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A Shortcut Method for Modeling Multi-Component Distillation in an Existing Column

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Abstract A shortcut method suitable for modeling multicomponent distillation in an existing reboiled or steam-stripped column is presented in this paper. The model employs a new approach to convert industry specification into key component recoveries suitable for application in shortcut distillation modeling. It computes flowrates, compositions and temperatures of product fractions, as well as the heat duties of the column, and generally avoids iterative calculations that can result in convergence problems when applied to optimization. Application of the method to case studies involving a reboiled column and a steam-stripped column are discussed. The predictions from the model are considered to be in good agreement with those reported for rigorous HYSYS model, for both the reboiled and the steam-stripped columns.

Keywords Multicomponent distillation, Shortcut model, Key component recoveries, Existing column

1. Introduction

Engineering processes are usually complex; hence a simple change in one of the variables may result in complex and non-linear changes in other variables. This complex situation can be handled diligently by gaining an insight into a particular process using mathematical models. A mathematical model being a simplified mathematical representation of those aspects of an actual process that are being investigated [1].

Various rigorous and shortcut models have been proposed and applied to distillation operations. These models are usually based on the established physical relationships existing within the distillation column and its associated heat exchanger network, as well as some underlying assumptions. Rigorous distillation models are executed through stage by stage calculations, and are composed of equations which include total and component material balances and corresponding energy balances that account for heat losses, equilibrium equations, physical property equations and summation equations. Rigorous models though more accurate than the shortcut models, have convergence problems and are more difficult to apply in optimization schemes.

Shortcut distillation models relate the feed and product compositions in a distillation process to the number of stages employed, without considering the composition profile across the length of the column. They are quicker to solve, do not have significant convergence problems and are more robust than rigorous models for column optimization [2]. The Fenske–Underwood - Gilliland (FUG) model is the most commonly applied multi-component distillation shortcut model, and most other shortcut models are modifications of this. The limiting assumptions upon which this model is based include, (i) constant molar overflow within each column section, (ii) constant relative volatilities throughout the column, (iii) the column stages are equilibrium stages and (iv) two primary (key) components can be used to model the process [3]. The advantages of the short-cut methods over the more rigorous methods lie in the simplicity of calculation and robustness in convergence. Hence the shortcut methods have been extensively used to provide a good preliminary design, which is used to initiate a more rigorous design of a conventional column [4]. The FUG model was originally developed for simple distillation columns employing reboilers. Many industrial distillation columns have complex configurations, while some use live steam as the separating agent instead of a reboiler. A typical example is the atmospheric CDU of a refinery which employs live steam and has complex column configuration.

In recent times, a number of researchers have extended the application of the shortcut modeling approach to accommodate complex column configurations and operating conditions. Many of these methods employ the Fenske and Underwood equations in the models, and also apply stage by stage calculations in the stripping sections of steam-stripped columns ([5]; [2]; [6]; [7]). Application of the Underwood equation requires iterative procedures, which can result in convergence problems. Also, stage by stage calculation of the stripping section stages makes the methods semi-rigorous. The shortcut method presented in this work does not employ the Underwood equation, and does not require flash calculations in the stripping section of a steam-stripped column.

2. Model Development

The application of shortcut models to industrial distillation require, a suitable means of computing equilibrium relations; the selection of appropriate key components and determination of their associated recoveries that satisfy the plant specifications, and a means of computing the enthalpy of streams, for the estimation of the heat duties of the column. The shortcut modeling approach presented in this work combines, the Fenske equation, material balances in terms of component recoveries, energy balances for total streams, and summation equations to model distillation columns like the one depicted in Figure 1. Thermophysical properties are estimated from suitable established correlations. To account for the effect of stripping steam, a modified overall column efficiency is applied to the stripping section of a steam-stripped column instead of a stage by stage flash calculation.

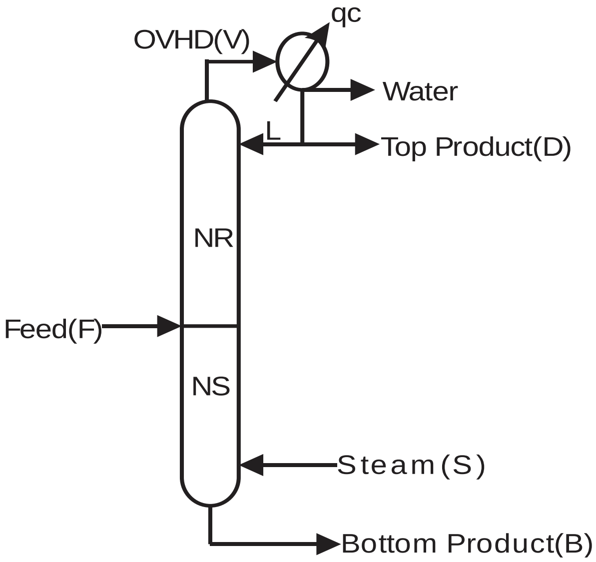

Figure 1: Simple Steam-stripped Column

2.1. Material and Energy Balances

Material and Energy balances can be written for the simple steam-stripped column shown in Figure (1) in terms of the fractional recovery of the key components (R_{LK} and R_{HK}).

Component balances:

$$R_{LK} = \frac{Dx_{dLK}}{Fx_{fLK}} \quad (1)$$

$$R_{HK} = \frac{Bx_{bHK}}{Fx_{fHK}} \quad (2)$$

Total material balance:

$$F = D + B \quad (3)$$

Energy balance (Total Stream):

$$Fh_f + SH_s = Dh_d + Bh_b + q_c \quad (4)$$

2.2. Estimation of the relative volatilities of components

The K-values are required for estimating the relative volatilities of the components in a stream or product fraction. The relative volatility of a component 'i' with respect to another component 'r' is defined as in Equation (5).

$$\alpha_{i-r} = \frac{K_i}{K_r} \qquad (5)$$

Various equations of state are commonly used to compute component K-values. Where the K-values are required to be calculated repeatedly, easy to use correlations having the form of Equation (6), such as the one proposed by [8] have being applied ([9]; [10]; [11]).

$$K_i = \frac{P_{ci}}{P}\exp[(1+\omega_i)f(T_{ri})] \qquad (6)$$

To compute relative volatilities in this work, the K-values were estimated from a modified form of the Wilson correlation which the author proposes as defined in Equation (7).

$$K_i = \left(\frac{P_{ci}}{P}\right)^{0.745}\exp\left[5.37(1+\omega^{0.714})\left(1-\left(\frac{T_{ci}}{T}\right)^{0.755}\right)\right] \qquad (7)$$

2.3. Selection of Key Components and Computation of their recoveries

In the industry, product quality is specified in terms of the boiling point range, temperature gaps (i.e. T5:T95 gap), and cut points, while shortcut methods use key components and their recoveries to specify separation (i.e. LK, HK, R_{LK} and R_{HK}). In themethod applied, a procedure described by [7] is used to select the key components, while the recoveries of the key components are determined by a new approach proposed below.

The Fenske equation can be written in terms of the key component compositions as,

$$N_{min} = \frac{\mathrm{Log}\left[\frac{(x_{dLK})(x_{bHK})}{(x_{dHK})(x_{bLK})}\right]}{\mathrm{Log}\left(\frac{\alpha_{LK}}{\alpha_{HK}}\right)} \qquad (8)$$

Equation (8) can be partitioned into two, to give the minimum number of stages for the rectifying and stripping sections respectively as follows,

$$N_{min\,(R)} = \frac{\mathrm{Log}\left[\frac{(x_{dLK})(x_{FSHK})}{(x_{dHK})(x_{FSLK})}\right]}{\mathrm{Log}\left(\frac{\alpha_{LK}}{\alpha_{HK}}\right)} \qquad (9)$$

$$\frac{\mathrm{Log}\left[\frac{(x_{bHK})(x_{FSLK})}{(x_{bLK})(x_{FSHK})}\right]}{\mathrm{Log}\left(\frac{\alpha_{LK}}{\alpha_{HK}}\right)} \qquad (10)$$

Where x_{FSHK} and x_{FSLK} are the liquid compositions of the heavy and light key components at the feed stage respectively.

The ratio of the liquid compositions of the key components at the feed stage may be approximated by the ratio of the key components compositions in the feed, so that Equations (9) and (10) can be written in terms of the feed compositions. This approximation will be more accurate if the feed tray had been optimally located, and if the feed is predominantly liquid. Rearranging these equations so that they are expressed in terms of the key component recoveries gives;

$$R_{LK} = (1 - R_{HK})\alpha_{LK-HK}^{N_{min}(R)} \qquad (11)$$

$$R_{HK} = (1 - R_{LK})\alpha_{LK-HK}^{N_{min}(S)} \qquad (12)$$

Equations (11) and (12), can be solved simultaneously to obtain the key components recoveries in terms of the minimum number of stages in the two sections of the column as,

$$R_{LK} = \frac{\alpha_{L-H}^{Nmin\ (R)}\left(1-\alpha_{L-H}^{Nmin\ (S)}\right)}{1-\left(\alpha_{L-H}^{Nmin\ (R)}\alpha_{L-H}^{Nmin\ (S)}\right)} \qquad (13)$$

$$R_{HK} = \frac{\alpha_{L-H}^{Nmin\ (S)}\left(\alpha_{L-H}^{Nmin\ (R)}-1\right)}{\left(\alpha_{L-H}^{Nmin\ (S)}\alpha_{L-H}^{Nmin\ (R)}\right)-1} \qquad (14)$$

Hence, if the minimum numbers of stages for the two sections of the column are known, then Equations (13) and (14) provide simple expressions for estimating the recovery of the key components in the column overhead and bottom products.

The separation to be achieved in a typical plant distillation column can be estimated by setting the minimum number of stages equal to 60% of the equilibrium number of stages of the column ([12]; [13]). The equilibrium number of stages in a column can be related to the actual number of stages in a column, by overall column efficiency.

$$N_{eq} = \varepsilon_o \times N_{ac} \qquad (15)$$

Since the actual number of stages in an existing column is fixed, applying O'Connell's correlation for efficiency gives the minimum number of stages for each section of the column as

$$N_{min(R)} = (0.6)\left(\frac{51-32.5\text{Log}\left(\mu_{av}\,\alpha_{L-H}\right)}{100}\right) \times \left(N_{ac\,(R)}\right) \qquad (16)$$

$$N_{min(S)} = (0.6)\left(\frac{51-32.5\text{Log}\left(\mu_{av}\,\alpha_{L-H}\right)}{100}\right) \times \left(N_{ac\,(S)}\right) \qquad (17)$$

Equation (16) is applied to the rectifying section of the column, while Equation (17) can be applied to the stripping section of a reboiled column. To account for the effect of steam in a steam stripped column, the average viscosity (μ_{av}) in Equation (17) is replaced by an effective viscosity of the form$\mu_{eff} = f\left(\mu_{av}, \mu_s\right)$, so that the minimum number of stripping stages is estimated from Equation (18).

$$N_{min(S)} = (0.6)\left(\frac{51-32.5\text{Log}\left(\mu_{eff}\,\alpha_{L-H}\right)}{100}\right) \times \left(N_{ac\,(S)}\right) \qquad (18)$$

Hence, using the $N_{min(R)}$ and $N_{min(S)}$ obtained from Equations (16) and (17) or (18), the key component recoveries are estimated from Equations (13) and (14).

2.4. Recovery of Non-key Components

The non-key components that are lighter than the LK-component, and the non-key components that are heavier than the HK-component, are assumed not to be distributed. Hence, all components lighter than the LK-component appear only in the top product, while all components heavier than the HK-component will appear only in the bottom product [3].The recoveries of the non-key components with volatilities that lie between those of the LK-component and the HK-component are estimated from;

$$\frac{R_i}{1-R_i} = \frac{1-R_{HK}}{R_{HK}}\alpha_{i-H}^{N_{min(R)}} \qquad (19)$$

The Colburn's method [14], is combined with the Gilliland's correlation to compute reflux ratio. The ratio of the key components on the feed stage is approximated by their ratio in the feed in applying the Colburn equation. The temperatures of the product fractions are computed from dew and bubble point calculations as described in [3].

The Lee-Kesler method is used for the calculation of enthalpies of streams ([15]; [16]; [17]), while the pressure effect on enthalpy is computed from the Pitzer and Curl correlation [17].The enthalpy of striping steam (Hs) is computed from the correlation presented in [18], while enthalpy of vaporization is estimated from the Trouton model. For the determination of mixture properties, the mixing rule in Equation (20) is applied.

$$PP_{mix} = \sum x_i pp_i \qquad (20)$$

3. Model Application

Case 1: Simple Reboiled Multicomponent Distillation

The illustrative example discussed below is taken from the work of Gadalla [19]. A simple reboiled column (Figure 2) is used to separate a mixture of aromatic hydrocarbons into two products. Benzene is to be separated from toluene with a 99% recovery of both components in the distillate and bottom respectively. A reflux ratio of 2.082 is specified, while the feed data and column specifications are reproduced in Table (1).

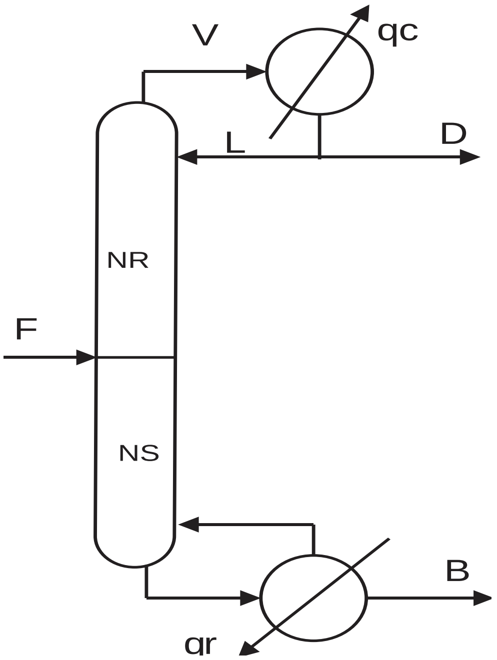

Figure 2: Simple reboiled column

Table 1: Feed data and column specifications for reboiled column.

Feed Mixture	**Flow rate (Kmol/hr)**
Benzene	200
Toluene	100
Ethyl benzene	100
M-Xylene	200
O-xylene	100
Total	700
Feed conditions	
Pressure (Bar)	2.0
Temperature (^oC)	135.9
Column specifications	
No of rectifying stages	15
No of stripping stages	15
Column pressure (Bar)	2.0

Gadalla [19], assumed a tray efficiency of 100% for this problem, hence overall column efficiency was also taken as 100% in the current work.The condenser duty 'q_c'was calculated by taking an energy balance around the condenser, defined by Equation (21)

$$q_c = VH_v - Lh_l - Dh_d \quad (21)$$

The condenser was assumed to be a total condenser, with the same vapour and liquid compositions. The liquid return was also assumed to be at the same temperature as the distillate.

The reboiler duty was calculated by taking an overall enthalpy balance around the column as presented in Equation (22)

$$q_r = Dh_d + Bh_b + q_c - Fh_f \quad (22)$$

The results from the shortcut model developed in this work, compared with those reported in [19] are summarized in Table (2).

Table 2: Comparison of results from the developed shortcut model and those reported in [19] for simple reboiled column

Parameter	**Gadalla's Model ****	**Rigorous Model ** (HYSYS)**	**Shortcut Model**	**ADV (%)**
Top product flow (Kmol/hr)	198.9	199.0	199.5	0.25
Top product temperature (^oC)	104.4	104.4	111.0	6.32
Condenser duty (KW)	5,002	5,003	4,996	0.14
Bottom product flow (Kmol/hr)	501.1	501.3	500.5	0.10
Bottom product temperature (^oC)	158.8	158.7	167.4	5.48
Reboiler duty (KW)	5427	5431	5485	0.99
Recovery of benzene (%)	98.92	99.00	99.46	0.46
Recovery of toluene (%)	98.87	99.00	99.46	0.46
Reflux ratio	2.082*	2.082*	2.082*	

*: Fixed value

**: values from [19]

The last column of Table (2), gives the percentage absolute deviation (ADV) between the values calculated by the shortcut model in this study and the values reported for HYSYS rigorous model. The percentage deviations of all the parameters determined were below 1%, except for the top and bottom product temperatures. The difference in these temperatures and those reported for rigorous HYSYS model were below 10^oC. The results from the shortcut model were generally in good agreement with those reported for rigorous HYSYS simulation. Hence, the developed shortcut model presented here can be used to model a multicomponent distillation in an existing column employing a reboiler.

Case 2: Simple Steam-Stripped Multicomponent Distillation

This example is also taken from Gadalla [19]. The objective is to separate an equimolar C8 – C23 mixture of normal paraffin into two products, using steam as the stripping agent.95% of n-C14 and 95% of n-C19 are to be recovered in the top and bottom products respectively. The operating data and column specifications are given in Table (3).

Table 3: Operating data and column specification for example case 2

Feed	**Parameter value**
Flow rate (Kmol/hr)	1000
Pressure (Bar)	3.0
Temperature (^oC)	300
Steam	
Flow rate (Kmol/hr)	1540
Temperature (^oC)	160
Pressure (Bar)	3.0
Column Specification	
Rectifying Stage	6
Stripping Stages	8
Pressure (Bar)	3.0
Reflux Ratio	0.411

The existing steam-stripped column can be represented by Figure1. The condenser duty was obtained from an energy balance over the entire column, as defined in Equation (23).

$$q_c = Fh_f + SH_s - Dh_d - Bh_b \quad (23)$$

The results obtained from the model were compared with those reported in [19], and summarized in Table (4).

Table 4: Comparison of results from the developed shortcut model and those reported in [19] for steam-stripped column

Parameter	**Gadalla's Model ****	**Rigorous Model ** (HYSYS)**	**Shortcut Model**	**ADV (%)**
n-C14 in the top (Kmol/hr)	61.5	59.4	61.8	4.04
n-C19 in bottom (Kmol/hr)	59.9	59.4	60.9	2.53
Top product flow (Kmol/hr)	564.0	564.6	565.1	0.09
Top product temperature (^oC)	131.4	130.4	138.9	6.52
Bottom product flow (Kmol/hr)	435.9	435.4	434.9	0.12
Bottom product temperature (^oC)	225.8	224.6	216.8	3.47
Condenser duty (MW)	40.4	40.0	39.1	2.25

The percentage absolute deviations for all the parameters were below 7%. The deviations observed for the product flow rates were below 0.2%, while those for the recovery of the LK and HK components were within 4%. The deviations for the top and bottom temperatures were lower than 10^oC. Again, the results from the shortcut model are in good agreement with those reported for rigorous HYSYS model, indicating that the shortcut model can be used to model multicomponent distillation in an existing column employing steam as a stripping agent.

4. Conclusions

The shortcut model presented can predict product flow rates, product compositions and column heat duties with sufficient accuracy, and is also able to predict product temperatures within 10^oC of the values predicted from rigorous HYSYS model, for both reboiled and steam-stripped columns. The model does not involve any stage-by-stage calculations in the stripping section of a steam-stripped column, and generally excludes iterative calculations that can lead to convergence problems when applied to optimization.

Notations

h	Enthalpy of liquid
H	Enthalpy of vapour
N_{ac}	Actual number of stages in a column
N_{eq}	Number of equilibrium stages
N_{min}	Minimum number of stages in a column
P_c	Critical pressure
P_r	Reduced pressure
P	Total pressure
PP_i	Property of component i
PP_{mix}	Mixture property
R_i	Recovery of component i
T	Temperature of stream
T_c	Critical temperature
T_r	Reduced temperature
x_{bi}	Mole fraction of component i in bottom product
x_{di}	Mole fraction of component i in top product
x_{fi}	Mole fraction of component i in feed
ε_o	Overall column efficiency
ω	Accentric factor

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