequences with minimum utility use in example problems 1 and 2 given in Andrecovich and Westerberg (1985a).

For sequence A/BC-B/C of example problem 1, the minimum

TABLE 2. VALUES OF z_{ij} FOR THE SEQUENCE A/BC–B/C OF EXAMPLE PROBLEM 1[*]

Interval	Fraction of Interval Assigned to Task	
	A/BC	B/C
353–363	1.0	0.0
363–373	1.0	0.0
373–383	1.0	0.0
383–393	1.0	0.0
393–403	0.0	1.0
403–413	0.0	1.0
413–423	0.0	1.0
423–433	0.0	1.0
433–443	0.0	1.0
443–453	0.410	0.590
453–463	1.0	0.0
463–473	1.0	0.0
473–483	1.0	0.0
483–493	1.0	0.0
493–503	1.0	0.0
503–523	1.0	0.0
513–523	1.0	0.0

[*] Andrecovich and Westerberg (1985a).

utility use obtained from the corrected $Q\Delta T$ method is 5.49 MM kJ/hr. The values of z_{ij} associated with this solution are shown in Table 2. These values of z_{ij} suggest first performing task A/BC at the lowest temperatures, next performing task B/C at the intermediate temperatures, and then finishing task A/BC at the higher temperatures. One feasible distillation system which is compatible with this information is shown at the left in Figure 4. The minimum utility use of this sequence obtained by more detailed analysis is 5.96 GJ/h, which is 9% greater than the bound on the minimum utility use. It is also clear in this figure that task A/BC limits further decrease in the utility use. Another column of type A/BC must be added to decrease utility use further. The values of z_{ij} indicate that it should be added at high temperature since the previous solution did not use all of the temperature intervals assigned to task A/BC. Adding this column and modifying the structure to maintain feasibility and to keep the utility use of task B/C about the same results in the distillation system shown at the right in Figure 4. The utility use of this system is 5.49 GJ/h which is equal to the bound.

TABLE 3. VALUES OF z_{ij} FOR SEQUENCE 8 OF EXAMPLE PROBLEM 2[*]

Interval	Fraction of Interval Assigned to Task			
	ABC/DE	D/E	A/BC	B/C
315–335	0.0	0.402	0.598	0.0
335–355	0.0	0.468	0.0	0.532
355–375	1.0	0.0	0.0	0.0
375–395	0.169	0.0	0.0	0.831
395–405	1.0	0.0	0.0	0.0
405–425	1.0	0.0	0.0	0.0
425–445	0.0	1.0	0.0	0.0
445–465	0.0	0.998	0.0	0.0

[*] Andrecovich and Westerberg (1985a).

The same principles apply in analyzing sequence 8 of example problem 2. The minimum utility use for this sequence obtained using the corrected $Q\Delta T$ method is 25.6 MM kJ/hr. The values of z_{ij} associated with this solution are given in Table 3. It is obvious from these values that task A/BC should be done at the lowest temperature possible. In the linear program solution task A/BC can be satisfied by assigning half of interval 1 to it, but in an actual solution task A/BC requires parts of intervals 1, 2, and 3. A minimum utility solution must use the remaining area in each of these intervals, and the z_{ij}'s indicate that tasks D/E and B/C should be used. Task ABC/DE should be included next, but it cannot use the whole width because that would force task B/C to be performed at a temperature higher than the critical temperature of both the distillate and bottoms. Performing tasks ABC/DE and B/C in parallel satisfies the critical temperature requirement of task B/C and the indications that task ABC/DE should be performed next.

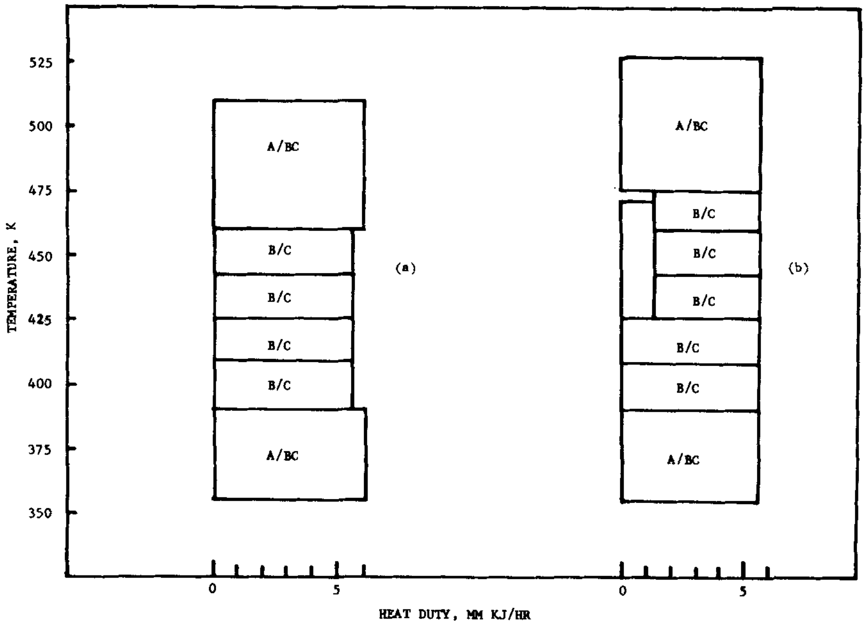

Figure 4. Synthesis of example problem 1 using corrected $Q\Delta T$ method.

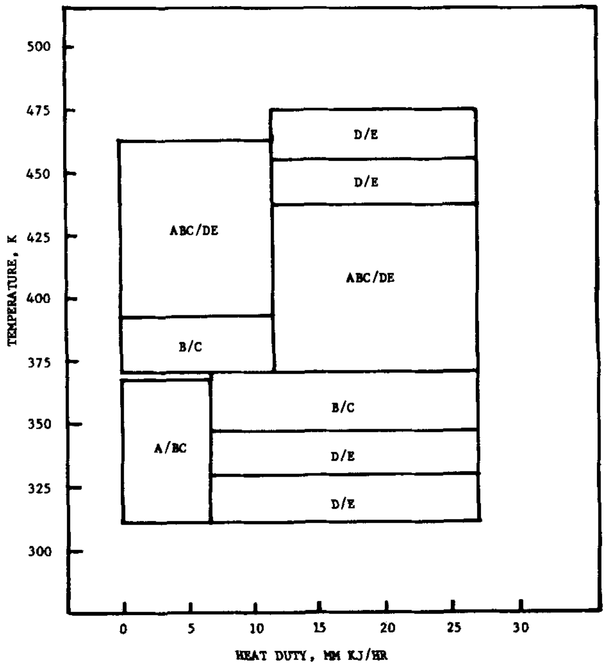

Figure 5. Synthesis of sequence 8 of example 2 using corrected $Q\Delta T$ method.

The z_{ij}'s suggest continuing to perform task *ABC/DE* until it is complete, then finishing task *D/E*. The distillation system shown in Figure 5 is compatible with the ordering of tasks suggested by the minimum utility use solution and has a minimum utility use of 27.0 GJ/h, within 5% of the bound on the utility use. Significant improvement to this solution seems unlikely since the utility use is nearly constant throughout the temperature range is used.

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NOTATION

a,b,c = Coefficients, Eqs. 7 to 9
m = Slope for linear equation relating $Q(T^*)$ to Q_0
Q = Rate of heat degraded by a column; i.e., the heat entering the column reboiler and leaving the column condenser, assuming both duties to be about equal
Q_0 = Rate of heat degraded across a column at the reference temperature T_0
Q_G = Guess for the width of the column stack when calculating the minimum utility bound
T = Temperature
T^* = Temperature T minus reference temperature T_0 for a column
$T^*_{\max}$ = Maximum feasible reboiler temperature for a distillation task
$T^*_{\min}$ = Minimum feasible condenser temperature for a distillation task
T_0 = Reference condenser temperature for a column
z_{ij} = Fraction of temperature interval j assigned to task i

Greek Letters

ΔT = Temperature drop across a column; i.e., reboiler temperature minus condenser temperature
ΔT_0 = Temperature drop across a column at reference temperature T_0
$\Delta T_{\min}$ = Minimum temperature difference allowed for heat exchange
η = Normalizing factor, Eq. 10
μ = Slope for linear equation relating $\Delta T(T^*)$ *to* ΔT_0
ϕ = Fraction of distillation task accomplished by an area of width Q and height ranging from T_1^* to T_2^*
ϕ_{ij} = Fraction of distillation task i that can be accomplished by a unit area in temperature interval j

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