PLATE EFFICIENCIES OF INDUSTRIAL SCALE DEHEXANISER

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ABSTRACT

In open literature the majority of measured data of distillation columns is on binary systems and from small-scale columns. Data from large industrial columns are scarce. In this paper the measurements of an industrial scale dehexaniser column with diameter of 3.7 m are presented. This column in operation has 40 valve plates of NYE-type. The behaviour and the stability of this column were monitored, liquid compositions, flow rates, pressure and temperature profiles were recorded and reconciled. This data were used to validate a mathematical model of a distillation column. The model describes the behaviour of real plates of distillation. It is based on a multicomponent point efficiency model and includes a mixing model of the phases on large plates. The aspects of simulation of a large-scale industrial column with such a model are discussed.

INTRODUCTION

In the modeling of a distillation column the concept of equilibrium stage is often used. In equilibrium stage approach the mass transfer on a distillation stage is described by the assumption that vapor and liquid phases leaving the plate are in thermodynamical equilibrium. However, the real plates do not behave ideally and therefore the departure from the equilibrium is usually handled by introducing column or stage efficiencies. It has been shown experimentally that in multicomponent mixtures the efficiencies can vary from plate to plate and also from component to component even on the same plate. When component efficiencies vary the distillation cannot be modeled using the concept of fixed value of efficiency. To overcome this problem one suggestion is to include multicomponent plate efficiency calculations into the equilibrium stage model. These calculations are based on multicomponent mass transfer models and estimation of binary NTUs (Number of Transfer Units). The efficiency-based model used in this study is based on the work by Aittamaa [1]. Several other authors have also presented simulation models based on efficiency calculations (see Taylor and Krishna [2] for a review of these). In these days the most extensive studies of applying the efficiency based model we know are those of Ilme [3, 4, 5].

Another approach is the rate-based approach in which the heat and mass transfer including multicomponent interactions between the components are directly calculated using heat and mass transfer coefficients. In this approach, the film theory and the generalized Maxwell-Stefan equations for diffusion are applied, too. The rate-based modeling concept was first introduced by a series of papers by Krishnamurthy and Taylor [6, 7, 8, 9]. Since then the development of the rate-based model has dominated the development of distillation modeling. The rate-based model was further developed to a second-generation model Taylor *et al.* [10]. Recently hydrodynamic aspects for cross flow operation of distillation columns have been studied in the papers by Kooijman and Taylor [11], Higler *et al.* [12], and Muller and Segura [13].

The common feature of both the efficiency based and the rate-based distillation column models is that the quality of the models is dependent on the quality of the NTU or mass transfer correlations. These correlations have often been developed from binary data and small-scale columns. More often than not these distillation models have also been tested against data obtained in small scale.

New high capacity distillation trays have successfully been applied to increase column capacities. Depending on the conditions, high capacity trays can increase unit throughput by 10 % to 25 % over a good standard tray design. To successfully maximize capacity revamps requires knowledge and information about the distillation process and especially equipment being used. The principles of the operation of the high capacity tray, capacity and limitations must be known to successfully utilize high capacity trays in column revamps.

The aim of the present paper is to present rarely published data of an industrial size distillation column employing high capacity trays and to discuss aspects of applying a rigorous efficiency based distillation model for simulation of such a column.

COLUMN AND MEASUREMENTS

The column under consideration is a dehexaniser column from Fortum Oil and Gas Oy's oil refinery in Porvoo, Finland. The column has 40 trays, reboiler, and a total condenser. The operating pressure was about 200 kPa (abs.). See Figure 1. for a simplified flowsheet of the column. The diameter of the column was 3.7 m.

Plates were NYE-type two pass trays (see Figure 2. for a schematic of NYE-trays). Compared to traditional trays both the contact and disengagement zones have been enlarged by replacing the downcomer seal with a modified inlet panel (i.e. NYE-panel). Vapour enters at the bottom of this modified area. It is redirected and it flows through perforations in the vertical face to the tray above. The bottom of the downcomer is elevated, and it acts as a ceiling over the modified area. Thus the downcomer of the NYE-tray is truncated and increases the active area on the tray. The more detailed description of the NYE-trays are given in the references Nye and Gangriwala [22] and Bruyn et al. [23]. Details of the trays used in this study are given in Table 1.

The column operation was observed during 48 hours. All together six composition samples were taken from the feed, distillate and bottoms product of the column. The hour average values for the flow rate and temperature of feed, distillate, reflux and bottoms were read from the automation system of the plant. Three stage temperatures were read from the automation system in the column along with the temperature of the overhead vapor. The automation system provided also time average data for the pressure of the top and bottom of the column.

From the observation time a five and a half hour period was chosen to represent a steady state operation. The measured time average data was reconciled. This data of the composition measurements are presented in Table 2. Figure 1. shows a simplified flowheet and experimental data of the column. A more detailed set of the measured data is found in Ahlgren [14].
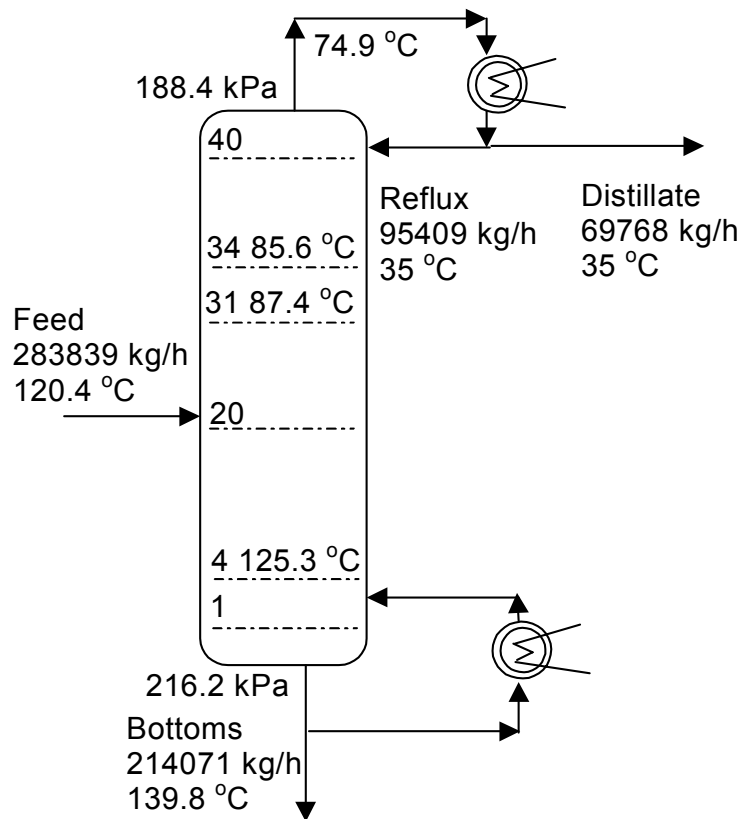
Figure 1. A simplified flowsheet and experimental data of the dehexaniser column.
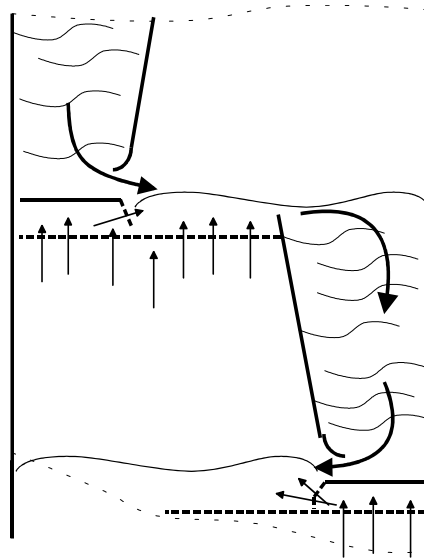

Figure 2. Schematic figure of the NYE-tray.

Table 1. Details of the two pass NYE-trays of the dehexaniser column

Downcomer area	1.142 m^2
Total hole area	1.676 m^2
Active area	8.58 m^2
Column inside diameter	3.672 m
Hole diameter	2.54 cm
Plate spacing	60.0 cm
Distance of weirs	1.178 m
Height of weir	5.675 cm
Total length of weir	6.318 m

Table 2. The reconciled compositions of feed, distillate and bottoms flow

Component	Feed - w%	Distillate - w%	Bottoms - w%
i-butane	0.003	0.013	0.000
n-butane	0.384	1.560	0.000
i-pentane	4.613	18.738	0.009
n-pentane	5.998	24.345	0.019
2,2-dimethylbutane	0.109	0.425	0.006
2,3-dimethylbutane	1.144	4.634	0.006
2-methylpentane	3.142	12.161	0.202
3-methylpentane	1.870	6.825	0.255
n-hexane	5.118	15.602	1.701
Methylcyclopentane	3.663	8.302	2.151
Benzene	1.221	2.961	0.653
Cyclohexane	3.527	3.821	3.432
2-methylhexane	2.575	0.255	3.331
trans-1,2-dimethylcyclopentane	3.102	0.154	4.063
3-methylhexane	1.885	0.088	2.471
n-heptane	4.418	0.029	5.848
Methylcyclohexane	6.791	0.029	8.995
Toluene	6.123	0.011	8.114
2-methylheptane	5.749	0.011	7.619
n-octane	6.379	0.008	8.455
n-propylcyclopentane	4.811	0.013	6.375
m-xylene	8.328	0.010	11.039
n-nonane	6.541	0.007	8.671
n-decane	12.142	0.000	16.099
n-undecane	0.368	0.000	0.488
Total	100.000	100.000	100.000

MODELLING

The mass transfer on an equilibrium stage is limited by the condition that the streams leaving the stage are in thermodynamic equilibrium. It is well known that usually this is not the case. To overcome this gap between the model and the reality, efficiencies are introduced into the model. In binary systems the efficiencies in small diameter columns often vary from 50 to 80 %, but in large plates efficiencies exceeding 100 % have been measured. In multicomponent systems, analogous definition of Murphree vapor phase efficiency can be given by the equation (1).

$$E_{m,ij} = \frac{Y_{i,j} - Y_{i,j-1}}{Y_{i,j}^* - Y_{i,j-1}} \tag{1}$$

The sum of the component fractions is equal to one thus one of the plate efficiencies is bound and in a nc-component system nc-1 plate efficiencies are independent. See for example Lockett [15] for a review of different approaches for tray efficiencies.

The point efficiencies are calculated from the matrix of overall number of transfer units. If the matrix of overall number of transfer units is considered constant in the horizontal direction on the distillation plate the point efficiencies are expressed in the following matrix generalization from a binary system Krishna *et al.* [16].

$$[E_{OV}] = [I] - \exp([-NTU_{OV}]) \tag{2}$$

In this study we consider a large-scale column and the concentration gradients on the tray are considerable, we will use equation (3) by Gautreaux and O'Connel [17] to relate the point efficiency to the plate efficiency

$$E_{m,ij} = \frac{[1 + (\lambda E_{0V}/N)]^N - 1}{\lambda}, \tag{3}$$

where λ is the stripping factor and N number of the mixed pools.

The two film theory for mass transfer can be used to relate the overall mass transfer units to the vapor and liquid phase mass transfer units, see Taylor and Krishna [2].

$$[NTU_{ov}]^{-1}[\beta_V]^{-1} = [NTU_V]^{-1}[\beta_V]^{-1} + \frac{V}{L}[K][NTU_L]^{-1}[\beta_L]^{-1}, \tag{4}$$

where the inverse matrix $[NTU_V]^{-1}$ is defined by equations (5) and (6) and the liquid side $[NTU_L]^{-1}$ is defined in a similar manner

$$NTU_{V,ii}^{-1} = \frac{Y_i}{NTU_{V,inc}} + \sum_{k=1,k\neq i}^{nc} \frac{Y_k}{NTU_{V,ik}} \tag{5}$$

$$NTU_{V,ij}^{-1} = -Y_i\left(\frac{1}{NTU_{V,ij}} + \frac{1}{NTU_{V,inc}}\right) \tag{6}$$

The rigorous efficiency calculation model is implemented into our distillation simulator (see Ilme [5] for further details of the implementation in a flowsheeting environment FLOWBAT). The characteristic feature of this implementation is that the multicomponent tray efficiencies are calculated together with the complete distillation model.

SIMULATIONS

The simulations were performed with 22 components out of the 25 main components that were found in the analysis. I-butane was lumped with n-butane, 2,2-dimethylbutane with 2,3-dimethylbutane and n-undecane with n-decane.

The thermodynamic model used in the simulation was the well-known Soave-Redlich Kwong (SRK) model. The parameters and models for calculation of physical properties were obtained from our in-house database.

The mass transfer units in the vapor and liquid phase are here calculated with the method of Chan and Fair [18, 19]. These correlations were recommended by Ilme [5] for hydrocarbons and are used here since no transfer units correlations specifically for NYE-trays are available that the authors are aware of.

The column was calculated first with these mass transfer correlations and the point efficiencies were obtained from equation (2). These point efficiencies where then used to model the behavior of the whole plate (i.e. point efficiencies instead of plate efficiencies). Figure 3. shows the comparison of the reconciled liquid compositions [w%] and calculated compositions of the key components of bottoms and distillate of this simulation.
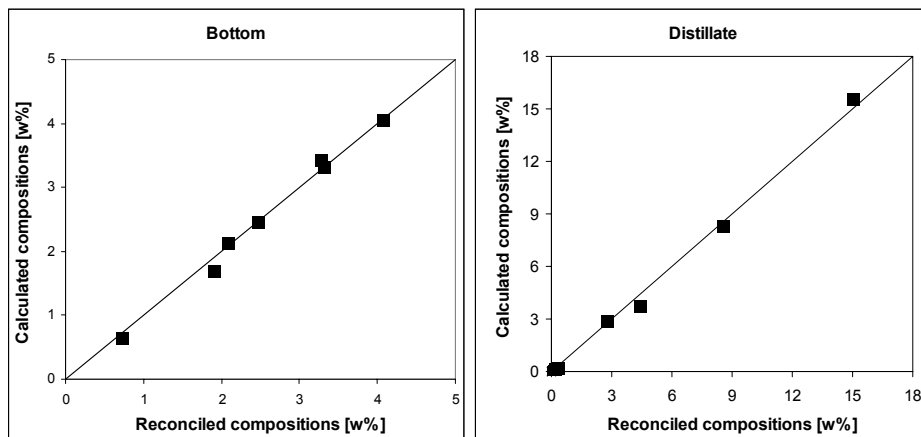
Figure 3. Comparison of reconciled and calculated liquid compositions [w%] of key components for bottoms and distillate. Calculated values were obtained by rigorous tray efficiency model using point efficiency as plate efficiency.

The agreement between the calculated column separation based on point efficiencies and the reconciled compositions is surprisingly good. One would expect that the plate efficiencies deviate significantly from the point efficiencies because the liquid mixing on plate is not complete. This should enhance the separation and increase the plate efficiency compared to point efficiency. Typically the calculated multi-component efficiencies varied between 0.75 and 0.85. The good agreement and the rather high values of the point efficiencies might indicate that the Chan and Fairs correlations [18, 19] may predict optimistic values for the NTUs on a NYE-tray.

In the next simulation the rigorous tray efficiency model was used and the plate efficiency was calculated according to equation (3). The number of the mixed pools was estimated from the eddy diffusion correlation of Welch *et al*. [20]. Again this correlation was used for the reason that no specific correlations for NYE-trays were at hand. Figure 4. shows the comparison of reconciled liquid compositions [w%] and calculated values of the key components in bottoms and distillate flow. In this case plate efficiencies were averaged on each plate and they varied typically between values of 0.85 to 1.1 showing the incomplete mixing on the plates. The agreement is not as good as in the calculations based on the point efficiency model.
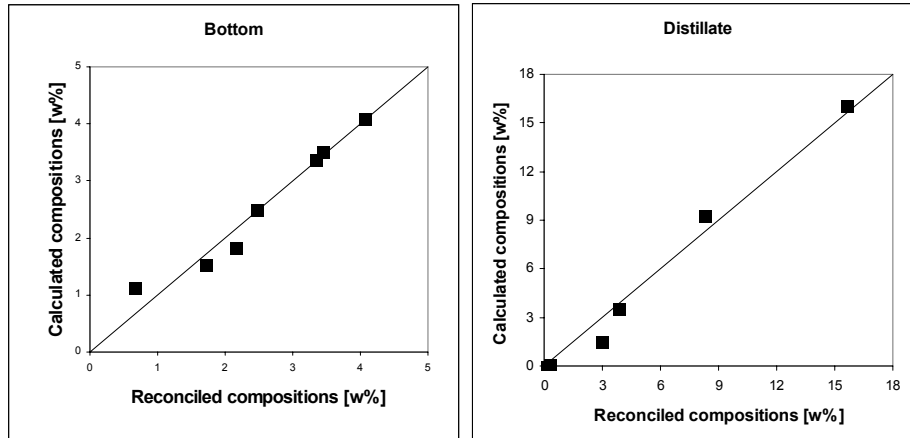
Figure 4. Comparison of reconciled and calculated liquid compositions [w%] of key components for bottoms and distillate. Calculated values were obtained by rigorous tray efficiency model using averaged plate efficiency.

As reference calculation the dehexaniser column was simulated with constant plate efficiencies of 0.75. Figure 5. shows the comparison of reconciled and calculated liquid compositions [w%] of the key components of bottoms and distillate. The good agreement with the measured and calculated compositions indicates that the plate efficiencies of the components lie around 0.75 – 0.85 as the point efficiency calculations also indicate.
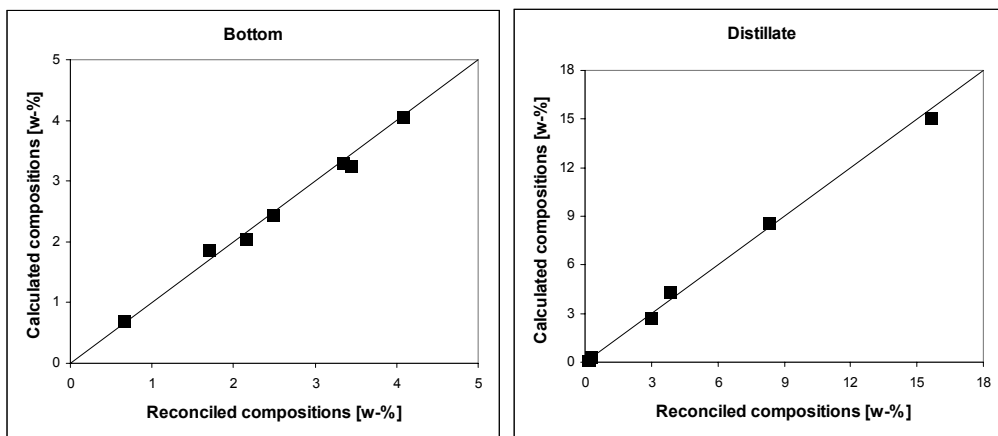
Figure 5. Comparison of reconciled and calculated liquid compositions [w%] and of key components for bottoms and distillate. Calculated values were obtained with constant plate efficiency 0.75.

DISCUSSION AND CONCLUSIONS

In open literature the majority of published measured data of distillation columns is on binary systems and from small-scale columns. Data from large industrial columns is scarce. In this paper the reconciled measurements of an industrial scale dehexaniser column of diameter of 3.7 m are presented. This column in operation has 40 two-pass valve trays of NYE-type. This type of data is important for development and validation of the type of distillation simulators presented in this paper as well as in the ongoing development of rate-based distillation models.

The data were used to test an implementation of a rigorous efficiency based distillation column model. The column was simulated with a rigorous point efficiency model (complete mixing) and by a rigorous tray efficiency model (incomplete liquid mixing on plate). It is rather surprising that the calculated values using the point efficiencies (complete liquid mixing) gave an excellent agreement with the measured values. These values were typically between 0.75-0.85. One possible explanation is that the NTU correlations by Chan and Fair [18, 19] used in the calculations overestimate the separation on the NYE-trays. These correlations were developed before NYE-trays came into market. One feature of the NYE-tray is that they have a larger capacity compared to traditional plates. In the Chan and Fair [18, 19] correlation the fractional approach to flooding is taken into account. This might be one reason why high values for the point efficiency were predicted by this correlation.

It is also an open question if the traditional mixing models and correlations are able to handle the effect of partly horizontal vapor flow on NYE-tray. It is likely that the calculated results presented in this paper indicate a too optimistic point efficiency of the model. It is evident that a more thorough analysis and experimental information are required for the prediction of the behavior of the NYE-tray.

ACKNOWLEDGEMENT

NOMENCLATURE

E_m	Murphree vapor phase efficiency
E_{OV}	Point efficiencies
$[E_{OV}]$	Matrix of point efficiencies
$[I]$	Identity matrix
$[K]$	Diagonal matrix of vapor/liquid equilibrium K-values
L	Liquid flow rate, mol/s
N	Number of mixed pools
$[NTU_L]$	Matrix of liquid phase transfer units
$[NTU_{OV}]$	Matrix of overall number of transfer units
NTU_V	Vapor phase transfer units
$[NTU_V]$	Matrix of vapor phase transfer units

V	Vapor flow rate, mol/s
X	Liquid molar fraction
Y	Vapor molar fraction
$Y*$	Vapor molar fraction in equilibrium with liquid at the point considered

Greek letters

$[\beta_L]$	Bootstrap matrix for the liquid phase
$[\beta_V]$	Bootstrap matrix for the vapor phase
λ	Stripping factor, $\lambda = m\dfrac{V}{L}$, where m is the slope of the vapor/liquid equilibrium curve

Subscripts

i, j, k, m	component
nc	number of component

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