

DELUMPING PROCEDURE FOR PREDICTION OF DISTRIBUTION OF PRODUCTS IN DISTILLATION USING A SHORT-CUT MODEL

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ABSTRACT

Short-cut models of distillation are useful in screening design options for separation of petroleum fractions at conceptual design stage. A methodology for prediction of detailed product distribution for distillation processes using short-cut calculations of distillation is developed in this work. The proposed delumping procedure is explained in this paper, and an illustrative example is presented to elucidate the application in modeling of distillation using short-cut calculation methods. The proposed methodology helps retain molecular information of composition of petroleum fractions and may help extend the premise of molecular components-based modeling to separation processes such as distillation.

KEYWORDS: *Distillation; Delumping; Short-cut model; Design; Product distribution*

INTRODUCTION

Distillation columns are an extension of single equilibrium stage separation using a cascade of stages in which the more volatile components transfer to vapour phase while the less-volatile components to liquid phase. The liquid needed to feed the cascade at the top is produced by condensation of the vapour leaving the top stage through a condenser. The vapour needed to feed the cascade at the bottom is produced by a reboiler. It is commonly assumed that the liquid and vapour streams leaving each stage are in equilibrium¹.

Distillation column models may be classified as rigorous and short-cut models. Rigorous models take into account mass and energy balances, and equilibrium relationship at every stage and solve these non-linear equations simultaneously. These models provide more accurate results compared to short-cut models but the calculations are time-consuming and dependent on good initial guess. Short-cut distillation models do not have convergence problems and consume less computation time. However, the results are less accurate. Short-cut models offer the opportunity to explore various design scenarios and are thus more suitable for design and optimisation at the con-

ceptual design stage¹. Once the screening of various design options has been carried out using short-cut models, a detailed simulation, of distillation process, with rigorous model is possible using the solution of short-cut model as an initialisation.

Modeling of refinery separation processes, such as distillation and single stage flash separation, is traditionally carried out by lumping petroleum fractions into pseudo-components using bulk properties such as true boiling point and specific gravity. This pseudo-component approach using physical properties, as opposed to the chemical lumps employed in conventional models for reaction systems, makes the two lumping strategies incompatible². In order to retain the molecular level information of the reactor effluent obtained using molecular level models for the reaction system, while utilising the existing tools for modelling of separation processes requires a delumping mechanism. A new methodology is developed for prediction of detailed product distribution, for simple distillation columns, using a short-cut model.

SHORT-CUT MODEL FOR DISTILLATION

The short-cut model for distillation employed in this work is based on the models developed by Fenske³,

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Gilliland⁴, and Underwood⁵. In this method constant molar overflow and constant relative volatilities are assumed for the whole column. For simple column design, i.e. a distillation column with one feed, one top product, and one bottom product the key components and their recoveries are specified first. The *light key* is the component to be recovered in the top product according to some specification while the *heavy key* is the component to be recovered in the bottom product according to some specification¹. The Underwood equation describes the minimum reflux condition, i.e. the minimum allowable reflux for a specified separation⁶, and is used to find all the roots between the relative volatilities of light and heavy key components:

$$\sum \frac{\alpha_i x_{F,i}}{\alpha_i - \theta} = 1 - q \tag{1}$$

where α_i is the relative volatility of component i .

$x_{F,i}$ is the mole fraction of the component i in the feed stream.

q is the liquid fraction of feed stream.

θ is the root of the Equation 1.

The minimum vapour flow in the top section and the distribution of components between the two key components is determined by Equation 2:

$$\sum \frac{\alpha_i d_i}{\alpha_i - \theta} = V_{\min} \tag{2}$$

Where d_i is the molar flow of the component i in the top product.

V_{\min} is the minimum vapour flow in the top section.

The minimum reflux ratio (R_{\min}) is calculated as:

$$R_{\min} = \frac{V_{\min}}{D} - 1 \tag{3}$$

where D is the molar flow rate of the top product. The minimum vapour flow in the bottom section (V'_{\min}) is calculated using Equation 4:

$$V'_{\min} = V_{\min} - (1 - q)F \tag{4}$$

where F represents the feed flow rate.

The total reflux condition is described by the Fenske equation to determine the minimum number of stages:

$$N_{\min} = \frac{\ln \left[\frac{R_{LK} / (1 - R_{LK})}{(1 - R_{HK}) / R_{HK}} \right]}{\ln [\alpha_{LK} / \alpha_{HK}]} \tag{5}$$

where N_{\min} is the minimum number of stages,

R_{LK} is the recovery of light key component in the overhead product,

R_{HK} is the recovery of heavy key component in bottom product.

α_{LK} , α_{HK} are the relative volatilities of the key components, respectively.

The distribution at the total reflux condition is estimated using Equation 6, derived from the Fenske equation⁷:

$$d_i = \frac{\alpha_i^{N_{\min}} f_i \left(\frac{d_{HK}}{b_{HK}} \right)}{1 + \alpha_i^{N_{\min}} \left(\frac{d_{HK}}{b_{HK}} \right)} \tag{6}$$

where f_i is the molar flow of component i in the feed stream, d_{HK} and b_{HK} are the molar flows of the heavy key in the distillate and bottom products respectively.

The Underwood equation tends to underestimate the value of the minimum reflux ratio because of the simplifying assumption of constant molar overflow¹. Suphanit⁸ proposed a modification for compensating the variation in molar overflow. In the modification proposed by Suphanit⁸ an enthalpy balance is carried out around the top section of the column to estimate the condenser duty and the minimum vapour flow. An overall enthalpy balance is carried out to obtain the reboiler duty and finally an enthalpy balance around the reboiler calculates the minimum vapour flow in the bottom section.

The distribution of components at finite reflux may be approximated by linear interpolation between their distributions at minimum reflux and total reflux conditions as suggested by Treybal⁹. The theoretical number of stages can be estimated from N_{\min} and R_{\min} using the graphical, empirical relationship of Gilliland⁴. This correlation may be represented analytically¹⁰:

$$\psi = 1 - \exp \left[\left(\frac{1 + 54.4\zeta}{11 + 117.2\zeta} \right) \times \left(\frac{\zeta - 1}{\zeta^{0.5}} \right) \right] \quad (7)$$

where

$$\zeta = \frac{R - R_{\min}}{R + 1} \quad (8)$$

$$\psi = \frac{N - N_{\min}}{N + 1} \quad (9)$$

The feed stage location can be determined by the empirical equation of Kirkbride¹¹:

$$\ln \left(\frac{N_R}{N_S} \right) = 0.206 \times \ln \left[\left(\frac{B}{D} \right) \cdot \left(\frac{x_{f,HK}}{x_{f,LK}} \right) \cdot \left(\frac{x_{b,LK}}{x_{d,HK}} \right)^2 \right] \quad (10)$$

where N_R and N_S are the number of theoretical stages in the rectifying and stripping sections respectively.

The short-cut model discussed here may be employed for predicting the performance of distillation columns. For example, Ahmad¹² demonstrated the application of short-cut calculations of distillation in modeling of the separation system for hydrotreating process streams. The computational time required for solving these models depends on the number of components in a given mixture¹³. In order to reduce the computational time for optimisation purposes, the components of mixtures are lumped into pseudo-components. However, in order to retain detailed information of process streams while modeling the separation processes using pseudo-components a delumping strategy is needed to obtain the composition information of mixtures in terms of the original components from the information available for the pseudo-components generated to represent the mixtures.

PSEUDO-COMPONENT DELUMPING

Leibovici et al.,¹⁴ proposed a delumping procedure for the prediction of detailed product distribution performing a flash calculation on a lumped mixture. The delumping approach developed by Leibovici et al.,¹⁴ assumes that the component fugacities may be treated as a linear combination of pure component parameters with coefficients depending on mixture properties. This can be expressed mathematically as¹⁴:

$$\ln \left[\frac{f_i}{x_i \cdot P} \right] = C_0 + \sum_{k=1}^{k=n} C_k \cdot p_{i,k} \quad (11)$$

Where f_i is the fugacity of a component in a mixture consisting of N components, $1 < i < N$.

x_i is the component mole fraction of component i .

$p_{i,k}$ is the component parameter for any equation of state $P = f(T, V)$ involving n parameters, $1 < k < n$.

C_0 and C_k are the coefficients of Equation 11.

The criterion for equilibrium has to be fulfilled for all components of a system:

$$f_i^V = f_i^L \quad (12)$$

The equilibrium ratio (K_i), that relates the vapour and liquid mole fractions of a component, can therefore be expressed by¹⁴:

$$\ln [K_i] = \Delta C_0 + \sum_{k=1}^{k=n} \Delta C_k \cdot p_{i,k} \quad (13)$$

where

$$\Delta C_k = C_k^L - C_k^V \quad (14)$$

For two-parameter equations of states such as the Peng-Robinson equation of state¹⁵ (PR-EOS) the values of $p_{i,1}$ and $p_{i,2}$ are $\sqrt{a_i}$ and b_i , respectively. For the PR-EOS the analytical expressions for ΔC_0 , ΔC_1 and ΔC_2 are¹⁴:

$$\Delta C_0 = \ln \left[\frac{v^V - b^V}{v^L - b^L} \right] \quad (15)$$

$$\Delta C_1 = \frac{\sqrt{a^V}}{\sqrt{2b^V}RT} \ln \left[\frac{v^V + (1 + \sqrt{2})b^V}{v^V + (1 - \sqrt{2})b^V} \right] - \frac{\sqrt{a^L}}{\sqrt{2b^L}RT} \ln \left[\frac{v^L + (1 + \sqrt{2})b^L}{v^L + (1 - \sqrt{2})b^L} \right] \quad (16)$$

$$\Delta C_2 = \frac{Z^L - 1}{b^L} + \frac{a^L}{2\sqrt{2}b^{L2}RT} \ln \left[\frac{v^L + (1 + \sqrt{2})b^L}{v^L + (1 - \sqrt{2})b^L} \right] - \frac{Z^V - 1}{b^V} - \frac{a^V}{2\sqrt{2}b^{V2}RT} \cdot \ln \left[\frac{v^V + (1 + \sqrt{2})b^V}{v^V + (1 - \sqrt{2})b^V} \right] \quad (17)$$

where a and b are the parameters of the PR-EOS, R represents the universal gas constant, T represents the temperature, v is the molar volume, Z is the compressibility factor, and the superscripts L and V represent the liquid and vapour phase respectively.

The delumping procedure is summarised into the following steps¹⁴:

1. Lump the mixture into pseudo-components.
2. Perform flash calculation for pseudo-components.
3. Determine $\ddot{A}C_k$ values from the lumped system using the above equations.
4. Calculate K_i values using Equation 13 for all the N components of the full system, i.e. the original mixture without lumping of components.
5. Calculate the vapour fraction and the vapour and liquid mole fractions of all N components of the original mixture, using these K_i values respectively¹⁶.

The delumping procedure proposed by Leibovici et al.,¹⁴ can be employed to derive composition information for mixtures, with a large number of components, while performing a flash calculation on pseudo-components. However, this methodology has been developed by Leibovici et al.,¹⁴ for single-stage separation and therefore not applicable directly for predicting detailed product distribution for distillation columns using short-cut models. More recently, delumping approaches have been developed and extended for multi-phase flash calculations¹⁷, and for equations of state with non-zero interaction parameters¹⁸. However, the approach developed, in this work, for predicting detailed product distribution for distillation columns using the short-cut model discussed may be helpful in conceptual design stage, particularly when detailed characterization of petroleum fractions is required. A molecular components based representation developed by Ahmad et al.,¹⁹ demonstrates the importance of detailed characterization techniques.

PREDICTION OF DETAILED PRODUCT DISTRIBUTION FOR DISTILLATION

In this section a new methodology is presented for prediction of the detailed product distribution for simple distillation columns. The proposed methodology uses the Fenske-Underwood-Gilliland method for performing short-cut calculations of distillation using pseudo-components. The information, in terms of pseudo-components, for the products of distillation is delumped to obtain composition in terms of the original

components of process streams by employing the delumping procedure.

For a reasonable prediction of product distribution in distillation columns we need to take into account two operating limits for the distillation process⁹. The first is the total reflux condition where the entire overhead vapour is refluxed back to the column and corresponds to the minimum number of stages required for desired separation. The second limiting operating condition is the minimum reflux condition which corresponds to minimum internal flows in the column and an infinite number of stages. Once the product distribution at these limiting operating conditions is predicted, the distribution of components at any actual reflux ratio R may be estimated by linear interpolation between the distribution at minimum and total reflux⁹.

Estimation of detailed product distribution at total reflux condition

At total reflux condition the minimum number of stages required can be estimated using the Fenske equation³. The Fenske equation assumes constant relative volatilities which is not the case in practice. The change in relative volatilities may result from changes in composition, temperature and pressure through the column. An average value of relative volatilities needs to be calculated and utilized¹. The distribution of components at total reflux conditions is estimated using the Hengstebeck-Geddes method²⁰. The distribution ratio of a component i (d_i/b_i) is given by Equation 18:

$$\ln\left(\frac{d_i}{b_i}\right) = A + C \cdot \ln\left(\frac{\alpha_i}{\alpha_{HK}}\right) \tag{18}$$

Where α_i is the relative volatility of component i with respect to heavy key. The coefficients of Equation 18 are calculated using the light and heavy key components:

$$A = \ln\left(\frac{d_L}{b_L}\right) \tag{19}$$

$$C = \frac{\ln\left(\frac{d_{LK}}{b_{LK}}\right) - \ln\left(\frac{d_{HK}}{b_{HK}}\right)}{\ln\left(\frac{\alpha_{LK}}{\alpha_{HK}}\right)} \tag{20}$$

The distillate flows can be calculated using the distribution ratios from Equation 21:

$$d_i = \left[\frac{\frac{d_i}{b_i}}{\frac{d_i}{b_i} + 1} \right] \cdot x_{f,i} \cdot F \quad (21)$$

where F is the molar flow of the feed, $x_{f,i}$ the mole fraction of component i in the feed.

The stepwise approach proposed for the prediction of the detailed distribution of components at total reflux conditions based on the distribution of pseudo-components is as follows:

1. Calculate the minimum number of stages, based on the lumped system, and the coefficients of the Hengstebeck-Geddes equation.
2. Calculate the K_i values of the full system, i.e. the mixture before lumping, using the delumping procedure.
3. Calculate the relative volatilities of the full system using the K -value of the heavy key from the calculation for the lumped system.
4. Estimate the distribution of components of the full system at total reflux conditions with the Hengstebeck-Geddes method using the relative volatilities calculated in Step 3.

Estimation of detailed product distribution at minimum reflux conditions

The Underwood equations (Equation 1 and 2) are widely applied for estimation of minimum reflux, and distribution of key components at minimum reflux conditions. The Underwood equations assume that the relative volatility of components and molar over flow remain constant between the pinches, i.e. constant composition zones.^[1] The relative volatilities at feed conditions are generally recommended over average values based on distillate and bottoms compositions because the location of pinches is often close to the feed stage¹.

In order to estimate the distribution at minimum reflux it may be assumed that components lighter than the light key end up almost completely in the overhead product and components heavier than the heavy key in the bottoms product¹⁷. Equation 1 is solved for the θ values. Each θ value lies between an adjacent pair of relative volatilities. For the case with non-adjacent key components the number of θ values required is one more than the number of components between the light and heavy key¹. The equation 2 is then written for each θ value and this set of equations is solved simultaneously to obtain minimum reflux and the mole fraction of components between the key components in the overhead product at the minimum reflux condition.

Leibovici et al.,¹⁴ observed that if lumping does not affect, or only slightly affects, the phase parameters then the delumping coefficients (ΔC_k) are the same for the lumped system and the full system. The approach developed for the estimation of the distribution of components at minimum reflux conditions is based on the analogy to this observation.

If a given petroleum fraction is lumped into pseudo-components appropriately i.e. satisfying the above criterion. It may be observed that the distribution curve (plot of distribution ratios of components vs. the relative volatilities) of pseudo-components matches closely with the distribution curve of the original mixture.

The stepwise procedure proposed for the prediction of the detailed distribution of components at minimum reflux conditions based on the distribution of pseudo-components is as follows:

1. Calculate the minimum reflux and the distribution of the lumped system at the minimum reflux condition.
2. Calculate the distribution ratios for the distributing components as well as the key components.
3. Calculate the K -values of the full system using the delumping procedure explained in Section 3.
4. Calculate the relative volatilities of the components of the full system using the K -value of the heavy key from the calculation for the lumped system.

5. Interpolate for distribution ratios of components of full system which are distributing.
6. Calculate the distillate flows of components using Equation 21.

Once the composition information of the products of the distillation, in terms of the original components of a given mixture, is obtained using the proposed methodology the distribution of components at any actual reflux ratio is estimated using linear interpolation between the distribution at minimum and total reflux conditions. An example is presented to elucidate the application of the methodology developed in this work for predicting detailed product distribution for simple distillation columns.

RESULTS AND DISCUSSION

A mixture of normal alkanes from C_1 to C_{12} is used to illustrate the application of the proposed approach for predicting the detailed distribution of components in distillation using the short-cut model. The components and the composition of the mixture under consideration are shown Table 1.

Table 1: Composition of mixture of normal alkanes from C_1 to C_{12}

Components	mole fractions
CH_4	0.01
C_2H_6	0.04
C_3H_8	0.05
$n-C_4H_{10}$	0.06
$n-C_5H_{12}$	0.13
$n-C_6H_{14}$	0.11
$n-C_7H_{16}$	0.125
$n-C_8H_{18}$	0.16
$n-C_9H_{20}$	0.1
$n-C_{10}H_{22}$	0.11
$n-C_{11}H_{24}$	0.095
$n-C_{12}H_{26}$	0.01

The mixture is lumped by generating one pseudo-component consisting of components from C_7 to C_9 . The composition of the lumped system is shown in Table 2.

Table 2 Composition of lumped system

Components	mole fractions
CH_4	0.01
C_2H_6	0.04
C_3H_8	0.05
$n-C_4H_{10}$	0.06
$n-C_5H_{12}$	0.13
$n-C_6H_{14}$	0.11
Pseudo-com1	0.385
$n-C_{10}H_{22}$	0.11
$n-C_{11}H_{24}$	0.095
$n-C_{12}H_{26}$	0.01

The shortcut model calculations are carried out at $T = 100^\circ C$, $P_{Condenser} = 2$ bar and $P_{Reboiler} = 3$ bar. $n-C_4H_{10}$ is the light key and $n-C_{10}H_{22}$ is the heavy key in the simulation of both original and lumped system. The degree of separation is specified by specifying recoveries of both keys as 95 %.

The results of the delumping approach proposed for modeling of distillation using short-cut model, are validated using the COLOM software version 2.1 (Centre for Process Integration, The University of Manchester). COLOM is a program for design and optimisation of separation systems at conceptual level of process design. The short-cut distillation model is employed in COLOM version 2.1. The strategy followed in this work, is simulation of the lumped system and prediction of detailed distribution at total and minimum reflux conditions using the proposed delumping approach. The results of the detailed prediction are then compared with the simulation of the original mixture in COLOM. The results of the prediction of the detailed distribution of components at the total reflux condition are shown in Table 3.

Table 3: Comparison of prediction of detailed distribution at total reflux conditions

Components	F(kmol/sec)	Predicted distillate flows (kmol/s)	Distillate flow using COLOM (kmol/s)	Absolute Error	% Error
CH ₄	0.1	0.0999	0.0999	3.3E-05	0.033
C ₂ H ₆	0.4	0.3977	0.3977	2.0E-05	0.005
C ₃ H ₈	0.5	0.4914	0.4914	2.6E-05	0.005
n-C ₄ H ₁₀	0.6	0.57	0.57	1.9E-05	0.003
n-C ₅ H ₁₂	1.3	1.1317	1.1317	2.0E-05	0.002
n-C ₆ H ₁₄	1.1	0.7796	0.7797	6.2E-05	0.008
n-C ₇ H ₁₆	1.25	0.5967	0.597	2.5E-04	0.042
n-C ₈ H ₁₈	1.6	0.4113	0.4117	3.8E-04	0.091
n-C ₉ H ₂₀	1.0	0.1182	0.1183	1.5E-04	0.124
n-C ₁₀ H ₂₂	1.1	0.0549	0.055	1.2E-04	0.207
n-C ₁₁ H ₂₄	0.95	0.0195	0.0195	1.9E-06	0.010
n-C ₁₂ H ₂₆	0.1	0.0009	0.0009	2.1E-05	2.319

Table 3 shows a good agreement for distillate flows of components with a maximum percentage error of 2.3 % because of the very small amount of n-C₁₂H₂₆ in the overhead product. The comparison at minimum reflux conditions is shown in Table 4.

Table 4 shows a good agreement for results of delumping products of distillation column using short-cut model at minimum reflux conditions. The percentage error for components heavier than the heavy key could not be calculated as they end up completely in the bottoms product.

Table 4: Comparison of prediction of detailed distribution at minimum reflux conditions

Components	F(kmol/sec)	Predicted distillate flows (kmol/s)	Distillate flows using COLOM (kmol/s)	Absolute Error	% Error
CH ₄	0.1	0.1	0.1	0	0
C ₂ H ₆	0.4	0.4	0.4	0	0
C ₃ H ₈	0.5	0.5	0.5	0	0
n-C ₄ H ₁₀	0.6	0.57	0.57	0	0
n-C ₅ H ₁₂	1.3	1.0565	1.0591	2.6E-03	0.245
n-C ₆ H ₁₄	1.1	0.6932	0.6969	3.7E-03	0.531
n-C ₇ H ₁₆	1.25	0.5561	0.5465	9.6E-03	1.760
n-C ₈ H ₁₈	1.6	0.4143	0.4179	3.6E-03	0.867
n-C ₉ H ₂₀	1.0	0.1332	0.1326	6.1E-04	0.460
n-C ₁₀ H ₂₂	1.1	0.055	0.055	0	0
n-C ₁₁ H ₂₄	0.95	0	0	0	-
n-C ₁₂ H ₂₆	0.1	0	0	0	-

The results of the illustrative example show that the proposed approach may be used to predict the detailed product distribution for simple distillation columns within a reasonable accuracy. The proposed methodology provides a framework for retaining molecular level information while modelling distillation process with short-cut distillation model using pseudo-components. However, further testing may be required to evaluate the effect of increasing the number of lumps, or the number of components lumped together, on the accuracy of prediction of top and bottom product composition for distillation systems.

CONCLUSIONS

A new methodology has been developed for predicting detailed product distribution for simple distillation columns using Fenske-Underwood-Gilliland short-cut method. Promising results have been demonstrated through an illustrative example, indicating that the proposed methodology may be applied in modeling of separation systems for hydrocarbon conversion processes with a reasonable accuracy of design calculations. The proposed methodology needs to be tested rigorously through industrial case studies to determine the accuracy and practicability in conceptual design applications. The delumping methodology proposed in this work may provide a framework for retaining molecular level information while modeling distillation processes with short-cut distillation models using pseudo-components to represent petroleum fractions.

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NOMENCLATURE

A coefficient in equation 18 and 19
B flow rate of bottom product of distillation column
C coefficient in equation 18 and 20
d_i distillate flow of a component, kmol/sec
D flow rate of top product of distillation column, kmol/sec

DB_o number of olefinic double bonds
F feed flow rate for distillation column, kmol/sec
f_i molar flow of a component in feed stream, kmol/sec
K_i vaporisation equilibrium ratio of a component
N_{min} minimum number of stages at total reflux condition
N_R number of theoretical stages in rectifying section of a distillation column
N_S number of theoretical stages in stripping section of distillation column
P pressure, bar
P_{i,k} component parameter for an equation of state, used in equation 11 and 13
q liquid fraction of feed stream at feed stage of a distillation column
R reflux ratio of distillation column. Also used to represent the universal gas constant
R_{HK} recovery of heavy key component in bottom product
R_{LK} recovery of light key component in top product
R_{min} minimum reflux ratio
T temperature, °C
V_{min} minimum vapour flow in bottom section of a distillation column
V_{min} minimum vapour flow in top section of a distillation column
x_{F,i} mole fraction of a component in feed stream
Z compressibility factor

Greek letters:

ΔC_k delumping coefficients in equation 13
 α_i relative volatility of a component
 θ root of Underwood equations (1 and 2)

Subscripts:

F feed stream of a distillation column
HK heavy key component in distillation
i component of a stream
LK light key component in distillation
M make-up gas

Superscripts:

L liquid phase
V vapour phase

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