Graphic Exergy Analysis of Processes in Distillation Column by Energy-Utilization Diagrams

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The graphical construction called an energy-utilization diagram (EUD) is adopted for analyses of energy transformation and exergy losses in a distillation column. The overall exergy loss on one plate of a column can be decomposed into six kinds of exergy losses and are represented graphically. Two of them are caused by mixing and cooling in the vapor phase, and the other two by mixing and heating in the liquid phase. To display the remaining two yielded by condensation and evaporation of each component, the concept of the individual energy level is applied. The relationship between the individual energy level and the xy diagram is presented as well as effects of the reflux ratio and the feed location on the EUD for the whole column. Separation of n-hexane and n-octane is used to illustrate the methodology.

Introduction

To evaluate the energy efficiency of a process, energy analysis based on the first law of thermodynamics used to be considered. However, in the past two decades it has been found that the second law of thermodynamics, which is related directly to the term of exergy, can confirm the quality of energy in process analyses. Subsequently, the basic concept of exergy has been widely applied in chemical process analysis and synthesis. Processes using mainly thermal energy are good targets for exergy analysis. This is especially true and suitable for the integration of heat exchangers, for example.

The term exergy, used by Rant in 1956, is made up of two parts: ex—Latin prefix for *from* or *out*, akin to Greek $\epsilon\xi$(ex) or $\epsilon\xi$o (exo), and $\epsilon\rho\gamma$o∂ (ergon)—Greek for *work*. Thus exergy means the amount of work which can be obtained by using heat reservoir at the reference temperature T_o. Once the term "available energy" was used but now the term "exergy" is preferably accepted in the energy society.

The material balance and energy balance are basically taken into consideration for process design. When the exergy (kJ/s) concept is introduced, the quality of energy can be demonstrated. By this concept, the quality loss, i.e., exergy loss, can be elucidated and be helpful in the evaluation of process systems. Improvement of the process system can also be accomplished by tackling the large exergy loss first, for example.

In general, the distillation process has used a large amount of heat for a separation of a mixture. There were some works in which the methods to improve energy usage in the column were discussed. For example, the effect of the installation of side-cooling and side-heating on the reduction of exergy loss of the whole column was discussed by Naka et al. (1980). By trying to approach the behavior of an adiabatic column or a conventional column to an ideal column (sometimes called reversible column) exergy loss is also reduced significantly (Ishida and Ohno, 1983; Kaiser and Gourlia, 1985; Rivero et al., 1991). Some works were conducted by using the concept of heat integration with other processes or even inside the process itself (Umeda et al., 1979; Linnhoff et al., 1983). By applying heat pump to distillation (Gopichand et al., 1988; Supranto et al., 1988) heat can also be recovered from the column.

Analyzing exergy loss in a distillation column can provide a useful understanding and insights, which will lead to a better design of a distillation system as stated by Fitzmorris et al. (1980). The presentation of exergy loss of a distillation column in a graphic form, by which the information can be visualized more clearly, was discussed by Naka et al. (1980) on a $(1-T_o/T)-Q$, diagram, by Ishida and Ohno (1983) on a energy-direction factor diagram (later they changed the ordinate from direction factor D to energy level A where $A = 1 - D$ (Ishida and Nakagawa, 1985) and called the diagram energy-utilization diagram (EUD)) and by Rivero et al. (1991) on enthalpy-Carnot factor diagram.

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EUD can simultaneously describe the results of the first and the second laws of thermodynamics on a single diagram. Because of its extension from a diagram between $(1 - T_o/T)$ and Q which could provide only information about heat exchange, to a diagram between the energy level A and the energy transformation ΔH, it can be applied to all kinds of energy transformation including physical or chemical processes. The energy balance relations, the exergy losses with their total amount and their distribution, and the strength of forces to drive processes can be found from this diagram.

Ishida and Taprap (1992) had applied the EUD to classify the overall exergy loss into individual components. Following this work, the exergy loss of phase change of each component was presented on the EUD by Ishida and Taprap (1993) by introducing the concept of individual energy level. Recently, Dhole and Linnhoff (1993) have presented the vapor and the liquid composite curves to represent the combined heat- and mass-transfer loss in the column. However, they did not clarify that loss in detail.

In this article, we emphasize a methodology of analyzing the overall exergy loss into individual processes (such as evaporation or condensation of each component or cooling of vapor phase and mixing, etc.) and present their characteristics on the EUD. This graphical method can reveal exergy losses of every type of process that can occur inside a column. Furthermore, this study shows that there is an important relationship between the energy level of an individual process and a well-known xy diagram.

Demonstration of Calculation Model

Mass-transfer model for distillation

Generally, solving a problem in a distillation column is based on an equilibrium model. The reason is because it is simple, and there is no need to compute mass fluxes. However, if one wants to predict more detailed behavior, the equilibrium calculation is insufficient. In this article, a mass-transfer model based on the method of Ito and Asano (1982) is applied. The main assumption of their model is that the rate of evaporation or condensation is vapor-phase controlled. The physical picture of a binary mixture is shown in Figure 1. The model and definitions of each term are explained in Appendix A.

Demonstration of a base case study

A binary mixture used here composes of n-hexane and n-octane (given as component 1 and 2, respectively), and the feed is introduced at the middle of the column by the rate of 100 mol/s with the mole fractions of 0.50 for both components for this base case. The condenser is considered as a total condenser. The reboiler is treated as an equilibrium stage. The total number of plates in this column is chosen as 11 for simplicity. Plate 1 is the condenser, plate 6 the feed, and plate 11 is the reboiler. The reflux ratio R_d is 1.0. The column is assumed to be operated at constant pressure, 1 atm. The compositions of bottoms and of distillate have to be calculated whereas their flow rates are fixed at 50 mol/s.

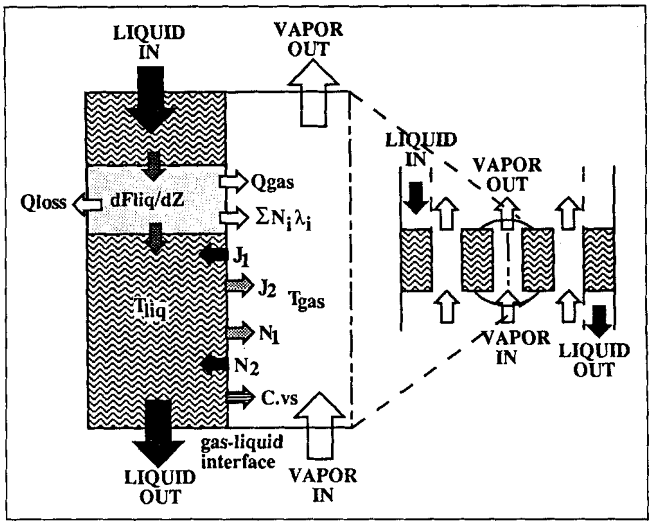

Figure 1. Mass transfer on an individual tray.

The simulation is conducted from the top condenser to the bottom reboiler. The initial values are set at the top of column, such as composition of each liquid component. The specification of each plate is illustrated in Figure 1. At plate 2, for example, the variables at the upper boundary such as the flow rate of liquid phase $F_{\text{liq},1}$ and the flow rate of vapor phase $F_{\text{gas},2}$ have been specified. Then, the mass balance and heat balance in liquid phase or vapor phase are obtained. From the calculation based on the mass flux definition, the amount of each component changed, for example, from liquid phase to vapor phase, can be identified. Then the flow rates of liquid out and of vapor in at the lower boundary in Figure 1 can be calculated. At the same time, by knowing the mole fractions of both phases, the temperatures of the vapor phase and the liquid phase, respectively, can be calculated as the dew-point and bubble-point temperature. Once the calculation for one plate is finished, the next lower one can be calculated similarly. At the reboiler, the calculation is performed by assuming equilibrium. The calculation is repeated until the given criteria for calculation error at the bottom of column is satisfied.

Figure 2 shows the calculated mole fractions of each component in both vapor and liquid phases on the xy diagram by choosing the light component, n-hexane as component 1 and the heavy component n-octane as component 2. Two curves above the diagonal line are for component 1. The uppermost curve is plotted by using the relationship of equilibrium value that is $y_{i,\text{eq}} = K_i x_i$, where the K-value, K_i $(= P_i^o/P)$, is calculated from the thermodynamics properties of each component. Each point on this curve is plotted by using K_i evaluated at liquid temperature of that plate. The second curve shows the simulation result $(x_{j,i}, y_{j,i})$ based on the mass-transfer model, where j refers to a plate and i refers to the component (1: light and 2: heavy one). This curve is generally located below the first curve at every point except at the reboiler, because the equilibrium model is assumed at the reboiler whereas the mass-transfer model are applied to other plates. The deviation between the first and the second curves results from the mass-transfer resistance. The third and the fourth curves, respectively, correspond to the results from the calculation based on the mass-transfer model and the equilibrium relation for component 2. It has a mirror-image to

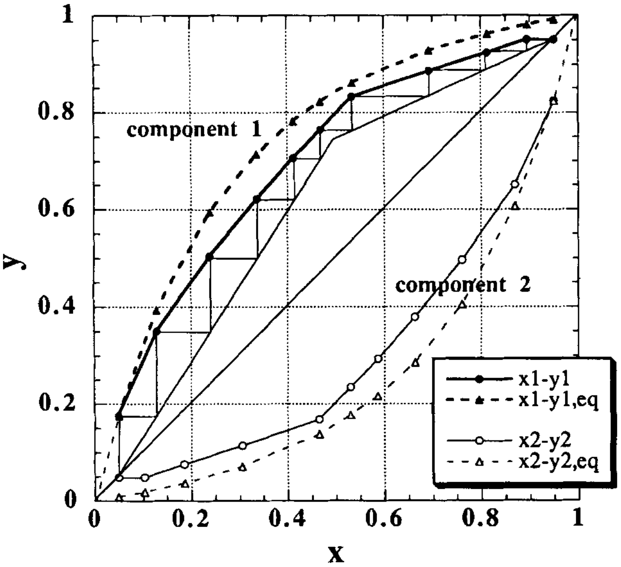

Figure 2. xy diagram of *n*-hexane and *n*-octane for a base case $R_d = 1.0$

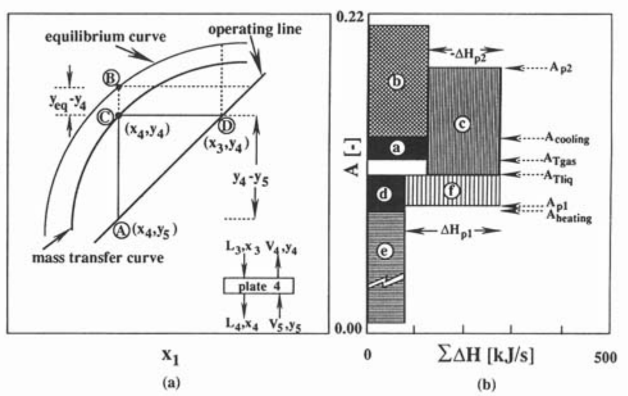

Figure 3. (a) *xy* diagram; (b) EUD diagram of plate 4.

component 1, because $x_2 = 1 - x_1$ and $y_2 = 1 - y_1$, for a binary case. Those curves, (x_1, y_1), $(x_1, y_{1,\text{eq}})$, (x_2, y_2) and $(x_2, y_{2,\text{eq}})$ will be used in the section on the relationship between individual energy level and xy diagram.

Demonstration of Exergy Loss by Heating, Cooling and Mixing

EUD

A EUD has been utilized as a graphic tool in a chemical process analysis. Its fundamental concept is based on the combination of the first law and the second law of thermodynamics. Its abscissa displays the amount of transformed energy/enthalpy of the process. Every process must donate or accept energy at some energy level. The process which donates energy is called energy donor and the one accepts energy be called energy acceptor. Based on the first law of thermodynamics, the amount of transformed energy between these two processes must be equal. If not, the extra part of this energy is called heat loss.

Hence the EUD's characteristic represents the amount of energy transformed from an energy donor to an acceptor by the width along the abscissa (presented by ΔH_{ea}), while their energy levels, A (defined by $1 - T_o \Delta S / \Delta H$) is by the height along the ordinate, i.e., the energy level of an energy donor must be greater than or at least equal to that of an energy acceptor. The exergy loss or exergy destruction caused by this energy transformation is represented by the amount of the area between the energy-donating line and energy-accepting line. Moreover, the driving force to promote the process can be shown by the difference between their energy levels.

The construction of the EUD derived from the concepts of the first law and the second law of thermodynamics is given in Appendix B.

Distribution of exergy loss by heating, cooling and mixing

Figure 3a shows the xy diagram of the light component for plate 4 from the top of the column. Point B is a location of $(x_4, y_{4,\text{eq}})$ on equilibrium curve whereas point C is located on the mass-transfer curve (x_4, y_4). Points A and D, respectively, are (x_4, y_5) and (x_3, y_4) located on the operating line.

Figure 3b shows the distribution of exergy losses of plate 4 on the EUD. There are six kinds of exergy losses (EXL). Those losses are accompanied by the cooling process of the vapor phase, the heating process of the liquid phase, the mixing process of the vapor phase, the mixing process of the liquid phase, the condensation of heavier component, and the evaporation of the lighter component. In this section the former four kinds are demonstrated.

Exergy Loss of Cooling Process of Vapor Phase. The vapor phase which comes from plate 5 has higher temperature and donates heat to plate 4. The donated heat $\Delta H_{\text{cooling}}$ is calculated based on the enthalpy change which is

$$\Delta H_{\text{cooling}} = V_5 \Sigma y_{5,i} [h_{G4,i} - h_{G5,i}] \tag{1}$$

Their average energy level is given by Eq. B4

$$A_{\text{cooling}} = 1 - T_o \Delta S_{\text{cooling}} / \Delta H_{\text{cooling}} \tag{2}$$

where the entropy change is given by

$$\Delta S_{\text{cooling}} = V_5 \Sigma y_{5,i} [s_{G4,i} - s_{G5,i}] \tag{3}$$

The released heat is accepted as heat at the temperature of the vapor phase on plate 4 of which energy level is given by Eq. 4 because the relation $\Delta H = T \Delta S$ holds for heat.

$$A_{T\text{gas}} = 1 - T_o / T_{\text{gas},4}. \tag{4}$$

When we draw the horizontal lines at A_{cooling} (energy level of energy donor) and $A_{T\text{gas}}$ (energy level of energy acceptor) with the width of $\Delta H_{\text{cooling}}$, the exergy loss of cooling process is given as the area ***a*** in Figure 3b.

Exergy Loss of Mixing Process of Vapor Phase. We calculate the exergy loss of mixing of the vapor phase by assuming that the vapor phase from plate 5 is mixed with the huge amount of vapor phase on plate 4. The meaning of this assumption called the premixing concept will be mentioned later in the relation to the phase change, i.e., the condensation and the evaporation. This exergy loss (EXL, kJ/s) shown as area ***b*** is calculated by

$$EXL_{\text{mixing}} = T_o \Delta S_{\text{mixing}}. \tag{5}$$

According to the premixing concept (Ishida and Chuang, 1990), ΔS_{mixing} can be calculated from the relation of

$$\Delta S_{\text{mixing}} = -R\Big[(V_5 + V_{ex,4}) \sum y_{ex,4,i} \ln y_{ex,4,i} - V_5 \sum y_{5,i} \ln y_{5,i} - V_{ex,4} \sum y_{4,i} \ln y_{4,i}\Big]. \tag{6}$$

The term $V_{ex,4}$ is the assumed stream of the abundant amount of which the composition, temperature and pressure are the same as stream V_4 and having an enormous flow rate compared to the stream V_5. When the term $V_{ex,4}$ is very large and the term $y_{ex,4,i}$ approaches $y_{4,i}$, the above relation can become (Ishida and Taprap, 1992)

$$\Delta S_{\text{mixing}} = -RV_5 \sum [y_{(5,i)}\{\ln y_{(4,i)} - \ln y_{(5,i)}\} - \{y_{(4,i)} - y_{(5,i)}\}]. \tag{7}$$

For an ideal solution, ΔH_{mixing} is zero and the value of A_{mixing} ($= 1 - \Delta S_{\text{mixing}}/\Delta H_{\text{mixing}}$) cannot be evaluated. Hence the exergy loss of mixing is displayed as the area on EUD by using the scale on abscissa as same as the amount of ($-\Delta H_{\text{cooling}}$) and setting the height as $EXL_{\text{mixing}}/(-\Delta H_{\text{cooling}})$. Hence the ordinate value for vapor mixing has no physical meaning except the area ***b*** which represents its exergy loss.

Exergy Losses of Heating and Mixing Processes of Liquid Phase. The procedure to obtain the exergy losses of the heating process and of the mixing process of the liquid phase is similar to that of the vapor phase. The liquid phase which comes from plate 3 has lower temperature and accepts heat from plate 4. The accepted heat $\Delta H_{\text{heating}}$ is also calculated based on the enthalpy change which is

$$\Delta H_{\text{heating}} = L_3 \sum x_{3,i}[h_{L4,i} - h_{L3,i}] \tag{8}$$

Their average energy level is given by Eq. B4

$$A_{\text{heating}} = 1 - T_o \Delta S_{\text{heating}}/\Delta H_{\text{heating}} \tag{9}$$

where $\Delta S_{\text{heating}}$ is computed by

$$\Delta S_{\text{heating}} = L_3 \sum x_{3,i}[s_{L4,i} - s_{L3,i}]. \tag{10}$$

The heat is donated at the temperature of the vapor phase of plate 4 of which energy level is given by $A_{T\text{liq}} = 1 - T_o/T_{\text{liq},4}$ is represented by the upper line of block ***d***. The energy level of heating process A_{heating}, i.e., energy acceptor, is represented by the lower line of the block ***d***. When we draw the horizontal lines at A_{heating} and $A_{T\text{liq}}$ with the width of $\Delta H_{\text{heating}}$, the exergy loss of heating process is given as the area ***d*** in Figure 3b.

The procedure for drawing the exergy loss of the mixing process in the liquid phase, area ***e***, is obtained in the same manner as in drawing area ***b*** for the vapor phase.

Demonstration of Exergy Loss by Evaporation and Condensation

Individual energy level

This concept (Ishida and Taprap, 1993) is based on the changes of partial enthalpy and partial entropy for phase change of each component. By using this concept, the exergy analysis of condensation or evaporation of each component in a distillation column can be obtained and its exergy loss can be shown as an area on the EUD. The detail of this concept is given in Appendix C.

Distribution of exergy loss by evaporation and condensation

The other two kinds of exergy losses are caused by phase changes, i.e., evaporation and condensation. For condensation of the heavier component 2, for example, the energy released by condensation is calculated by $-\Delta H_{p2}$ whereas its individual energy level is given by A_{p2} as explained in Appendix C.

$$-\Delta H_{p2} = -n_{p2}\Delta h_{p2}$$

$$A_{p2} = 1 - (T_o \Delta s_{p2}/\Delta h_{p2}). \tag{11}$$

The terms of Δh_{p2} and Δs_{p2} correspond to $(\bar{h}_{2,G} - \bar{h}_{2,L})$ and $(\bar{s}_{2,G} - \bar{s}_{2,L})$, respectively, and n_{p2} denotes the number of moles condensed per unit time for the present plate.

It is assumed that the condensation of component 2 takes place at the temperature (K) of liquid T_{liq}. Its energy level $A_{T\text{liq}}$ is given as $A_{T\text{liq}} = 1 - T_o/T_{\text{liq}}$. Hence the exergy loss of the condensation is represented by the area ***c***. Since the condensation of component 2 acts as the energy donor, its energy level A_{p2} should appear above the energy level of the acceptor $A_{T\text{liq}}$. We may say that once component 2 has its energy level A_{p2} higher than the energy level of the liquid phase $A_{T\text{liq}}$, it means condensation of component 2 may occur.

Similarly, the exergy loss of the evaporation of component 1, the lighter component may be drawn as area ***f*** on the diagram. The width of the block ***f*** corresponds to the amount of energy required for evaporation of component 1. Its energy level is shown by the level at A_{p1}. When the evaporation takes place, it receives energy. Hence, the evaporation of this component acts as the energy acceptor. Consequently, its energy level appears below the line of $A_{T\text{liq}}$.

The difference of the energy level between each component A_{pi} and of liquid temperature level $A_{T\text{liq}}$ shows the driving force of that process. The larger the driving force is, the easier the process can generally occur. In Figure 3b, for example, component 1 has a smaller driving force than component 2 (the gap between level A_{p1} and level $A_{T\text{liq}} <$ the gap between A_{p2} and $A_{T\text{liq}}$), meaning that the former cannot proceed so easily as the latter. However, the mole fraction x_1 ($= 0.6939$) is much higher than y_2 ($= 0.1143$), giving rise to the result that the rate of evaporation of component 1 which is proportional to ΔH_{p1} is larger than the rate of condensation of component 2 which is proportional to $-\Delta H_{p2}$.

In the above calculation, we used the constant concentration on a plate for both the vapor phase and the liquid phase. By the premixing concept, the vapor phase rising from the lower plate has been assumed to be mixed with the abundant amount of the vapor phase of the present plate; hence, the composition of the vapor may be considered constant.

Figures 3a and 3b show the implicit information. The path AC in Figure 3a is related to the change of the vapor phase which is composed of the exergy losses of both area ***a*** (cooling process) and ***b*** (mixing process); the path CD is related to the change of the liquid phase which is composed of exergy losses of area ***d*** (heating process) and ***e*** (mixing process). The path BC is related to the exergy loss of evaporation of component 1 and this point is discussed in detail in the next section.

Relationship between individual energy level and xy diagram

The definition of an individual energy level of component i, A_{pi}, is given as

$$A_{pi} = 1 - \frac{T_o \Delta \bar{s}_i}{\Delta \bar{h}_i} \tag{12}$$

where the partial enthalpy change of component i in mixture $\Delta \bar{h}_i$ and the partial entropy change $\Delta \bar{s}_i$ (kJ/mol·K) are represented by the following equations, say for its evaporation

$$\Delta \bar{h}_i = \bar{h}_{g,i} - \bar{h}_{l,i} = h^o_{g,i} - h^o_{l,i} = \Delta h^o_i \tag{13}$$

$$\begin{aligned} \Delta \bar{s}_i &= \bar{s}_{g,i} - \bar{s}_{l,i} \\ &= (s^o_{g,i} - R \ln y_i) - (s^o_{l,i} - R \ln x_i) \\ &= \Delta s^o_i - R \ln (y_i/x_i) \end{aligned} \tag{14}$$

For equilibrium of component i, we have $\Delta g_{i,eq} = 0$, yielding the following equation

$$\Delta h_{i,eq} - T \Delta s_{i,eq} = 0 \tag{15}$$

where $\Delta h_{i,eq} = h^o_{g,i} - h^o_{l,i}$ and $\Delta s_{i,eq} = \Delta s^o i - R \ln (y_{i,eq}/x_i)$. By inserting Eqs. 13 and 14 in Eq. 12 and using Eq. 15, we can have the final relationship where A_T is defined as $(1 - T_o/T)$ or $(1 - T_o \Delta s_{i,eq}/\Delta h_{i,eq})$.

$$A_T - A_{pi} = \frac{RT_o}{\Delta h^o_i}\left[\ln \frac{y_{i,eq}}{x_i} - \ln \frac{y_i}{x_i}\right]$$

$$\Delta A = \frac{RT_o}{\Delta h^o_i}[\ln y_{i,eq} - \ln y_i] \tag{16}$$

The lefthand side of Eq. 16 represents the driving force of the process. The righthand side gives its physical meaning: when we plot the *xy* relation on logarithmic scale as shown in Figure 4, the difference of $(\ln y_{i,eq} - \ln y_i)$ is proportional to the driving force of that process. It is to be noted that Eq. 16 can hold for a ternary or a general multicomponent mixture. So this equation may give a clear image for the driving force of phase change ΔA.

The xy diagram is very intuitive and convenient. However its convenience is limited only to a binary system. The driving force given by the difference between the individual energy level and the level of liquid temperature is proportional to $(\ln y_{eq} - \ln y)$. Hence this driving force for condensation or evaporation on the EUD is found to inherit the advantage of xy diagram.

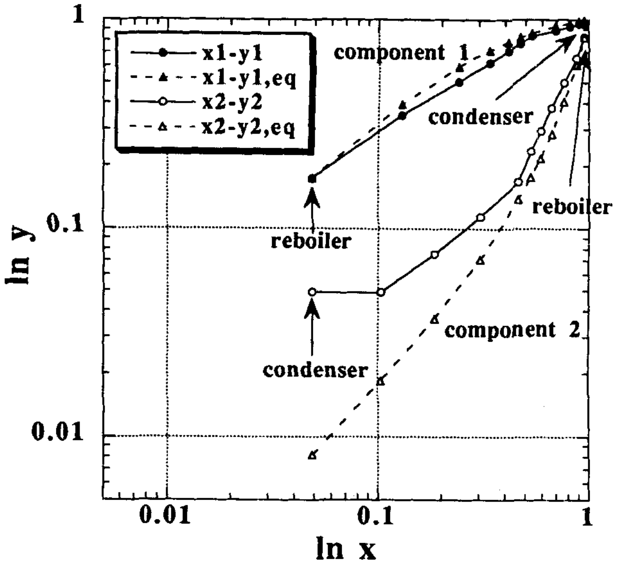

Figure 4. ln x-ln y diagram of *n*-hexane and *n*-octane for a base case $R_d = 1.0$.

Demonstration of Exergy Loss for a Whole Column

Distribution of overall exergy loss for a base case

Figure 5 shows the EUD of the whole column for a base case. Each small frame represents the EUD of each plate and its order from top to bottom is from left to right. For the condenser (plate 1: the leftmost) and the reboiler (plate 11: the rightmost), the width of the frame is set at 5,000 kJ/s, while the width of the other blocks for other plates at 700 kJ/s. This figure illustrates the following tendencies of the exergy loss of individual processes for the separation of n-C_6H_{14} and n-C_8H_{18}.

Heating and Cooling

- The exergy loss by the heating of the liquid phase and by the cooling of the vapor phase is not significant for both in the rectifying section and the stripping section.

Mixing

- The exergy loss by mixing is significant.

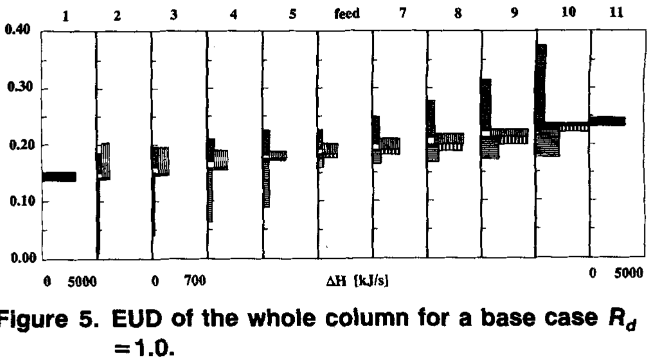

Figure 5. EUD of the whole column for a base case $R_d = 1.0$.

- In the stripping section, this loss in both vapor and liquid phases increases with increasing plate number.
- In the rectifying section, this loss in both vapor and liquid phase is not significantly changed with increasing plate number.

Phase Change: Evaporation and Condensation

- The exergy loss caused by the phase change is comparable to the exergy loss of mixing in this case.
- For each component, the width represents ΔH (enthalpy change, kJ/s) and hence it is proportional to the amount of evaporation or condensation. In the stripping section, $-\Delta H_{p2}$ is generally larger than ΔH_{p1}, meaning that the amount of condensation exceeds that of evaporation. On the contrary, in the rectifying section, ΔH_{p1} is generally larger than $-\Delta H_{p2}$, meaning that the amount of evaporation exceeds that of condensation.
- For the heavy component, component 2, the gap between A_{p2} and $A_{T\text{liq}}$ is the greatest at the plate 2, and decreases with increasing plate number whereas the light component, component 1, shows the opposite tendency except at the plate next to the reboiler. This gap corresponds to the driving force for evaporation or condensation and comparison between Figures 4 and 5 shows that it is proportional to $(\ln y_{1,eq} - \ln y_1)$ or $(\ln y_2 - \ln y_{2,eq})$.

For the binary base case, $y_{1,eq} - y_1$ is equal to $y_2 - y_{2,eq}$. But $A_{p2} - A_{T\text{liq}}$ is greater than $A_{T\text{liq}} - A_{p1}$ except in the plate near the reboiler because $\ln y_2 - \ln y_{2,eq}$ is greater than $\ln y_{1,eq} - \ln y_1$ for $y_2 < y_1$.

When we look at the EUD of Figure 5, we can find for this binary mixture that the biggest loss of exergy on each plate of the column is the mixing process especially in the stripping section. The exergy losses of the cooling process and heating process are quite small since the temperatures of vapor phase and of liquid phase are slightly changed from plate to plate (see the white block in the middle of the graphic display). The potential of phase change, i.e., the condensation of component 2 and the evaporation of component 1, can be found from the height and the width of each block for each component. This kind of information can be helpful for process design and operation. In this manner, the EUD reveals the energy distribution as well as its exergy loss of each subprocess from plate to plate in a distillation column. From this point of view, we can visualize the process phenomena by a graphic display and we can pinpoint where we should pay attention such as where the exergy loss is large or where the driving force is small and so on.

We may summarize the features of the EUD as follows:

- Visualization of the amount of energy transformation by width.
- Visualization of the exergy loss by area.
- Visualization of the energy level of each component by height.
- Visualization of the driving force by gap.

Effect of reflux ratio

Figure 6 shows the mole fraction of the component 2 in the distillate and the heat supplied by the reboiler when the reflux ratio is changed by keeping other conditions the same with the exception of the product composition. The minimum of $x_{2,d}$ means the maximum of the separation performances.

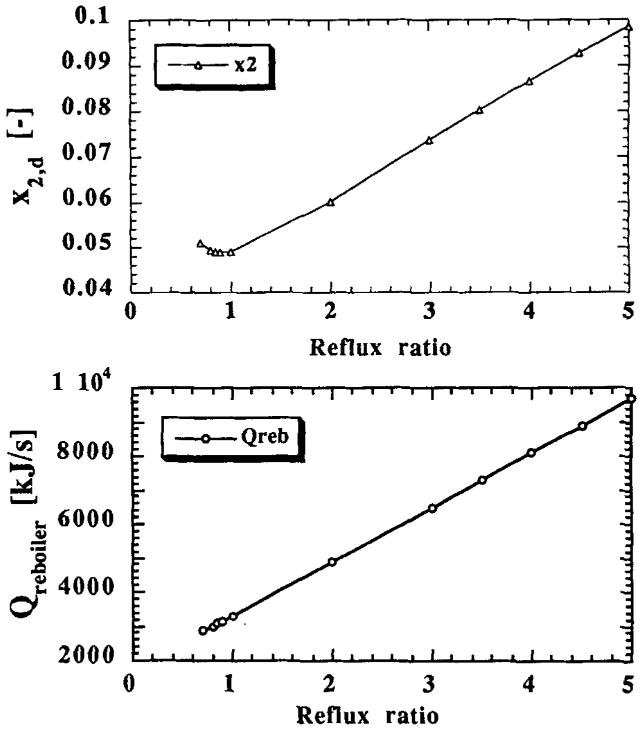

Figure 6. Separation performance and heat requirement at reboiler for different reflux ratio.

When the reflux ratio is too great, both heat requirement and $x_{2,d}$ are great. Figures 7 and 8 show the EUDs when the reflux ratios are 2.0 and 0.85. The exergy loss of each plate is large when the reflux ratio is 2.0. Hence too much exergy loss is found to yield low separation performance. However, when the reflux ratio is as small as 0.85, as shown in Figure 8, the gap between $A_{T\text{liq}}$ and A_{p1} becomes nearly zero at plate 5. So too small a driving force, i.e., pinch in mass transfer, is found to make separation performance poor.

Effect of feed location

Figure 9 shows the mole fraction of the component 2, $x_{2,d}$ in the distillate and the heat supplied to the reboiler when the feed location is changed by keeping other conditions the same except the product composition. The maximum performance can be seen when the feed is at the middle of the column. When the feed location is too close to the condenser or to the reboiler, $x_{2,d}$ becomes large. Figures 10 and 11, respectively, show the EUDs when plates 5 and 8 are the

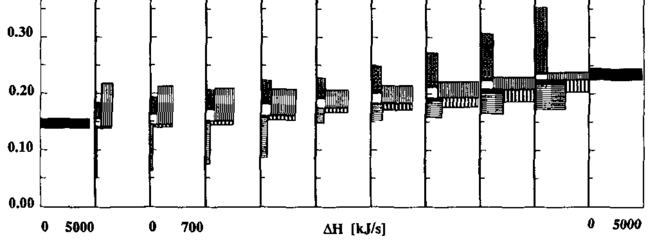

Figure 7. EUD of the whole column when $R_d = 2.0$.

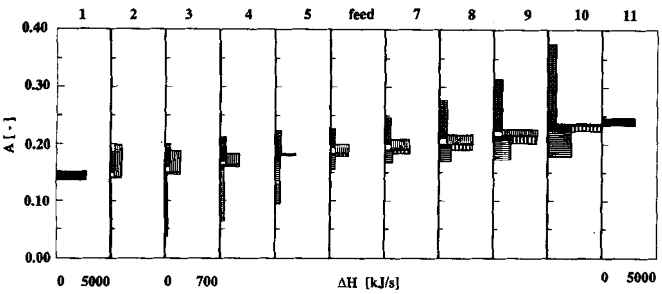

Figure 8. EUD of the whole column when $R_d = 0.85$.

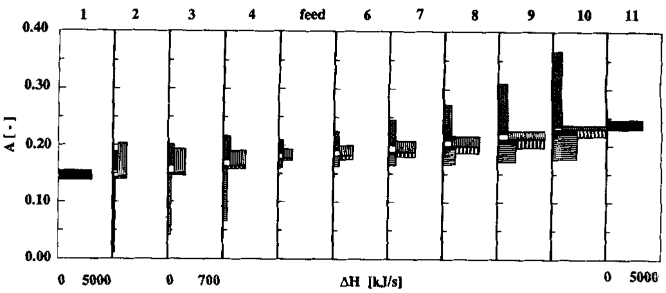

Figure 10. EUD of the whole column when feed location is at plate 5.

feed locations. We can see that the heat exchange for phase change i.e., $-\Delta H_{p2}$ and ΔH_{p1} at plate 5 in Figure 10 and at plate 7 in Figure 11 are very small. This means enough evaporation or condensation does not take place on those plates. Hence very small heat exchange for some plate in the column yields low separation performance.

Drawing of EUD Based on Experimental Data

We have demonstrated the characteristic features of the EUD for a distillation column based on the simulation result from the mass-transfer model. And by introducing the individual energy level concept, we have displayed the energy level and exergy loss of the phase change of each component graphically. However, the EUD can be generated from any model if there are available simulation data or even experimental data. One can draw an EUD of a distillation column as will be explained step by step as follows:

(1) Assume that we have the following experimental data; the amount of distillate and its composition (D (mol/s), x_d), the amount of bottoms and its composition (B, x_b) and, at each plate j, temperature (T_j), pressure (P_j (Pa)), composition of outlet stream of liquid phase as well as of vapor phases ($x_{j,i}$ and $y_{j,i}$) of all components.

(2) From (1), we can have flow rates of liquid phase (L_j (mol/s)) and of vapor phase (V_j (mol/s)) at any plate by mass balance from the following equations.

$$V_{j+1} = L_j + D$$

$$V_{j+1} y_{j+1,i} = L_j x_{j,i} + D x_{d,i}$$

$$V_j + L_j = V_{j+1} + L_{j-1}$$

$$V_j y_{j,i} + L_j x_{j,i} = V_{j+1} y_{j+1,i} + L_{j-1} x_{j-1,i}$$

(3) From thermodynamic properties, we can calculate enthalpy and entropy of the inlet streams and the outlet streams at plate j. Then, the enthalpy change and the entropy change of the heating process and the cooling process can be obtained by applying Eqs. 1 through 3 for cooling (area ***a*** in Figure 3b) and Eqs. 8 through 10 for heating (area ***d*** in Figure 3b). Then we can draw the blocks with A_{cooling} and A_{heating}.

(4) Similar to step 3, exergy loss caused by mixing can be obtained by applying Eq. 7 (area ***b*** and ***e*** in Figure 3b). Then, mixing blocks can be also drawn on EUD.

(5) For phase change of each component, by knowing the flow rate and its composition for both phases, the amount of each component transferred from liquid to vapor phase, or vice versa, can be calculated. This amount is a mass flux of each component. By using Eq. 11, the amount of enthalpy change of condensation or evaporation of each component can be calculated. In addition, by using the advantage of the relationship of individual energy level and the xy diagram on logarithmic scale from Eq. 16, the EUD for phase change (area ***c*** and ***f*** in Figure 3b) can be drawn immediately.

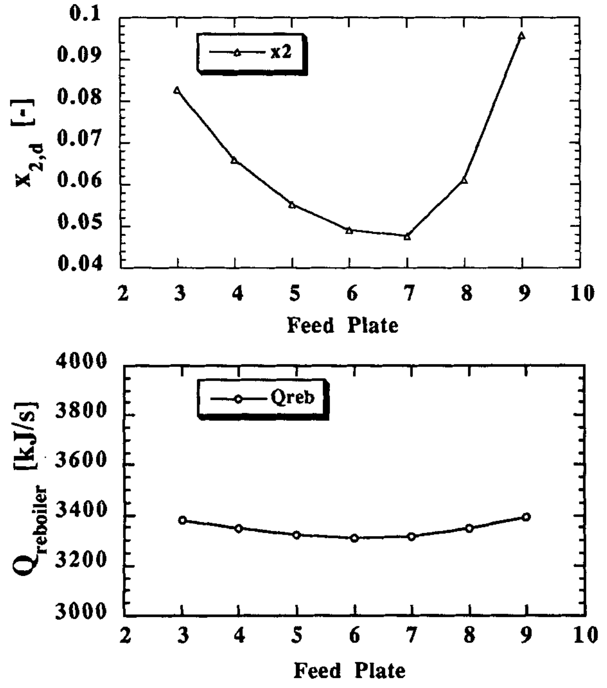

Figure 9. Separation performance and heat requirement at reboiler for different feed location.

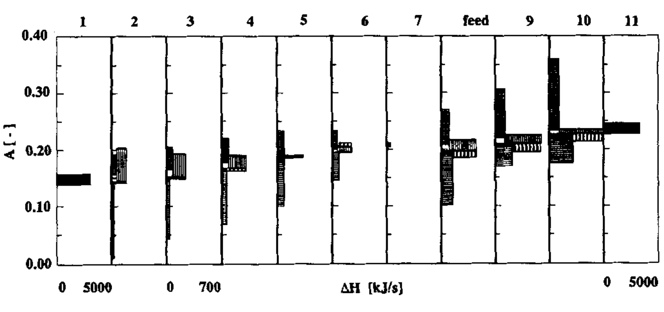

Figure 11. EUD of the whole column when feed location is at plate 8.

Conclusion

Starting from a mass-transfer model coupled with mass and heat balance, we are able to develop the EUD for a distillation column with relation to the xy diagram in logarithmic scale. The diagrams identify the amount of energy transformation and exergy loss of an individual process, as well as the heating and mixing of the liquid phase, cooling and mixing of the vapor phase and phase changes. The optimal separation performance is found to be obtained by decreasing exergy loss, avoiding too small driving force for phase change, i.e., pinch in mass transfer, and avoiding too small heat exchange at a certain plate. The EUD can be drawn also on experimental data.

Notation

B = flow rate of bottoms stream, mol/s
D_{ij} = binary diffusion coefficient, m^2/s
F = flow rate of feed, mol/s
$h_{Gj,i}$ = molar enthalpy of ith component in vapor phase, kJ/mol
$h_{Lj,i}$ = molar enthalpy of ith component in liquid phase, kJ/mol
J_i = diffusional flux of ith component, $mol/m^2 \cdot s$
N_i = mass (molar) flux of ith component, $mol/m^2 \cdot s$
P_i^o = vapor pressure of ith component, Pa
Q = heat added or removed at jth plate, kJ/s
R = gas constant, $kJ/mol \cdot K$
$s_{Gj,i}$ = molar entropy of ith component in vapor phase, $kJ/mol \cdot K$
$s_{Lj,i}$ = molar entropy of ith component in liquid phase, $kJ/mol \cdot K$

Subscripts

c = condenser
d = distillate
ea = energy acceptor
ed = energy donor
N = reboiler
o = reference state (298.15 K)
p = subprocess
s = vapor-liquid interface

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Appendix A: Mass Transfer Model for Distillation

It is assumed that the rate of phase change is determined by the mass transfer in the vapor phase and that the mass flux N_i is composed of the diffusional flux J_i and the convective flux $Cv_s y_{si}$

$$N_i = J_i + Cv_s y_{si} \tag{A1}$$

where C (mol/m^3) is the molar concentration of vapor phase, v_s (m/s) is the interfacial velocity from liquid phase to vapor phase, and y_{si} is the mole fraction of vapor phase at interface. To solve Eq. A1, Ito and Asano (1982) applied the following equation for mass transfer in a cylindrical wall

$$Sh_i\left(\frac{J_i}{N_i}\right) = \frac{J_i D_o}{CD_i(y_{si} - y_i)}$$

$$= \left[3.66 + \frac{0.0668[\pi/4G_i]^{-1}}{1 + 0.04[\pi/4G_i]^{-2/3}}\right] \cdot \exp(-0.1098\ Re \cdot Sc) \tag{A2}$$

where D_o is a diameter of a hole through which vapor phase goes up and G_i is Graetz number. The term $\pi/(4G_i)$ can be equal to $D_i Z/D_o^2 U$ where U (m/s) is vapor phase velocity and Z (m) is an average height of vapor phase. Re is Reynolds number and Sc is Schmidt number.

The values of the parameters used in this study are as follows: $D_o = 0.003$ m; $Z = 0.10$ m. We indirectly use Re and Sc (in Eq. A2) as the term of interfacial velocity (v_s), diffusion coefficient (D_i), and hole diameter (D_o) (m^2) from the relationship of $\exp(-0.1098\ Re \cdot Sc) = \exp(-0.1098\ v_s \cdot D_o/D_i)$.

D_i (m^2/s) is an effective diffusion coefficient of component i in the multicomponent mixture calculated from Wilke's equation

$$\frac{1}{D_i} = \sum_{j \neq i} \frac{1}{D_{ij}} \left(y_{sj} - \frac{J_j}{J_i} y_{si} \right) \tag{A3}$$

Ito and Asano (1982) integrated the mole fraction of the vapor phase along the axial height, but in this article Sh_i is obtained at the average height for simplicity.

Appendix B: EUD

Every process donates or accepts energy at some energy level. Based on the first and second laws of thermodynamics, the following equations are obtained, respectively (Ishida and Kawamura, 1982).

$$\Delta H_{ed} + \Delta H_{ea} = 0 \tag{B1}$$

$$\Delta S_{ed} + \Delta S_{ea} \geq 0 \tag{B2}$$

The exergy change of energy donor ($\Delta \epsilon_{ed}$) or of energy acceptor ($\Delta \epsilon_{ea}$) is defined by the following equation, where T_o is the environmental temperature

$$\Delta \epsilon_k = \Delta H_k - T_o \Delta S_k = \Delta H_k A_k \quad (k\text{: } ed \text{ or } ea) \tag{B3}$$

where A_k is the energy level indicating the quality of energy donated or accepted, defined as follows

$$A_k = \Delta \epsilon_k / \Delta H_k = 1 - T_o \Delta S_k / \Delta H_k \tag{B4}$$

For energy exchange between an energy donor and an energy acceptor, we have exergy loss as

$$\begin{aligned} EXL &= -\sum_k \Delta \epsilon_k = -\sum_k (\Delta H_k A_k) \\ &= -\Delta H_{ed} A_{ed} - \Delta H_{ea} A_{ea} \\ &= \Delta H_{ea}(A_{ed} - A_{ea}) \geq 0 \end{aligned} \tag{B5}$$

Since ΔH_{ea} is always positive, the energy level of the donor A_{ed} should be greater than or equal to that of the acceptor A_{ea}. Equation B5 is the feature of EUD. The value of ΔH_{ea} is plotted on the abscissa and the value of A_{ed} and A_{ea} are plotted on the ordinate. Hence, the area on the diagram represents the exergy loss.

Appendix C: Individual Energy Level

Generally, the enthalpy change ΔH_p and the entropy change ΔS_p are described as

$$\Delta H_p = H_{\text{out}} - H_{\text{in}} = \Sigma n_{i,\text{out}} \bar{h}_i - \Sigma n_{i,\text{in}} \bar{h}_i \tag{C1}$$

$$\Delta S_p = S_{\text{out}} - S_{\text{in}} = \Sigma n_{i,\text{out}} \bar{s}_i - \Sigma n_{i,\text{in}} \bar{s}_i \tag{C2}$$

When the process p consists of two subprocesses $p1$ and $p2$, the above relation can be converted to

$$\Delta H_p = \Delta H_{p1} + \Delta H_{p2} = n_{p1} \Delta h_{p1} + n_{p2} \Delta h_{p2} \tag{C3}$$

$$\Delta S_p = \Delta S_{p1} + \Delta S_{p2} = n_{p1} \Delta s_{p1} + n_{p2} \Delta s_{p2} \tag{C4}$$

where n_{p1} and n_{p2}, respectively, denote the extent of the subprocesses p_1 and p_2 where n is positive for evaporation and negative for condensation. The enthalpy change Δh_{pj} and entropy change Δs_{pj} for each subprocess can be obtained by applying the partial molar enthalpy and entropy. For example, the evaporation of light component 1 Δh_{p1} and Δs_{p1} are described as

$$\Delta h_{p1} = \bar{h}_{1,G} - \bar{h}_{1,L} \tag{C5}$$

$$\Delta s_{p1} = \bar{s}_{1,G} - \bar{s}_{1,L} \tag{C6}$$

Exergy loss for evaporation of component 1 and condensation of component 2 with heat supply ΔH_Q at the energy level A_Q is defined as

$$\begin{aligned} EXL &= -[n_{p1}(\Delta h_{p1} - T_o \Delta s_{p1}) + n_{p2}(\Delta h_{p2} - T_o \Delta s_{p2}) + \Delta H_Q A_Q] \\ &= -[n_{p1} \Delta h_{p1}[1 - (T_o \Delta s_{p1}/\Delta h_{p1})] + n_{p2} \Delta h_{p2}[1 - (T_o \Delta s_{p2}/\Delta h_{p2})] + \Delta H_Q A_Q] \\ &= -[\Delta H_{p1} A_{p1} + \Delta H_{p2} A_{p2} + \Delta H_Q A_Q] \end{aligned} \tag{C7}$$

where A_{pj} is the energy level of the individual process j represented by

$$A_{pj} = 1 - (T_o \Delta s_{pj}/\Delta h_{pj}) \tag{C8}$$

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