Shortcut Evaluation of ΔT and $Q\Delta T$ for the Synthesis of Heat Integrated Distillation Sequences

K. GLINOS,
M. F. MALONE, and
J. M. DOUGLAS

Department of Chemical Engineering
University of Massachusetts
Amherst, MA 01003

Among the many methods that have been proposed for the synthesis of distillation sequences that minimize cost, a recent one by Andrecovich and Westerberg (1983) has attracted our attention because of the potential applicability this approach can have in a variety of cases. The authors use the quantity $Q\Delta T$, which is the product of the reboiler duty Q and the temperature difference ΔT between the top and the bottom of a column, and the available utility temperatures to establish lower bounds on the cost either of single separation tasks (using multieffect distillation) or of several separation tasks (sequences of simple and multieffect columns are used). In the method it is assumed that the distillation sequences for a problem can be specified. This is true when we deal with sharp splits, but if we are also to consider sloppy splits, we have essentially an infinite number of alternatives, and the method does not give a way to choose or define the separation tasks. However, it is not inherently restricted to pure splits. Also, the method is based on the assumption that the product $Q\Delta T$ is constant, which is not exactly correct, especially if the key components are not close boilers.

A disadvantage of all methods of the above type is the large computational effort they require. For instance, to find the ΔT's, iterative bubble point calculations have to be done at the top and the bottom of each column. If Q, ΔT, and their product were available from simple algebraic equations, the method would be significantly accelerated and it would possibly allow for product or recycle purity optimizations. Here we present simple expressions to evaluate these quantities.

If we assume that the vapor in the column is ideal, that the molal volume of the liquid is negligible in comparison to that of the gas, and that the heat of vaporization of a component, ΔH_i, is insensitive to temperature for the narrow temperature range we are interested in, the Clausius-Clapeyron equation can be written in the form

$$P_i = P_{i,o} \exp\left\{-\frac{\Delta H_i}{R}\left(\frac{1}{T} - \frac{1}{T_o}\right)\right\} \tag{1}$$

Dividing both sides of Eq. 1 by the total pressure, we get the equilibrium Henry's law constants, K_i and $K_{i,o}$. It is also true that

$$K_i = \frac{P_i}{P_{\text{Tot}}} = \frac{\alpha_i}{\Sigma \alpha_j X_{j,k}} \tag{2}$$

where k is the stream or the tray that the above mole fractions correspond to. For ideal mixtures, the heat of vaporization is about the same for all components, and without much error we can substitute an average ΔH for ΔH_i. Actually, this assumption is already made, to have constant molal overflow in the column. If we substitute Eq. 2 into 1, we find the following expression for the temperature difference between locations 1 and 2:

$$\frac{1}{T_2} - \frac{1}{T_1} = \frac{R}{\Delta H} \ln\left(\frac{\sigma_2}{\sigma_1}\right) \tag{3}$$

where $\sigma_k = \Sigma \alpha_i X_{i,k}$. We can find several interesting results from Eq. 3. If we write it to relate the feed with the distillate temperature, we get

$$T_D = \left\{-\frac{R}{\Delta H} \ln\left(\frac{\sigma_F}{\sigma_D}\right) + \frac{1}{T_F}\right\}^{-1} \tag{4}$$

which gives the top temperature if T_F is known. In a similar way, we find the bottom temperature

$$T_B = \left\{\frac{R}{\Delta H} \ln\left(\frac{\sigma_B}{\sigma_F}\right) + \frac{1}{T_F}\right\}^{-1} \tag{5}$$

Subtracting Eq. 4 from 5, we easily find the temperature difference between the top and the bottom of the column. Moreover, if $\Delta H \gg RT_F$, we can approximately write

$$\Delta T = \frac{RT_F^2}{\Delta H} \ln\left(\frac{\sigma_D}{\sigma_B}\right) \tag{6}$$

The above equation is simple to use and gives accurate estimates of ΔT, as we show below. In addition, if we write Eq. 3 for the top and bottom temperatures, we get

$$\Delta T = \frac{RT_D T_B}{\Delta H} \ln\left(\frac{\sigma_D}{\sigma_B}\right) \tag{7}$$

and we see that Eq. 6 is exact if $T_F^2 = T_D T_B$. Even if the feed temperature is not known, we can still use Eq. 6 by assigning to T_F some rough average value that can be estimated from the boiling points of the pure components. Also, Eq. 6 shows ΔT to be proportional to the square of the temperature. However, α is also dependent on T, and our detailed analysis of binary mixtures showed that the overall effect of T on ΔT can be described by adding a linear to a square term. The contribution of the linear term usually will be more significant.

To illustrate the performance of Eq. 6, we calculated the ΔT's

TABLE 1

Column	ΔT (Approx.)	ΔT (Exact)
A/B	3.9	3.9
B/C	15.4	15.0
C/D	9.9	10.6
D/E	11.4	9.9
A/BC	13.7	13.4
AB/C	17.8	17.5
B/CD	17.4	17.0
BC/D	16.2	16.1
A/BCDE	18.9	18.9

for all the possible splits of the five-component mixture that Andrecovich and Westerberg present as an example in their work (Table 1). We give below some of the values they calculated (exact) and then our approximations. We'll see that these values are always very close. The value of ΔH we used is an average of the heats of vaporization of the pure components. Note that in the table and throughout this paper we don't add 10° C to the ΔT's found, as the above authors do in their calculations, to provide a driving force for heat transfer. This does not affect the above equations, and some ΔT as a driving force can be added later.

The heat input to the column is approximately equal to $Q = V\Delta H$, where V is the vapor rate. Then Eq. 6 can be written as

$$Q\Delta T = RVT_F^2 \ln\left(\frac{\sigma_D}{\sigma_B}\right) \qquad (8)$$

which is independent of ΔH. An anticipated deficiency of the method proposed by Andrecovich and Westerberg is that it is based on the assumption that the quantity $Q\Delta T$ is constant for a certain separation task, regardless of the number of effects (columns) used. However, this may not be quite true. The dependency of the logarithmic term of Eq. 8 on T turns out to be roughly the inverse of the dependency of V on T, and therefore they approximately cancel out, at least for small α values (expensive separations). Especially for binary mixtures, we can prove that roughly $Q\Delta T = (Q\Delta T)_0(T/T_0)^2$, if the α is close to unity. Therefore, the main reason that $Q\Delta T$ varies with temperature (pressure) is its linear dependence on the squared value of the average temperature at which each distillation effect takes place, or, more exactly, on the product $T_D T_B$, as we see from Eq. 7.

There is a simple way to take these variations into account, using the total entropy increase for a distillation task, ΔS, instead of $Q\Delta T$. Using Eq. 7 we find

$$\Delta S = Q\left(\frac{1}{T_D} - \frac{1}{T_B}\right) = RV \ln\left(\frac{\sigma_D}{\sigma_B}\right) \qquad (9)$$

Even with double effect distillation, variations of 10 or 20% in $Q\Delta T$ are usual. Although ΔS varies slightly, it is much less sensitive than $Q\Delta T$ because it is not directly dependent on the temperature and also more attractive to use since it is a physical quantity. In fact, ΔS varies proportionaly to the inverse of the temperature, but this dependence is not strong, particularly for components that are close boilers and over limited temperature ranges. We also want to note that Eq. 9 gives the entropy increase (exergy loss) in the column itself, and doesn't account for the reboiler and condenser. The entropy increase in the heat exchangers will depend on the ΔT's we wish to use as a driving force. The method of Andrecovich and Westerberg can be easily modified in terms of ΔS, for instance, by minimizing the total entropy increase (exergy loss) instead of $Q\Delta T$ and the T-Q diagrams will be replaced by $1/T$-Q diagrams.

Using the expressions we presented above, a significant amount of numerical work and iterative computations can be avoided. In addition, if we use shortcut equations that explicitly predict the vapor rate for any kind of split (Glinos and Malone, 1984), the evaluation of Q's and ΔT's for a multicomponent mixture becomes a trivial task, requiring only a pocket calculator. Another important feature of Eq. 6 or 8 is the insight offered into the factors influencing ΔT and $Q\Delta T$. Since ΔT is explicitly expressed as a function of the compositions, the expressions are also useful for the synthesis of distillation sequences performing sloppy splits, where the design of the system is dependent on product or recycle purity optimizations. Moreover, Eq. 9 can be used for quick estimations of the increase in the vapor rate, resulting from pressure shifts, if V is known at some other condition. Thus we can avoid repeating iterative or complex calculations. In the examples we tried, this method predicted V within 4% of its actual value. Finally, Eqs. 4 and 5 may be useful when heat integration is considered, since they yield accurate estimates of the temperatures at the reboiler and the condenser.

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NOTATION

P_i = vapor pressure of pure component i
P_{tot} = column operating pressure
V = vapor rate
Q = reboiler or condenser duty
R = universal gas constant
T_k = temperature at location or stream k
$X_{i,k}$ = mole fraction of component i in stream k

Greek Letters

α_i = relative volatility of component i
σ_k = a weighted by the mole fractions average of the relative volatilities, defined by $\sigma_k = \Sigma\alpha_i X_{i,k}$
ΔH_i = molal heat of vaporization of component i
ΔS = total entropy increase for a certain separation task
ΔT = temperature difference between the top and the bottom of the column

Subscripts

D, B, F = distillate, bottom, and feed conditions respectively

LITERATURE CITED

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