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Department of Chemical Engineering

TKP4171 – PROJECT DESIGN

Report

"How many stages should be used in a distillation column"

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Abstract

This report checks what ratio, between the real number of stages and the theoretical minimum number of stages, that gives the lowest cost for a distillation column. Two different cost methods were used to cost estimate the column, Sinnott and Turton. Sinnott gave a ratio of 1.9 for capital costs and 2.9 when energy was included. For Turton the numbers were 2.3 and 3.1, respectively. The average ratios were 2.1 with no energy cost included and 3.0 with energy cost. Norwegian electricity was used to calculate the energy cost. A more expensive energy source would give a higher optimum N_{ratio} .

Data for the cost estimation were found by simulating separation of binary mixtures in a distillation column in UniSim. 20 different binary mixtures were separated to generalize the prediction for the optimum N_{ratio} . In the simulation of the mixtures, feed fraction, distillate fraction, quality of the feed and the numbers of stages were varied. An equation, $\frac{V}{V_{min}} = \frac{b}{N/N_{min}-1} + 1$, was developed to curve fit the results. It showed to be an inadequate fit.

Due to the sources of error in the simulations and the cost analyzes, the suggested N_{ratio} is inaccurate, but it indicates that the N_{ratio} should be higher than the suggested value of two from literature.

Preface

This report was written as a part of the course TKP4170, "Process Design", during the spring semester 2012. The project is a study of the relation between the actual numbers of stages in a distillation column and the minimum numbers of stages. The report requires basic knowledge in chemical engineering, Matlab and UniSim.

The group would like to thank Ph.D candidate Maryam Ghadrhan for helpful guidance throughout the process, and Professor Sigurd Skogestad for setting the project on the right track.

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1 Introduction

Choosing the correct number of stages in an industrial distillation column is essential for a good design. Several shortcut methods to give an estimate of the numbers of stages needed in a distillation column have been published. These methods calculate and approximate numbers of stages in the column as a function of the reflux ratio and the minimum number of stages. This report will try to validate the correlation found by Gilliland and find an improved correlation. This was done by running many different rigorous simulations in UniSim and changing feed fraction, distillate fraction, feed quality, numbers of stages and the components separated.

A cost estimation based in the simulated data is also carried out. Previously published reports have suggested that two times the theoretical minimum number of stages is a good estimate for the number of stages a column. In this report this rule of thumb is discussed, and an improved value is proposed. This is done by looking into both the construction cost and the operating cost. The energy consumption increases when the numbers of stages in the column decreases. In this report the cost estimation methods developed by Sinnott and Turton are used.

2 Theory

Distillation is a common separation technique in chemical industry. The method exploits that a boiling mixture consisting of components with different boiling points, the composition in the liquid and the gas will be different. The mixture can be vaporised and condensed several times to reach a desired purity.

2.1 Outline of a continuous distillation column

A continuous distillation column consist of a vertical shell house together with a condenser and a re-boiler, see figure 2.1.

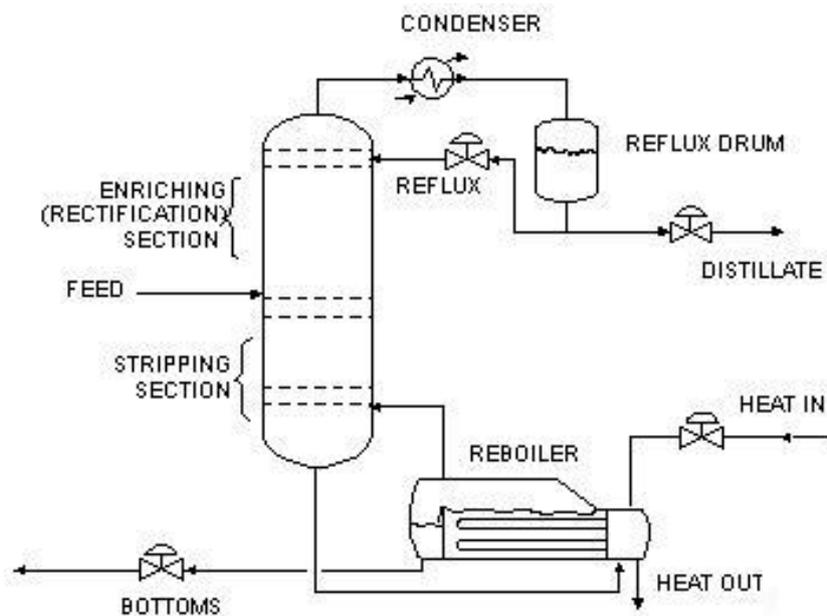


Figure 2.1: Standard setup of an industrial distillation column, together with reboiler and condenser [2]

The column is either filled with a packing material or consisting of stages, both to maximize the vapor-liquid contact. Improving contact between the vapor and liquid phase makes each stage closer to the equilibrium, and enhances the performance of the column. Thus reducing the numbers of stages needed to reach the specified purity and reducing the energy consumption in the column.

2.2 Simulating a continuous column

Simulation of a column is dependent on how the phase equilibrium between vapor and liquid is calculated for each step. For ideal mixtures the vapor-liquid equilibrium can be derived from Raoult's law and mass balances. The equilibrium line for an ideal binary mixture is given in equation 2.1, [7].

$$y_A = \frac{\alpha x_A}{1 + (\alpha - 1)x_A} \quad (2.1)$$

α is the relative volatility, x_A is fraction of component A in the liquid and y_A is the fraction of component A in the vapor. The simulation program UniSim uses property packages that include equations that describe vapor-liquid equilibrium for real systems. A property package is a set of equations that describes the behavior of different chemicals. The property packages are designed to handle different types of chemicals, Peng-Robinson is for an example used for non-polar hydrocarbons.

2.3 Shortcut methods in UniSim

The shortcut method in UniSim can be used to give an indication of the minimum number of steps in a distillation column. The minimum numbers of trays occurs when the reflux ratio goes to infinity. UniSim uses Fenske's formula to estimate the minimum number of stages. This method assumes that the relative volatility α is constant. Fenske's formula for binary mixtures is given in equation 2.2 [7].

$$N_{min} = \frac{\ln\left(\frac{x_D}{1-x_D} \frac{1-x_B}{x_B}\right)}{\alpha} \quad (2.2)$$

Where x_B and x_D are the desired bottom and distillate liquid fractions respectively.

2.4 Gilliland

Gilliland's correlation is a graphical method for estimating the real number of stages, N , required for a separation at a given reflux ratio, R . In the correlation are the minimum numbers of stages, N_{min} , and the minimum reflux ratio, R_{min} , needed. The graphical method plots $\frac{N-N_{min}}{N+1}$ versus $\frac{R-R_{min}}{R+1}$. $\frac{R-R_{min}}{R+1}$ can also be written as $\frac{V-V_{min}}{V+1}$, where V is the vapor in the boil-up stream from the reboiler and V_{min} is the minimum size of the vapor stream, this can be done since $\frac{L}{D}$ is equal to R and V is $L + D$. L is the liquid stream that returns to the column after the condenser and D is the distillate stream from the condenser [8].

3 Simulation

Simulation of a distillation column was performed in UniSim to find the vapor flow in the column for 20 binary mixtures at different feed fractions, z_f , distillate fraction, z_d , quality of feed, q , and number of stages, N . The vapor flow is proportional to the energy consumption of the column. Quality of feed is a measurement of the state of the stream. When q is equal to zero the feed is saturated vapor, and when q is one the feed is saturated liquid. All combination of the cases presented in Table 3.1 were simulated. A case is defined as unique set of variables from Table 3.1 and change of components in the column.

Table 3.1: The fixed variables for each simulation

$z_f[\text{heavy}, \text{light}]$	$z_d[\text{heavy}, \text{light}]$	q	$z_b[\text{heavy}, \text{light}]$
[0.7, 0.3]	[0.01, 0.99]	0	[0.96, 0.04]
[0.5, 0.5]	[0.02, 0.98]	0.5	[0.96, 0.04]
[0.3, 0.7]	[0.04, 0.96]	1	[0.96, 0.04]

Figure 3.1 shows the process flow diagram for the simulation. The logical operation (VS box) applies the same conditions to the feed to the rigorous simulation (F1) and the feed to the short cut column (F2). The shortcut column gives an estimate for N_{min} by Fenske equation 2.2.

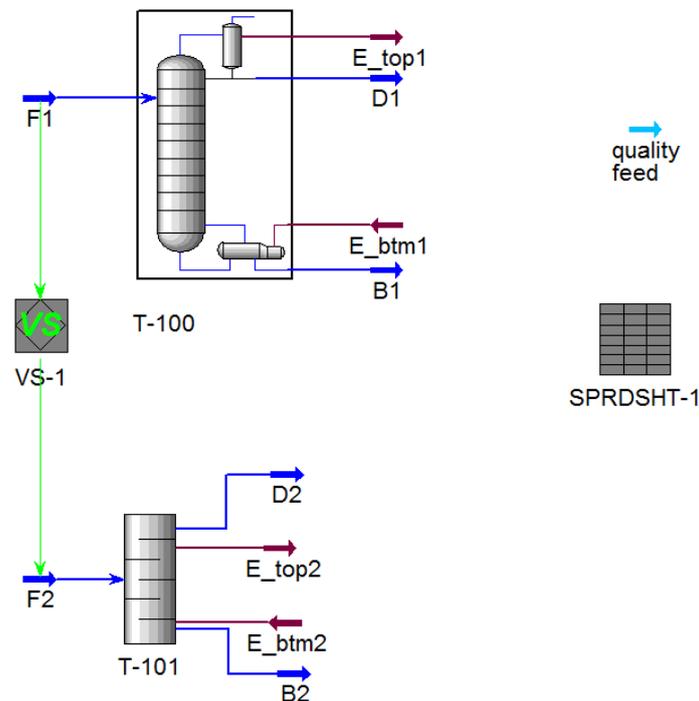


Figure 3.1: Setup of simulation in UniSim. The rigorous columns is T-100 and the shortcut column T-101.

The simulation was done with a basis of 100 kmol/h feed and a column pressure at 1 bar . The temperature in the feed flow is a function of the feed quality and the composition. The reboiler pressure was set

to 105 *kPa* and the pressure drop in the condenser to 5 *kPa*. Distillate composition and bottom fraction of the light component were used as the two degrees of freedom. It was assumed 100 % efficiency at each stage. Modified Inside-out was used as solver for the column for increased robustness. Table 3.2 shows the specifications of the column.

Table 3.2: Simulation setup for rigorous column

Degree of freedom 1	Fraction of heavy component in distillate
Degree of freedom 2	Fraction of light component in bottom
Column pressure	100 <i>kPa</i>
Reboiler pressure	105 <i>kPa</i>
Pressure drop condenser	5 <i>kPa</i>
Solver	Modified Inside-Out

3.1 Components and property packages

Different types of components were separated to generalize the conclusion for the optimum ratio, N_{ratio} , between the real number of stages and the theoretical number of stages. Alkanes, alkenes, alcohols, phenols, polyols (glycerol), ether, chlorinated hydrocarbons and aromatic hydrocarbons were simulated. These groups of components require different property packages for simulation. Peng-Robinson is the most common used property package for hydrocarbons, but it does not work well with polar components. For the alkanes, alkenes, ether and aromatic hydrocarbons Peng-Robinson was used as property package. NRTL (Non-random two-liquid) was used for the simulations with alcohols, phenols and chlorinated hydrocarbons, while for the polyols the glycerol package was used [5]. A complete overview of the components used in the simulation, the component types and the property packages used can be found in table 3.3.

Table 3.3: Setup simulation of rigorous column

Components	Type	Property package
1-butanol - 2-propanol	Alcohol	NRTL
Ethanol - methanol	Alcohol	NRTL
2,6 xylenol - phenol	Phenol	NRTL
2-chlorobutane - 1-chloropropane	Chlorinated hydrocarbon	NRTL
Ethylene dichloride - vinyl chloride	Chlorinated hydrocarbon	NRTL
Glycol - ethylene glycol	Polyol	Glycol package
1-butene - propene	Alkene	Peng-Robinson
m-cresol - phenol	Phenol	NRTL
Metyl-tert-butyl-ether - n-butane	Ether - alkane	Peng-Robinson
n-butane - propene	Alkane - alkene	Peng-Robinson
n-butane - n-propane	Alkane	Peng-Robinson
n-decane - n-nonane	Alkane	Peng-Robinson
n-nonane - n-octane	Alkane	Peng-Robinson
n-heptane - n-hexane	Alkane	Peng-Robinson
n-octane - n-heptane	Alkane	Peng-Robinson
n-pentane - n-butane	Alkane	Peng-Robinson
Propane - ethane	Alkane	Peng-Robinson
p-xylene - benzene	Aromatic hydrocarbon	Peng-Robinson
p-xylene - toluene	Aromatic hydrocarbon	Peng-Robinson
Toluene - benzene	Aromatic hydrocarbon	Peng-Robinson

3.2 Automation of the simulation

Changing z_f , z_d , q and N systematically and extracting V at the different conditions was done by connecting UniSim and MATLAB. MATLAB and UniSim were connected with object linking and embedding through ActiveX controls. The connection makes it possible to perform changes in and extracting data from UniSim through Matlab. Appendix B shows how the connection was established and contains the MATLAB scripts that performs the changes.

The sets of variables that were used in the simulation are presented in table 3.1. For each set of binary mixture all the different combination of the variables in table 3.1 were simulated. This gives a total of 27 simulations with the same variable set. For each fixed set of variables the number of stages were changed by multiplying N_{ratio} with an estimate of N_{min} , found by the shortcut column, and rounding up the number. This was done for comparison of the different simulations, because all the simulations would then have data for the same N_{ratio} . The N_{ratio} is defined by equation 3.1

$$N_{ratio} = \frac{N}{N_{min}} \quad (3.1)$$

The N_{ratio} values used for each simulation is presented in equation 3.2. As the critical area for cost estimation is expected to have a N_{ratio} around 2, the N_{ratio} interval is short in this area.

$$N_{ratio} = [1 \ 1.1 \ 1.2 \ 1.3 \ 1.4 \ 1.5 \ 1.6 \ 1.8 \ 1.9 \ 2 \ 2.1 \ \dots \quad (3.2)$$

$$2.2 \ 2.4 \ 2.6 \ 2.8 \ 3 \ 3.2 \ 3.4 \ 3.6 \ 3.8 \ 4 \ 8 \ 12]$$

Feed stage for each simulation was set by using equation 3.3. Fb is the molar flowrate of bottom and Fd is the flowrate of the distillate in kilomoles per hour. Equation 3.3 does give an optimal feed location, causing a higher vapor flow in the column than necessary [10].

$$\frac{N_{rectifying}}{N_{stripping}} = \left(\frac{z_{f_{light}}}{z_{f_{heavy}}} \right) \left(\frac{z_{b_{heavy}}}{z_{d_{light}}} \right)^2 \left(\frac{Fb}{Fd} \right)^{0.206} \quad (3.3)$$

$N_{rectifying}/N_{stripping}$ is the ratio between the number of steps in the rectifying and the stripping section. This ratio was used to calculate the location of the feed stage as shown in equation 3.4. The equation sets the feed location to the last stage in the stripping section. The plus one in the nominator corrects for the stage added by the reboiler and the feed stage is rounded up to the closest whole number, as the feed stage is an integer.

$$Feed \ tray = round \left\{ \frac{N + 1}{1 + \left(\frac{N_{rectifying}}{N_{stripping}} \right)^{-1}} \right\} \quad (3.4)$$

As previously mentioned, q , is a measurement of state of the feed flow, and it is calculated as shown in equation 3.5. $H_{vap,sat}$ is the enthalpy of the saturated vapor, H_f is the enthalpy of the feed and $H_{liq,sat}$ is entalpy of the saturated liquid [9].

$$q = \frac{H_{vap,sat} - H_f}{H_{vap,sat} - H_{liq,sat}} \quad (3.5)$$

3.3 Extracted data

Parameters needed for later analysis were extracted from UniSim. Those parameters are found in Table 3.4. Notice that some of the variables set by the MATLAB script are again extracted. This is to assure that the variables are inserted correctly and are not changed unintentionally during the simulation.

Table 3.4: List of variables extracted from the simulation

Symbol	Unit	Description
q		Quality of the feed
Ff	$kmol/h$	Feed mass stream
xf		Feed composition in mol fraction
Fd	$kmol/h$	Distillate mass stream
xd		Distillate composition in mol fraction
		Feed tray
V	$kmol/h$	Vapor flow from the reboiler
N		Number of steps
$Nmin_{curv}$		Nmin calculated by curve fitting and asymptote analysis
$Vmin_{curv}$		Vmin calculated by curve fitting and asymptote analysis
	kg/h	Mass flow from the reboiler
ρ_L	kg/m^3	Mass density of liquid in boil-up stream
ρ_V	kg/m^3	Mass density of vapour in boil-up stream
Q_R	kJ/h	Duty reboiler
Q_C	kJ/h	Duty condenser
T_{1R}	$^{\circ}C$	Temperature in to reboiler
T_{2R}	$^{\circ}C$	Temperature out of reboiler
T_{1C}	$^{\circ}C$	Temperature in to condenser
T_{2C}	$^{\circ}C$	Temperature out of condenser

3.4 Curve fitting and estimating N_{min} and V_{min}

Once the feed fraction, z_f , distillate fraction, z_d and the quality of feed, q , are fixed, the column has a N_{min} and a V_{min} independent of the column stages. V_{min} is found when the numbers of trays go to infinity and N_{min} is found when V goes to infinity. To find V_{min} and N_{min} , V is plotted against N . An example of this is shown in figure 3.2. The plot for the rest of the simulated cases is shown in appendix A.

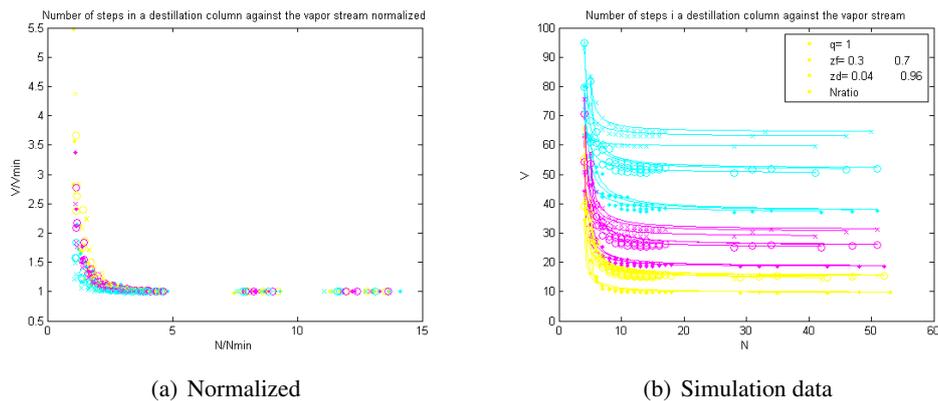


Figure 3.2: Simulated data of n-butane and propene. The left figure shows V/V_{min} plotted against N/N_{min} . The right figure show N potted against V .

For each of the series in figure 3.2, N_{min} and V_{min} are the horizontal and vertical asymptotes respectively. Approximate values for N_{min} and V_{min} were found by curve fitting equation 3.6 to the series. The curve

fitting was done by least square method. The Matlab script used for the curve fitting is in shown in appendix B.

$$V = \frac{b}{N - N_{min}} + V_{end} \quad (3.6)$$

V_{end} is the vapor flow at the largest N in each simulation series. V_{end} was used since the number of stages is large therefor close to the true V_{min} . For the simulation of the alcohols the simulation of the largest numbers of stages failed.

Equation 3.6 was the equation found that matched the path of the data points best. Three other equations 3.7-3.9 were also tested, but they did not give an adequate fit to the simulation data.

$$V = \frac{b_1}{a_1 N - N_{min}} + V_{min} \quad (3.7)$$

$$V = a_1 e^{-b_1 N} \quad (3.8)$$

$$V = a_1 e^{-b_1 N} + a_2 e^{-b_2 N} \quad (3.9)$$

3.5 Analysis of the simulated data

In order to validate the simulated data, the data were plotted varying only one of the three properties z_f , z_d and q . The two fixed variables were set to the middle of Table 3.1. Figure 3.3 shows number of stages plotted against the vapor flow for the n-Butane and Propene.

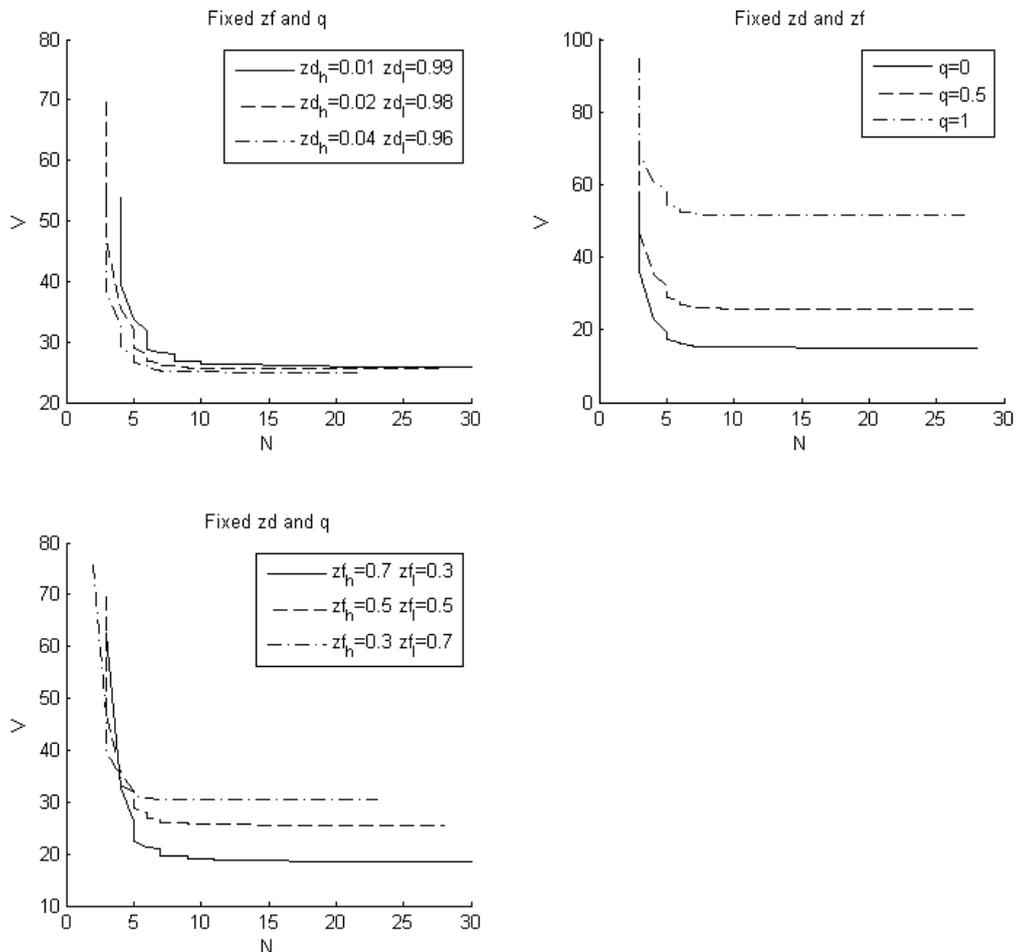


Figure 3.3: Numbers of stages plotted against the vapor flow, with the basis in the raw data. In the plot, two of the 3 degrees of freedom z_f , z_d and q is fixed to the middle simulated value.

When, q , is the only changed parameter, the plot indicates that N_{min} is independent of q , since it converges to the same vertical asymptote. This corresponds to classical distillation theory. This plot also shows that the vapor flow, which is proportional to the energy consumption, is higher when the feed contains more liquid.

Once z_f is the only adjusted variable the plot should converge to the same N_{min} , according to distillation theory. Unfortunately the simulation data those not give a smooth line and therefore do not give a clear result. This is probably due to error in choosing the correct feed stage. When it comes to the vapor flow, the plot shows that the vapor flow is lower once the feed contains more heavy component. This is due

to the specified composition in the bottom stream.

Once z_d is the only adjusted variable it is hard to see if it converges to the same V_{min} or not. Theoretically the vertical and horizontal asymptotes for all the variation of z_d should be different.

3.5.1 Trends between the different cases

A curve fit of the relation between N/N_{min} and V/V_{min} was made with the basis in all the collected data from the simulation for each binary mixture. The trend for six of the different binary mixtures are presented in figure 3.4. The equation used in the curve fitting is presented in equation 3.10, and is chosen since it match the plot of V versus N well, see section 3.4.

$$V/V_{min} = \frac{b}{N/N_{min} - 1} + 1 \quad (3.10)$$

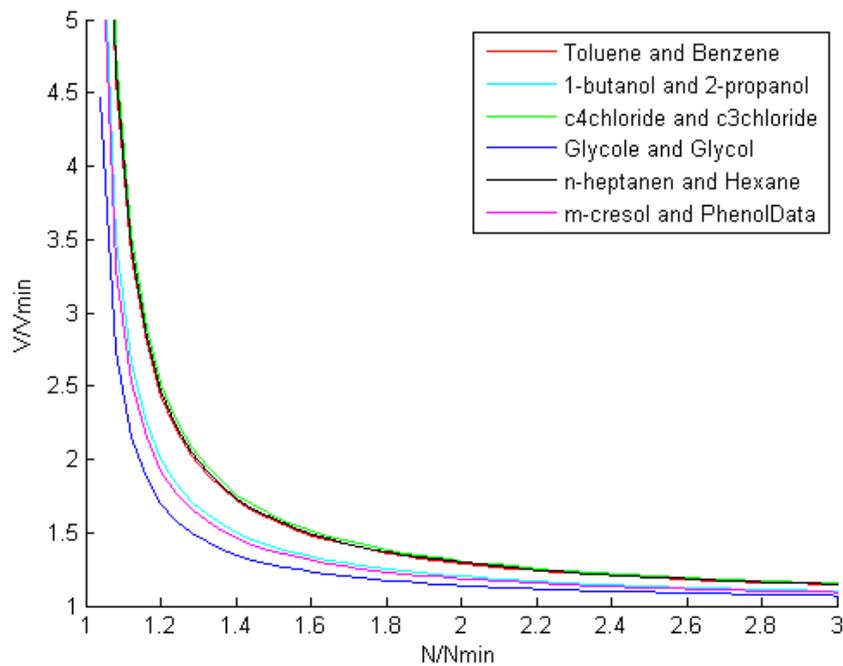


Figure 3.4: Curve fit of the relation between N/N_{min} and V/V_{min} for the simulated data for six different binary mixtures

3.5.2 Average for all the cases

An average value of V/V_{min} as a function of N/N_{min} for all cases was found by taking the average of the curve fit for the different binary mixtures. The function found is presented in equation 3.11.

$$V/V_{min} = \frac{0.22}{N/N_{min} - 1} + 1 \quad (3.11)$$

This equation can be used as a shortcut method for finding the number of stages in the column for a specific V/V_{min} , when N_{min} is known. However it is not a good approximation as it is strongly dependent on feed compositions, feed quality, type of components and distillate composition. This can be seen from the large scattering of the data in figure 3.2 where one of the mixtures is plotted. The difference between the different cases can be seen in figure 3.11.

3.6 Gilliland analysis

The data found by curve fitting was plotted as done by Gilliland [8], $(N - N_{min})/(N + 1)$ against $(V - V_{min})/V$. See also chapter 2.4. This plotting relieved a large scattering of the data in contrast to the results found by Gilliland. Many of the series in the data set also had trajectories that seemed to not go between the points [0,1] and [1,0] as seen in figure 3.5.

By definition of N_{min} and V_{min} , all the series should go between the points [0,1] and [1,0]. When V is equal to V_{min} N is infinite, and vice versa. This causes $(N - N_{min})/(N + 1)$ to approach 1 when V goes to infinity $(V - V_{min})/V$ is then zero. The same logic can be provided to the other corner. An example of the Gilliland plot with N_{min} and V_{min} found by curve fitting is shown in figure 3.5 to the right. The black line is the Molokanov equation 3.12 which is a curve fit of the data found by Gilliland [6].

$$y = 1 - \exp\left(\frac{1 + 54.4x}{11 + 117.2x}\right) \left(\frac{x - 1}{\sqrt{(x)}}\right) \quad (3.12)$$

Where y is $(N - N_{min})/(N + 1)$ and x is $(V - V_{min})/V$

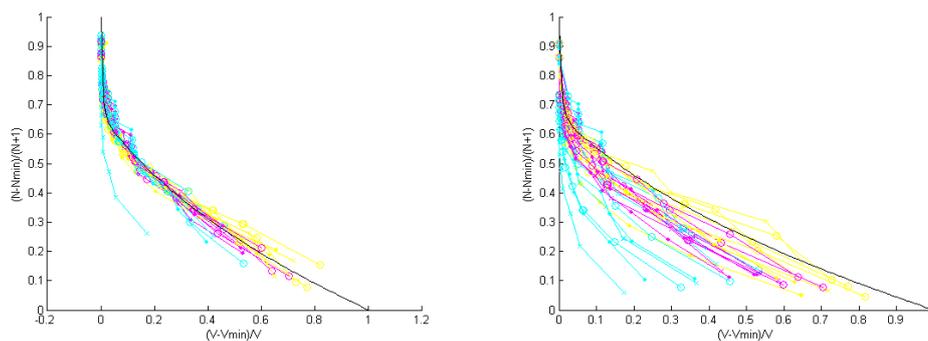


Figure 3.5: Simulated data of n-butanepropene plotted as done by Gilliland. The black line is the Molokanov equation which is a curve fit of the results by Gilliland

3.6.1 Curve fitting to the Gilliland plot

It is assumed that the scattering in the right plot of figure 3.5 is due to errors in the curve fitting method used in section 3.4. In addition notice that all the series go towards the point [0, 1]. This is a consequence of the assumption that V is equal to V_{min} on the largest simulated N in each series. The true V_{min} will be smaller than this approximated V_{min} .

In this particular simulated case most of the series lays below the Molokanov line. To make the series match the Gilliland plot N_{min} has to be larger if V_{min} is fixed. It is also possible to only adjust V_{min} keeping N_{min} constant, then V_{min} has to become larger. But this can not be correct as the true V_{min} is below the already chosen V_{min} .

3.6.2 Improving N_{min} and V_{min} by using Gilliland

As the cost analysis is dependent on a correct N_{min} to be reliable, it is essential to get a good value for this parameter. Gilliland was assumed to give a good description of the relationship between N , N_{min} , V and V_{min} , and used to find an improved N_{min} and V_{min} . This was done by minimizing the square error between the Molokanov equation and the simulated data. This operation is mathematically correct, but it might not find the physically correct values, even if the Molokanov equation is correct. This is caused by having two adjustable variables. If N_{min} is fixed V_{min} can be justed so it fits the Molokanov line. If V_{min} is fixed N_{min} can be adjusted so it fits the Molokanov equation. The minimizing has still been performed as it is assumed that it will mostly vary on N_{min} .

The curve fitting was proved to be very sensitive to the guess of N_{min} and V_{min} . In some cases it was not possible to find guesses that resulted in convergence for all series. The left figure in figure 3.5 shows an example of the data with the improved N_{min} and V_{min} . It can be seen that one of the series has not been converged.

4 Cost estimation

A cost estimation with the basis in the simulated data has been performed to find the N_{ratio} which gives the lowest total cost of the column. To do this it is essential to have a good method to determine the cost. In this project there have been used two different cost methods to calculate the fixed capital cost, those are the cost methods developed by Turton and Sinnott. Both methods are strongly dependent on a good size estimation.

4.1 Size calculations

The size calculations are based on data found from the simulation.

4.1.1 Calculation of Column Diameter

To estimate the column diameter equations from Sinnott [12] were used. The maximum allowable vapor velocity, u_w , is used to find the diameter. Equation 4.1 and 4.2 shows how the diameter. This equation is designed to optimize the column productivity, but still avoids flooding.

$$u_w = (-0.171l_t^2 + 0.27l_t - 0.047) \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \quad (4.1)$$

In the equation l_t the plate spacing between the trays and is chosen to be 0.9 m for every case. This value is chosen so it is large enough for easy maintenance of the column. ρ_L and ρ_V is the density of the liquid and vapor in the boil-up stream respectively. The diameter is calculated using the equation 4.2 below. In this equation the maximum allowable vapor velocity is used to calculate the diameter of the column, and it also is assumed that the vapor volume is much greater than the liquid volume.

$$D = \sqrt{\frac{4V_g}{\pi\rho_V u_w}} \quad (4.2)$$

V_g kg/s is the vapor rate, and is found in the boil-up stream from the reboiler. The density that is used in the equation is also found in the boilup stream and is given in kg/m³

4.1.2 Calculation of column size parameters

Then the height of the distillation column can be found by using equation (4.3)

$$L = N \cdot l_t \quad (4.3)$$

Where N is the number of stage in the column. The volume in the column is found by multiply the length of the column with the cross-sectional area in the column.

To estimate the column wall thickness, t equation 4.4 found in Sinnott [12] is used.

$$t = \frac{P_i D_i}{(2SE - 1.2P_i)} \quad (4.4)$$

P_i is the maximum allowed pressure in the column, and is assumed to be 10 bar in this project. In this equation, SE is the maximum allowable stress for type 304 stainless steel at 300 °F, which is assumed to be 15 Ksi which is equal to 103.42 N/mm², found in Table 13.2 in Sinnott [12].

The shell mass, M , is found by using the following equation 4.5.

$$M = \pi t_w \rho D_c L_c \quad (4.5)$$

Where t_w is the thickness of the wall, D_c is column diameter and L_c is the column height.

4.1.3 Calculation of heat transfer area in the reboiler and condenser

In the project it is assumed that the reboiler and condenser are counterflow shell and tube heat exchangers. Steam is used to heat the cold stream in the reboiler and water, from a source near the plant, is used to cool down the hot stream in the condenser. The area for the reboiler and condenser is found by using equation 4.6 given in [12].

$$Q = UA\Delta T_{lm} \quad (4.6)$$

The duty, Q , for the condenser or the reboiler is extracted from UniSim. A is the area in m², ΔT_{lm} is the logarithmic mean temperature. U W/m²°C is the overall heat-transfer coefficient given in W/m²°C. The value for the heat-transfer coefficient is given in Table 4.1 and is found in [3].

Table 4.1: Overall heat-transfer coefficient

U-tube	250 – 750	W/m ² °C
Kettle reboiler	500 – 1000	W/m ² °C

In this project the value 750 W/m²°C and 1000 W/m²°C is used for the U-tube and the kettle reboiler.

The logarithmic mean temperature difference, ΔT_{lm} , can be found be using equation 4.7 found in [12]

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} \quad (4.7)$$

ΔT_1 and ΔT_2 is the difference in the temperature between the two streams on both sides of the heat exchanger.

4.1.4 Temperature of the streams in and out of the condenser

The temperature of the hot streams in and out of the condenser is found in UniSim. The hot inlet stream in the condenser is found in the vapor stream in the top of the column. The cooled outlet stream in the condenser is found in the distillate stream.

In this project it is assumed that cooling water in the process is pumped up from a water source near the plant, and that the heated cooling water is returned to the water source. It is assumed that the temperature for the cooling water in the condenser goes from $T_{in}=10\text{ }^\circ\text{C}$ to $T_{out}=15\text{ }^\circ\text{C}$, due to the minimum temperature difference given in Sinnott [12]. The difference in the temperature, ΔT_{min} , in the to outlet streams for a condenser will usually be between $5\text{ }^\circ\text{C}$ and $7\text{ }^\circ\text{C}$ when cooling water is used as a cooling agent. For every case in this project it is assumed that the minimum temperature difference is $5\text{ }^\circ\text{C}$ or more. If this lower limit is not satisfied, the temperature in the cooling stream has to be changed to a lower value.

4.1.5 Temperature of the streams in and out of the reboiler

The temperatures of the in and out streams in the reboiler is also found in UniSim. The cold inlet stream in the reboiler is found in the liquid stream in the bottom of the column, and the heated outlet stream in the reboiler is found in the boil-up stream.

In the reboiler steam is used to heat the liquid stream. It is assumed that low pressure steam is used. Low pressure steam has a pressure at 4 bar and the temperature is $160\text{ }^\circ\text{C}$. According to this assumption the inlet temperature for the steam is set to $160\text{ }^\circ\text{C}$. The minimum temperature difference, ΔT_{min} , for a reboiler has to be between $10\text{ }^\circ\text{C}$ and $30\text{ }^\circ\text{C}$. In this project it is assumed that ΔT_{min} is $20\text{ }^\circ\text{C}$. According to this relationship the temperature for the steam out of the reboiler is set to be $20\text{ }^\circ\text{C}$ higher than the heated outlet stream in the reboiler. If the outlet temperature for the steam is higher than the temperature in low pressure steam, medium pressure steam or high pressure steam have to be used instead. Values for medium ($212\text{ }^\circ\text{C}$ and 20 bar) and high pressure ($250\text{ }^\circ\text{C}$ and 40 bar) steam is found in [12].

4.2 Cost calculations assumptions

N/N_{min} giving the lowest cost are found in two cases, with and without energy costs.

For both of these cases the cost evaluation is based on the following assumptions:

- The distillation column is a vertical process vessel, and the maximum operating pressure is 10 bar
- Sieve trays are used in the column

- The condenser is a U-tube heat exchanger and water is used as cooling agent
- The reboiler is a kettle reboiler and steam is used as heating agent
- Norwegian electricity is used to generate steam
- Equipment for the support systems to the column is not included
- The construction material is stainless steel
- The pay back time is 5 years
- The column is operating 8000 hours per year
- Increase in the costs due to loans are not included

In one of the cost method equations in Turton [13] is used to calculate the cost. The factors and equations that are used gives the cost in 2001 US gulf coast basis. In the other cost method equation in Sinnott [12] is used, which give the cost in 2001 US gulf coast basis. In both the methods the inflation is taken to considering to get the value to the present time by using equation 4.17 given in the chapter below.

4.3 Turton cost method

Equations given in Turton [13] is used to calculate the capital costs for the distillation column, including condenser and reboiler.

4.3.1 Purchased Equipment Cost

The value of purchased cost, C_p^0 , for the plant is calculated at ambient operating pressure and carbon steel is used as construction material. This material cost is later converted to the cost for stainless steel in chapter 4.3.3. Purchased cost can be calculated by using equation 4.8 given is [13]

$$\log(C_p^0) = K_1 + K_2 \log(A) + K_3 \log(A)^2 \quad (4.8)$$

In this equation A is the size parameter. K_n is purchased cost factors for different equipment, and is given in Table 4.2

Table 4.2: Equipment Cost Data, given in [13]

Equipment	K_1	K_2	K_3	Size parameter
Process vessels	3.4974	0.4485	0.1074	volume [m^3]
Sieve trays	2.9949	0.4465	0.3962	area [m^2]
U-tube	4.1884	-0.2503	0.1974	area [m^2]
Kettle reboiler	4.4646	-0.5277	0.3955	area [m^2]

4.3.2 Pressure factor

The cost for the process vessel is depending on the operating pressure in the column. The pressure factor, F_p is calculated by equation 4.9, which is a function of the column pressure and diameter.

$$F_p = \frac{\frac{(p+1)D}{2(849,6-1.2(p+1))} + 0.00315}{0.0063} \quad (4.9)$$

where p is the operating pressure *bar*g and D is the diameter m in the column. It has been assumed that the operating pressure was 10 *bar* in the column. The cost for the other equipment is independent of the pressure, when a low pressure is assumed.

4.3.3 Bare Module Cost

Bare module cost is the sum of direct and indirect cost for each equipment. The bare module cost for the heat exchanger and the process vessel can be calculated by using the equation 4.10

$$C_{BM} = C_p^0 F_{BM} \quad (4.10)$$

where F_{BM} is given in equation 4.11

$$F_{BM} = B_1 + B_2 F_M F_p \quad (4.11)$$

B_n is the bare module factor and F_M is the material factor. In this project there were assumed that all the equipments material are stainless steel. B_n and F_M for stainless steel are given in Table 4.3. F_p is the pressure factor given above. The cost of the heat exchanger is independent of the pressure, when the pressure is low, and F_p is then equal to one.

Table 4.3: Bare module factor and material factor for stainless steel and carbon steel

Equipment	B_1	B_2	F_M Stainless steel	F_M Carbon steel
Process vessels	2.25	1.85	3.33	1
Heat exchanger	1.63	1.66	2.7	1.33

The bare module cost for the sieve trays is calculated with equation 4.12.

$$C_{BM} = C_p^0 N F_{BM} F_q \quad (4.12)$$

F_{BM} is the bare module factor, which is dependent of the material for the equipment and are given in stainless steel for the trays. For sieve trays $F_{BM} = 1.33$. N is the number of actual trays in the column. F_q is a quantity factor for trays, and can be found by using equation 4.13.

$$\log(F_q) = 0.4771 + 0.08516 \log(N) - 0.3473 (\log(N))^2 \quad (4.13)$$

for $N < 20$

$$F_q = 1 \text{ for } N > 20$$

4.3.4 Total Module and Grass Roots Costs

Total module costs refers to the cost of making small-to-moderate expansion to an existing plant. Grass roots cost, also known as the fixed capital cost, refers to the cost to a completely new facility.

Total module cost can be found by using equation 4.14.

$$C_{TM} = \sum_{i=1}^n C_{TM,i} = 1.18 \sum_{i=1}^n C_{BM,i} \quad (4.14)$$

The grass root cost, C_{GR} , can be estimated by using equation 4.15.

$$C_{GR} = C_{TM} + 0.50 \sum_{i=1}^n C_{BM,i}^0 \quad (4.15)$$

In both equations n is the number of equipment. C_{BM}^0 in equation 4.15, can be found by calculating the bare module cost for the equipment with ambient pressure and carbon steel as material.

4.4 Sinnott cost method

In the second cost method the cost equations presented in Sinnott [12] are used to calculate the cost for the distillation column. The purchased cost, C_e , for the whole column, can be calculated by using eq.

(4.16)

$$C_e = a + bS^n \quad (4.16)$$

Where S is a size parameter, a and b are cost constants and n is the exponent for the type of equipment; all given in Table 4.4 . The calculation is done at ambient operating pressure and the construction material is Stainless steel 304. The factors and equations that are used give the cost in 2006 and US gulf coast basis.

Table 4.4: Equipment Cost Data

Equipment	a	b	n	Size parameter
Process vessels	15000	68	0.85	Shell mass [kg]
Sieve trays	110	380	1.8	Diameter [m]
U-Tube Condenser	24000	46	1.2	Area [m^2]
Kettle reboiler	25000	340	0.9	Area [m^2]

In the case of sieve trays, condenser and reboiler, the data of Table 4.4 is given for carbon steel and the equation needs a factor of 1.3 to be applicable for stainless steel. The cost estimated by equation 4.16 needs to multiply by a factor of 6 in order to get the total fixed capital cost.

4.5 Accounting for Inflation

Since the fixed capital cost calculated in the two methods is not in the value for the present time. The fixed cost have to be converted into value for the present time before the cost analyse can be done. This can be done be using the equation below 4.17, given in [13].

$$C_2 = C_1 \frac{I_2}{I_1} \quad (4.17)$$

in this equation, C_1 is the cost for the base time when the cost is known, C_2 is the cost value for the present time, I_1 is the cost index for the base time and I_2 is the cost index for the present time. The CEPCI-index gives the values for I_1 and I_2

The value for I_1 when the cost method in Turton is used is 397 [13]. The CEPCI-index when the cost method in Sinnott is used is 509.7 [12]. For I_2 the CEPCI-index for February 2012 is used. The value is 590.8 [4].

4.6 Effect of location factor

The equations and factors above give the cost in US Gulf Coast (USGC) basis. The total cost for a plant is dependent on the location for the plant. By using equation 4.18 [12] the cost for the plant built in an other country can be calculated [12].

$$\text{Cost of plant in location A} = \text{cost of plant in USGC} \cdot LF_A \quad (4.18)$$

LF_A is the location factor for location A relative to USGC basis.

In the case when the energy source in the reboiler is electricity, the cost for Norwegian electricity is used in the cost evaluation. The column is therefore located in Norway. It has been assumed that the location factor for Norway is 1.3 relative to USGC basis [11].

4.7 Operating cost

In this project, in the case of the operating costs, only the energy required in the reboiler that has been considered. It is assumed that the cooling water that is used in the process, has been pumped up from a water source near the plant. The cost of the electricity needed to pump up the water and the possible cost for returning the heated cooling water to the water source is not included in the calculation of the utility.

It has been assumed that steam is being used in the reboiler, and that electricity is used to heat water to steam. The amount of electricity needed in this process is found by using the duty needed in the reboiler and multiply it by 1.1 to account for a 10 percent heat loss. The cost for electricity was calculated by approximating the average value for the last four years in figure 4.1 for the blue line.

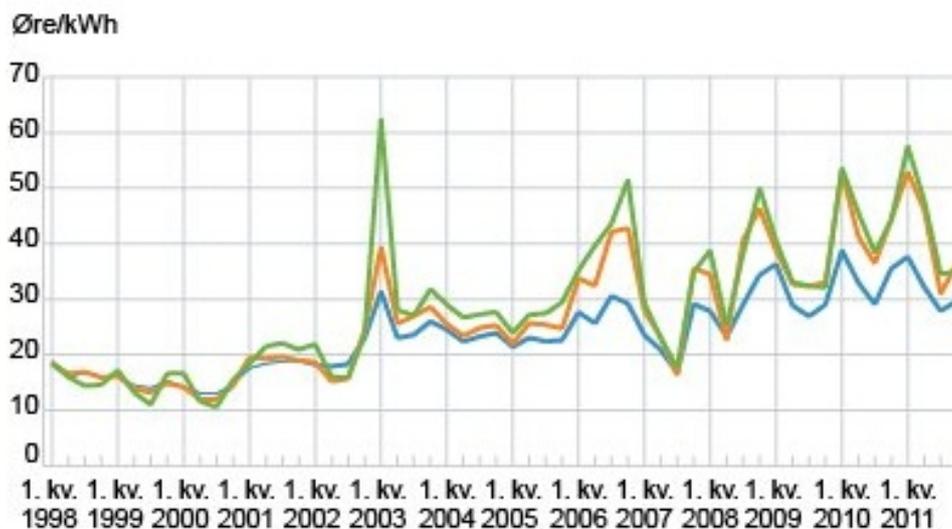


Figure 4.1: Price for the electric power in Norway. The green line is households, the orange line is service industry and the blue line is industry without high power industry and pulp and paper industry

The blue line in the figure show the price for the electric power in the Norwegian industry. In this project it has been assumed that the price for the electricity is $0.35 \text{ NOK}/kWh$, which is equal to $0.061 \text{ USD}/kWh$ when the currency is converted to USD [1].

5 Result from cost estimation

The cost estimation has been done for all the simulated mixtures in this project, except for the mixture with a boiling point below $0\text{ }^{\circ}\text{C}$ for atmospheric pressure, since that gives negative temperature values for the vapor entering the condensor. Another cooling agent than water has to be used in these situation. The cases filling these circumstances were discarded to from the cost estimation. That concerns the cases: n-Butane and Propane, Ethylene dicloride and Vinyl chloride, i-Butene and Propylene, Methyl tert-butyl ether and Butane, n-Butane and propylene, n-Pentane and Butane, Propane and Ethane.

Figure 5.1-5.3 shown below are the results from the simulation of the separation of Toluene and Benzene. The usage of colors and symbols are the same in all these three figures. The blue, red and green lines present the mole fraction for the binary mixture in the distillation stream in the top of the column. The red lines represent when zd is 0.01, the green lines when zd is 0.02 and the blue lines when zd is 0.04. The different symbols represent the changes in zf . The filled circle is when zf is 0.7, the unfilled circle when zf is 0.5 and the cross when zf is 0.3.

Figure 5.1 shows the N/N_{min} at the x-axis and the total capital cost at the y-axis. The optimal N/N_{min} is when the capital cost has a minimum. The minimum in fixed capital cost for toluene and benzene with different properties can be observed in the figure 5.1 shown below.

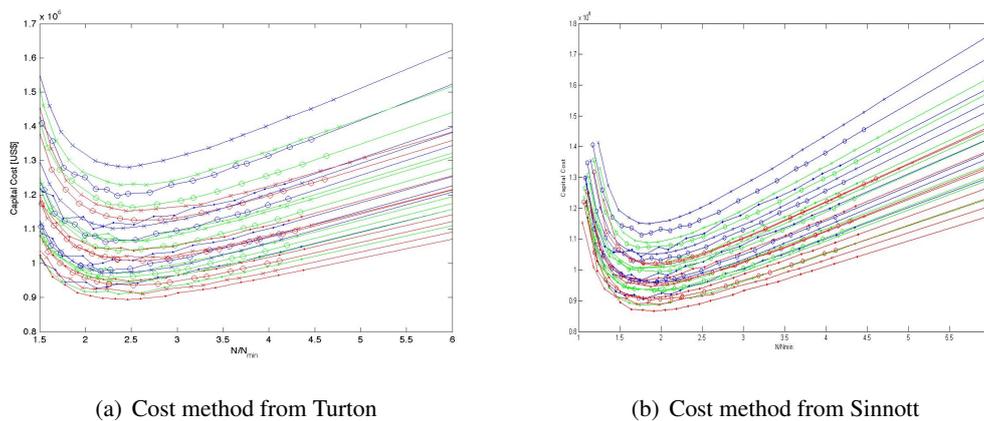


Figure 5.1: Fixed capital cost plotted against N/N_{min}

In figure 5.1 can it be seen that for the Turton cost method is the optimal N/N_{min} slightly higher than two, and for the Sinnott method is it slightly lower than two.

Figure 5.2 shows N/N_{min} plotted against the price for the energy needed in the reboiler in one year.

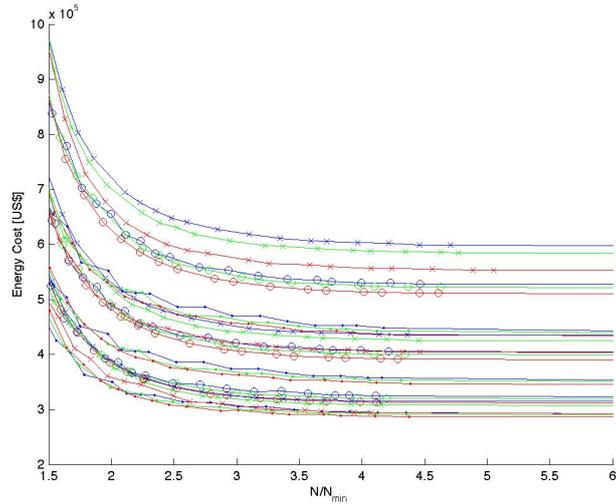
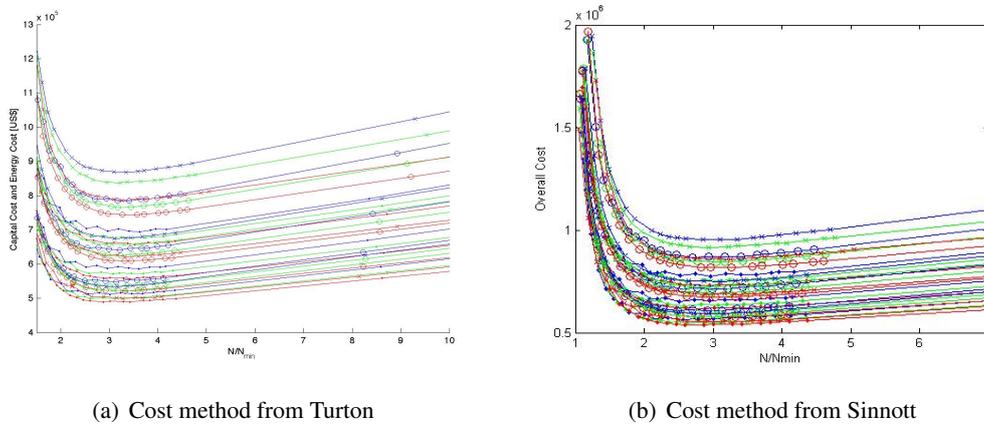


Figure 5.2: Energy cost plotted against N/N_{min}

From the theory it is known that the energy in a distillation column decreases when the height of the column increases. This correlation can be observed in Figure 5.2.

Figure 5.3 shows the N/N_{min} on the x-axis and the sum of the annualized capital cost and the energy cost on the y-axis.



(a) Cost method from Turton

(b) Cost method from Sinnott

Figure 5.3: Capital cost and energy cost plotted against N/N_{min}

In figure 5.3 it can be observed that the minimum for the overall cost has a higher value for the N_{ratio} compared to the case when only the capital cost was plotted against N_{ratio} . The optimal value for N_{ratio} is now closer to three than to two. This shows that increasing the energy costs increases the optimal N_{ratio} for both cost methods.

5.1 Distribution of cost

Figure 5.4 and 5.5 shows the cost distribution for column when the minimum total cost occurs for separation of Toluene and Benzene. This occurs when the mole fraction for the heavy component in the feed stream is 0.7, the feed stream is vapor and the mole fraction for the heavy component in the distillate is 0.04. In figure 5.4 the distribution for the capital cost is considered.

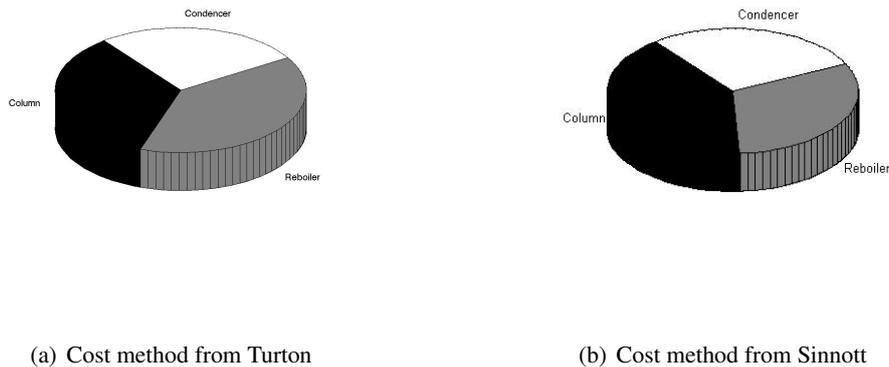


Figure 5.4: Distribution of capital cost

In the pie diagrams it can be observed that the cost for the column is lower when the Turton method is used compared to the cost method in Sinnott. The reason for this can be that when the Turton cost equations are used for the column, the volume of the column is the cost parameter, while the Sinnott method it is the weight of the column shell that is the cost parameter. It can also be observed in the diagrams that the cost for the reboiler is higher when the cost method from Turton is used compare to the cost method in Sinnott. In the both the cost equations for the reboiler, it is the area of the reboiler that is the cost parameter. These difference in distribution shows how the cost parameters are differently weighted in the two methods.

In figure 5.4 the cost for the energy is also included in the cost distribution.

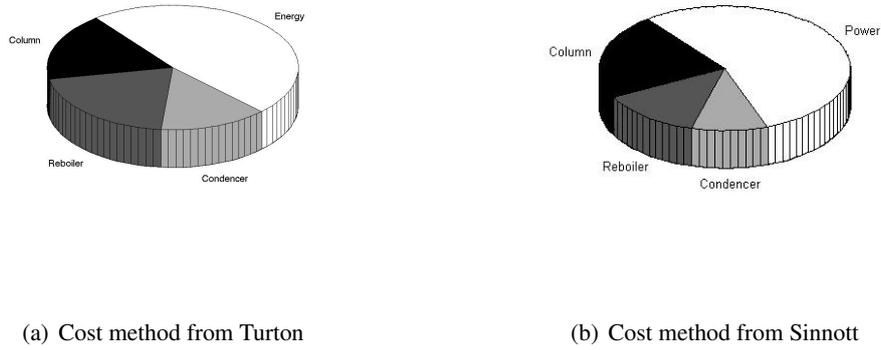


Figure 5.5: Distribution of the overall cost

The pie diagram shows that the cost for energy is the largest expense for the overall costs, accounting for over 50 % in both the methods. This is even though a cheap source of energy were used for generating steam to the reboiler.

5.2 Study parameters effect on the capital cost and the optimal N_{ratio}

Studies were done to check the effect of zf , zd and q on the capital costs and the optimal N_{ratio} for the capital costs and the overall costs. This was done by holding two of the parameters constant and varying the third.

5.2.1 The effect of changes in the parameters on the capital costs

Figure 5.6 is the result when zf is equal to 0.5, q is equal to 0.5 and zd is varied. The serie with circles is when zd is 0.01, the squares when zd is 0.02 and the triangle when zd is 0.04.

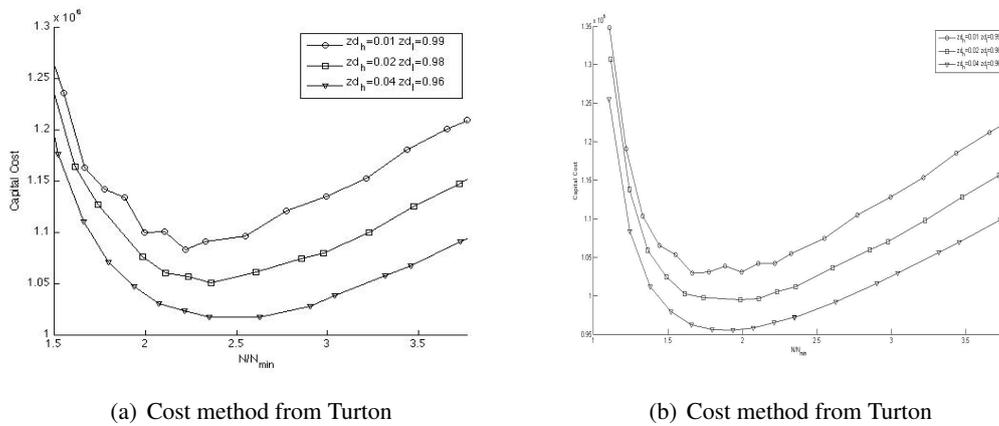


Figure 5.6: Fixed zf and q while zd varies. The sum of capital plotted against N/N_{min}

The result shows that the capital cost for the column, in both cost methods, increases when the product in the distillation stream becomes purer. This result is reasonable since a purer product needs a distillation column with a higher number of trays.

Figure 5.7 is the result when z_f is equal to 0.5 and z_d is 0.02. The serie with circles is when the feed stream is saturated vapor, the serie with squares is when the amount of vapor and liquid in the feed stream is equal, and the serie with triangles is when the feed stream is saturated liquid.

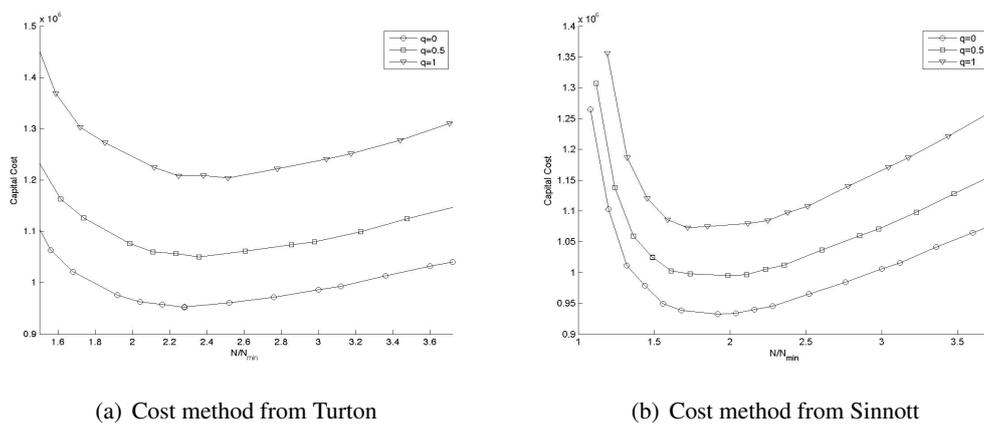


Figure 5.7: Fixed z_f and z_d while q varies. The sum of capital plotted against N/N_{min}

The results shows that the capital cost for the column increase when the feed quality goes from saturated vapor to saturated liquid. The trend can be seen for both cost methods. This result is reasonable since the energy requirement in the reboiler is higher when the inlet stream is liquid, and then the reboiler area then has to be larger, causing an increase in the cost for the reboiler.

In figure 5.8 is z_d and q kept constant at 0.02 and 0.5, respectively. The circles represent when z_f is 0.7, the squares when z_f is 0.5 and the triangles when z_f is 0.3.

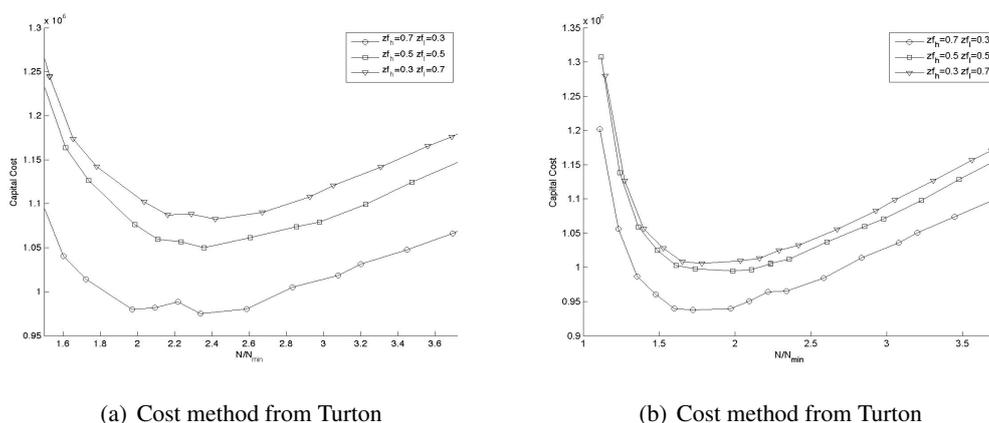


Figure 5.8: Fixed z_d and q with varying z_f . The sum of capital cost is plotted against N/N_{min}

In figure 5.8 it can be observed that the cost increase when the amount of heavy component in decreases.

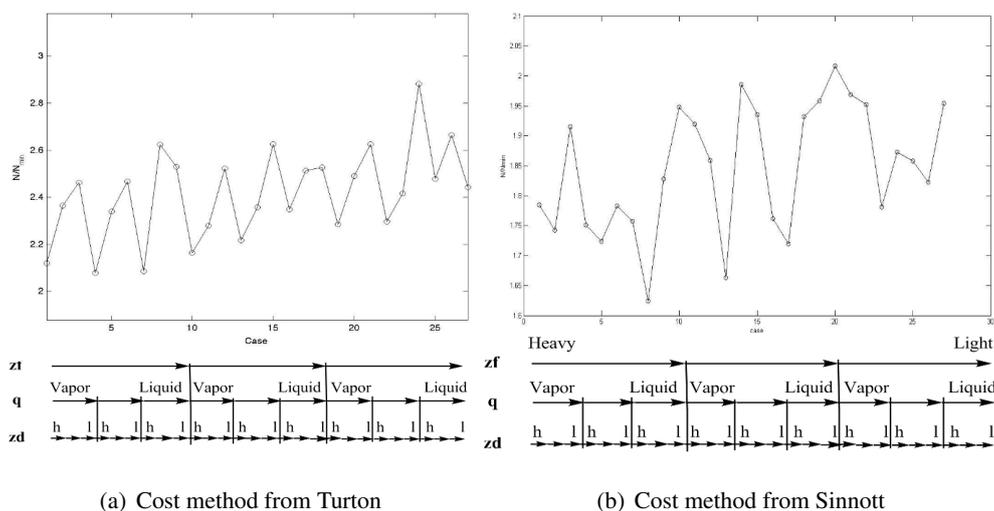
This is due to the setup of the simulation in UniSim. The size of the bottom stream and the purity is fixed, so in order to achieve the given specifications is it necessary to increase the fluid volume in the reboiler. Then more heat is required in the reboiler to vaporize the liquid and area of the reboiler increases.

5.2.2 Optimal N/N_{min} for capital and overall costs

Figure 5.9 shows the optimal N_{ratio} found from capital cost estimation for the 27 different simulation series in the separation of Toluene and Benzene. The cost estimation method on the left in figure 5.9 is for Turton and the right is for Sinnott. For the first three circles are the fraction of heavy in the distillate increased from 0.01 to 0.04, while q and z_f are kept constant. For the next three circles are z_f kept constant, q is increased to 0.5, while the cycle for z_d is repeated. In the next three circles are z_f still kept constant, q is increased to 1 and the cycle for z_d is repeated. Next is z_f decreased from 0.7 to 0.5 and the loops for q and z_d are repeated. The arrows below the graphs illustrates how the parameters are changed.

In the left graph it can be seen that a reduction in the purity of the product, the heavy fraction in the feed and the vapor fraction gives a higher N_{ratio} . Reducing the vapor fraction increases the area of the reboiler, due to an increased heat usage, giving higher capital costs for a low vapor fraction. Reducing the purity decreases N_{min} , according to distillation theory. The reduced N_{min} gives a higher optimal N_{ratio} . As previously mentioned does a decrease of the heavy fraction in the feed increase the capital cost, contrary to the distillation theory. This is due the specifications for the column in the simulation. The cost method for Sinnott does not show any clear trends, showing how the optimal N_{ratio} , in addition to be dependent upon the parameters, are dependent of the cost estimation method. Similiar graphs for all the cost estimated cases can be found in appendix B.5.3.

Figure 5.9: N/N_{min} vs. various cases of different compositions for the minimum amount of capital cost



The cost estimation series were not curve fitted, so the minimum costs were found for the N_{min} provided from the simulation data.

Figure 5.10 below shows the overall costs for the column, and it is built up in the same way as figure 5.9. Now is it the Sinnott cost estimation that shows the clear trends. The graph for the Sinnott method follows the same pattern as the Turton method described for figure 5.9. In appendix C can plots for the other cases be found.

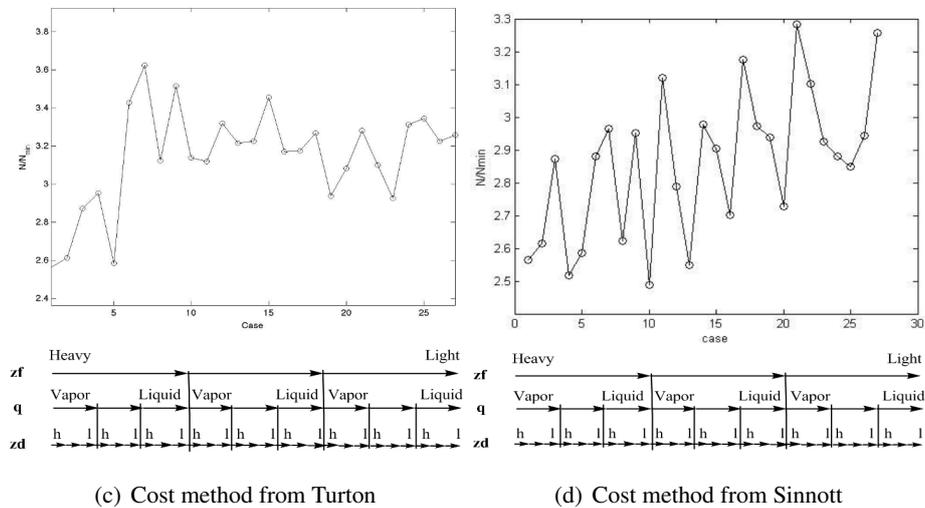


Figure 5.10: N/N_{min} vs. case, when capital cost and energy cost is considered

5.3 N/N_{min} when capital cost is considered

The data plotted in 5.2.2 were used to calculate an average optimal N/N_{min} for the capital cost for each of the cost estimated cases. The average for each of the cases are shown in Table 5.1.

Table 5.1: Average optimal N/N_{min} when different components are separated

Components	$N/N - min$	
	Cost method 1.	Cost method 2
Toluene and Benzene	2.3413	1.8451
1-Butanol and 2-propanol	2.5188	1.9805
26-xylenol and phenol	2.2085	1.7353
C4-Chloride and C3-Chloride	2.3170	1.8289
Ethanol and Methanol	2.2463	1.7979
Glycerol and Ethylene Glycol	2.3919	2.3515
m-cresol and phenol	2.1982	1.7727
n-Decane and n-Nonane	2.1150	1.7856
n-Heptane and Hexane	2.2554	1.8236
n-Nonane and n-Octane	2.0809	1.7728
n-octane and Heptane	2.2772	1.7875
p-Xylene and Benzene	2.5430	2.0297
p-Xylene and Toluene	2.3705	1.8587
Average N/N_{min}	2.3027	1.8746

The two different cost methods gives to different results for the average optimal N/N_{min} . The reason for this is that the cost for the column and reboiler are differently weighted in the two methods. In Turton the column have a lower price while the reboiler is more expensive, compared to Sinnott. This indicate that good cost estimation is necessary to find the number of stage in the column that gives the total minimum cost. The total average optimal N/N_{min} for the capital costs are 2.1.

5.4 N/N_{min} when overall cost is considered

The average optimal N/N_{min} corresponding the minimum overall cost is found for the cost estimation of the different binary mixtures. Table 5.2 shows the optimal N/N_{min} for each mixture, estimated by both the costs methods.

Table 5.2: Optimal N/N_{min} for the overall costs

Components	N/N_{min}	
	Cost method from Turton	Cost method from Sinnott
Toluene and Benzene	3.1423	2.8577
1-Butanol and 2-propanol	3.7093	3.3567
26-xylenol and phenol	2.8562	2.7089
C4-Chloride and C3-Chloride	3.0063	2.7839
Ethanol and Methanol	3.0515	2.9505
Glycerol and Ethylene Glycol	4.0877	4.1773
m-cresol and phenol	2.9820	2.8413
m-Decane and n-Nonane	2.8175	2.6893
n-Heptane and Hexane	3.0329	2.8227
n-Nonane and n-Octane	2.8612	2.7301
n-octane and Heptane	2.9266	2.8073
p-Xylene and Benzene	3.6442	3.2687
p-Xylene and Toluene	3.0691	2.8065
Average N/N_{min}	3.0916	2.8853

When the operating cost is included in the total cost, the average N/N_{min} for the two cost methods are more similar. The optimal N/N_{min} increases compared to the N/N_{min} for the capital costs. The average N/N_{min} for the two methods are 3. When capital costs are estimated, can the energy used be considered as free. The increase in the optimal N/N_{min} for the overall costs indicates that N/N_{min} should be higher than 2.

6 Discussion

All the calculations in this project is based on the simulation data from UniSim. Possible sources of errors in the simulation will therefore be important for the result. The property package used for each simulation, feed stage location and the tolerance in the equilibrium calculations in the column. Reducing these sources of error would decrease the uncertainties for the results and perhaps decrease the fluctuations. Optimizing the feed stage location would for an example decrease the energy usage in the column, and therefor affect the optimal N_{min} for the overall costs. z_f , z_d , q and N were varied to generalize the results from the simulations.

1 bar was used as feed pressure for the column, causing many of the components to have a bubble point below 0°C , giving negative temperatures in the condenser. Water was used as cooling agent in this project, and because that it was not possible to cool down the vapor in the condensor. Seven simulations were discarded from the cost analysis due to these circumstances.

The curve suggested by the group for curve fitting showed a decent fit to the simulation series. It did however estimate a too low N_{min} as well as a too high V_{min} . This was seen when the results were plotted with the same axes as Gilliland used. Using curve fitting to find N_{min} and V_{min} is a source of error for the recommended N_{ratio} , since the ratio is dependent upon N_{min} . The N_{min} found in this report is higher than the true N_{min} , making the recommended N_{ratio} lower than it should be.

The results found in the report is dependent on the cost estimations method by Turton and Sinnott. The energy source used to create steam for the reboiler is Norwegian electricity, which is a relative cheap energy source. Using a more expensive source of energy, would increase the recommended N_{ratio} . An increase in the capital costs would give a lower optimal N_{ratio} , since the capitol cost would be a larger portion of the total costs. The number of years for the pay back time of the column is also important. A longer pay back time would increase the recommended N_{ratio} .

Due to the sources of error is there uncertainties concerning in the optimal N_{ratio} that was found in the report.

For further analysis it is suggested that more accurate values are found for the overall heat-transfer coefficient, used in the cost estimation and for N_{min} . An improved value for N_{min} can be found by using McCabe-Thiele's method. Performing a similiar analysis for a multicomponent mixture would increase the generalization of the result.

7 Conclusion

This report have checked if the ratio between the real number of stages and the theoretical number of stages should be two, as mentioned in literature. A suggestion for a new ratio was found by simulating different binary mixtures in UniSim. Two different types of cost estimation methods, Sinnott and Turton, were used to check the ratio. With the Sinnott method it was found that the ratio giving the lowest capital cost is 1.9, and the ratio giving the lowest overall cost is 2.9. For the Turton method are the ratio for lowest capital cost and the lowest overall costs 2.3 and 3.1, respectively. The average ratio for capital cost is 2.1 and the average for the overall costs is 3.0 for both methods. Comparison of the two optimal ratios for capital costs and overall costs shows that the optimal N_{ratio} increases as the energy cost increases.

It was proposed an equation, $V/V_{min} = b/(N - N_{min})$, for curve fitting the simulation series and to be used as a shortcut method for finding N_{min} and V_{min} . The equation was found to not give a good fit, the N_{min} found is too low and the V_{min} is too high. To find a better estimate for N_{min} and V_{min} , the simulations series were curve fitted to the Molokonov equation in a Gilliland plot.

There are some sources of error concerning the N_{ratio} found in this rapport. The N_{ratio} found depend upon the results from the simulations, the sizing of the column and the thoroughness of the cost analysis. In the cost analyzes were many assumptions made for the column and the energy costs. Due to these sources of error it is not certain that the optimum N_{ratio} should be 3.0 for the overall costs, but the results shows that the N_{ratio} should be higher than two when the energy costs is included.

8 List of symbols

Table 8.1: List of symbols

Symbol	Unit	Description
α		Relative volatility
ρ_L	kg/m^3	mass density of liquid in boil-up stream
ρ_V	kg/m^3	mass density of vapor in boil-up stream
ΔT_{min}	$^{\circ}C$	Minimum temperature difference
a		constant curve fitting
a		constant Sinnott cost estimation
a_1		constant curve fitting
a_2		constant curve fitting
A		Size parameter for cost estimation
b		constant curve fitting
b		constant Sinnott cost estimation
b_1		constant curve fitting
b_2		constant curve fitting
C_p	US\$	Perched equipment cost
C_{BM}	US\$	Bare module cost
C_e	US\$	Purchased cost, Sinnott cost estimation
C_{GM}	US\$	Fixed capital cost
C_{TM}	US\$	Total module cost
D_c		Diameter column
F_{BM}		Bare module factor
F_p		Pressure factor used in cost estimation
F_q		Quantity factor for trays
H_f	kJ	Enthalpy feed
$H_{liq,sat}$	kJ	Enthalpy feed as saturated liquid
$H_{vap,sat}$	kJ	Enthalpy feed as saturated vapor
H_f	kJ	Enthalpy feed
K_1		Constant for cost estimation
K_2		Constant for cost estimation
K_3		Constant for cost estimation
l_t	m	Plate spacing in spacing
L	$kmol/h$	Liquid flow
L_C	m	Hight of distillation column

Symbol	Unit	Description
n		constant Sinnott cost estimation
N		Number of trays
N_{min}		Minimum number of steps
$N_{min_{curv}}$		N_{min} calculated by curve fitting and asymptote analysis
$V_{min_{curv}}$		V_{min} calculated by curve fitting and asymptote analysis
M	kg	Mass of column
$N_{rectifying}$		Number of stages in the rectifying section
N_{ratio}		Ratio between Number of steps and minimum number of steps
$N_{stripping}$		Number of stages in the stripping section
y_A		Vapor mol fraction of component A
P_i	N/mm^2	Maximum allowable column pressure
Q	W	Duty of re-boiler
q		quality of the feed
R		Reflux ratio
R		Minimumn reflux ratio
S		Size parameter in Sinnott cost estimation
SE	Ksi	Maximum allowable stress
t	m	Wall thickness
T_1R	C	Temperature reboiler in
T_2R	C	Temperature reboiler out
T_1C	C	Temperature condenser in
T_2C	C	Temperature condenser out
T_{lm}		Logarithmic middle temperature
u_w	m/s	Maximum allowable vapor velocity
V	$kmol/h$	Vapor flow
V_g	kg/s	Gas flow in boil-up for size calculation
V_{min}	$kmol/h$	Minimum vapor flow
x_A		Liquid mol fraction of component A
x_D		Liquid mol fraction in distillate
x_D		Liquid mol fraction in bottom
z^f		Feed composition in mol fraction
z^f_{heavy}		Feed heavy component in mol fraction
z^f_{light}		Feed light component in mol fraction
z^d		Distillate composition in mol fraction
z^b		Bottoms composition in mol fraction

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Appendices

A Results

The numbers of steps in the simulated column was potted towards the vapor flow. The graphs for the simulated cases is found in the figures right figure below. N_{min} and V_{min} was found by curve fitting, the procedure for this calculation is found in chapter 3. The normalized graphs with the N_{min} and V_{min} found by curve fitting is presented to the left in the following figures.

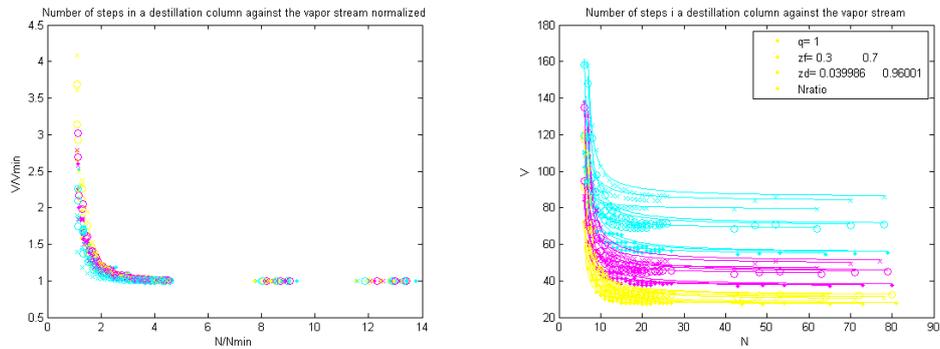


Figure A.1: Simulated data of 1-butanol2-propanol

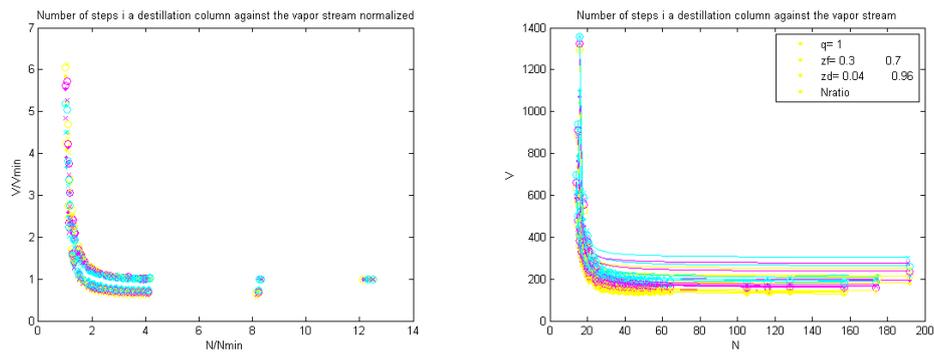


Figure A.2: Simulated data of 26-xylenolphenolfitted

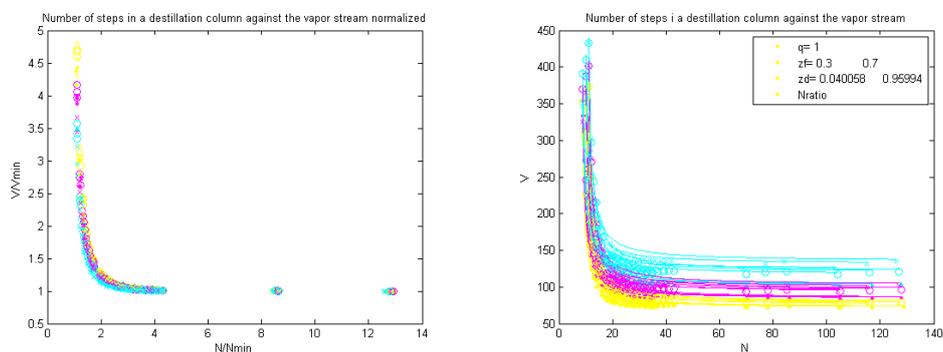


Figure A.3: Simulated data of c4chloridefitted

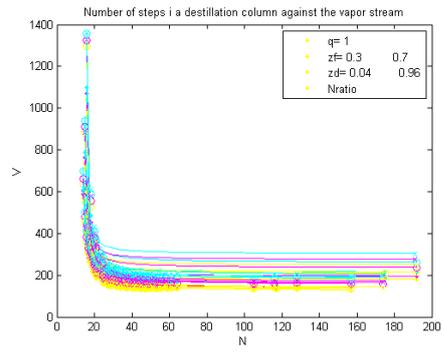
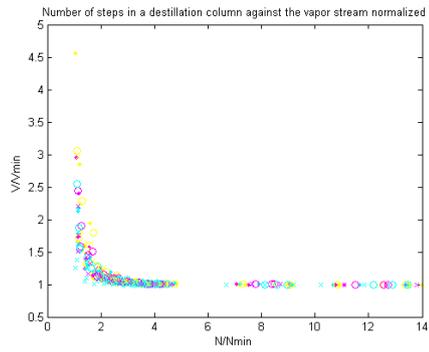


Figure A.4: Simulated data of edvcmfitted

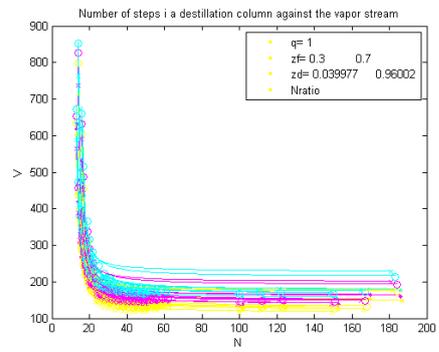
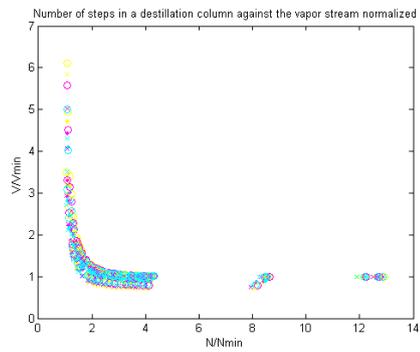


Figure A.5: Simulated data of ethanolmethanol

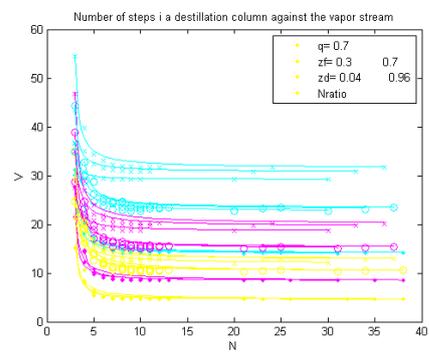
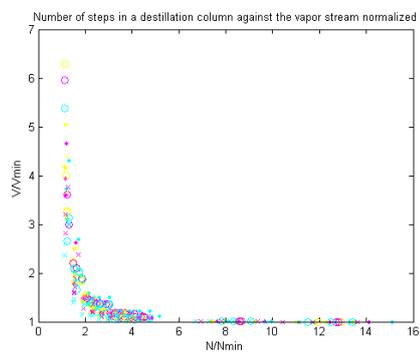


Figure A.6: Simulated data of glycoleglycol

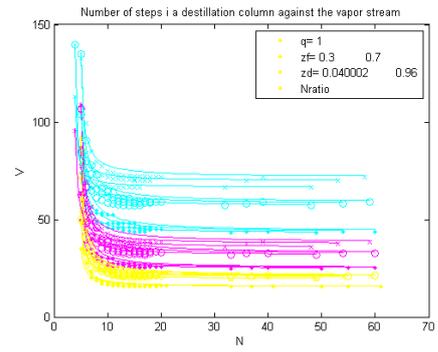
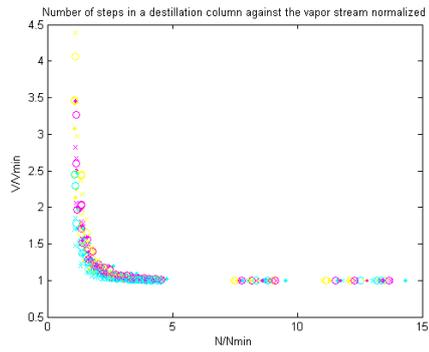


Figure A.7: Simulated data of i-butene/propene

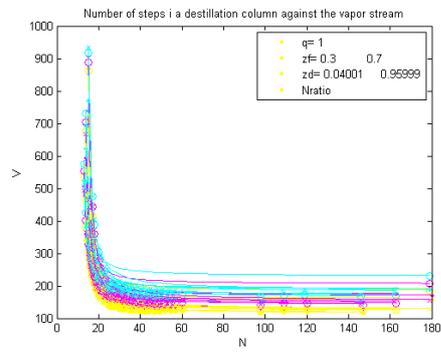
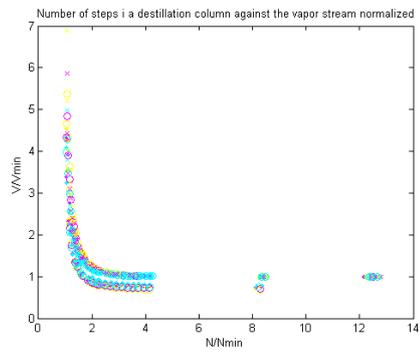


Figure A.8: Simulated data of m-cresol/phenol

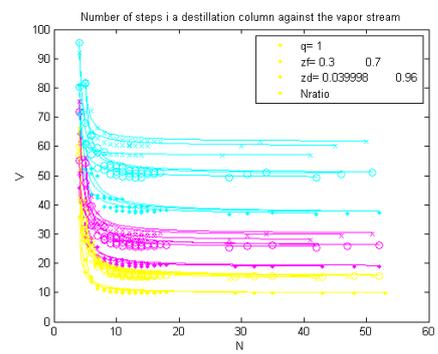
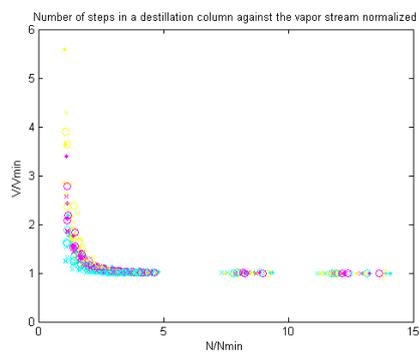


Figure A.9: Simulated data of MTBE/n-butane

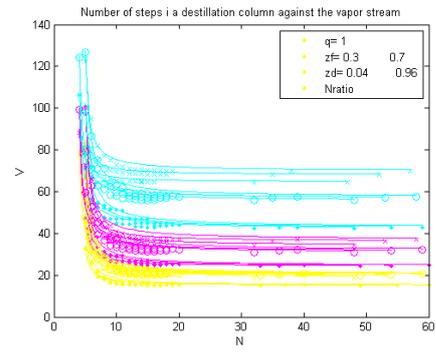
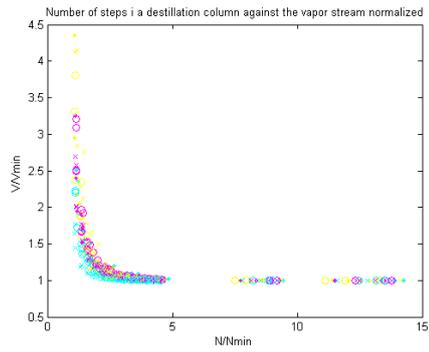


Figure A.10: Simulated data of n-butane-propane

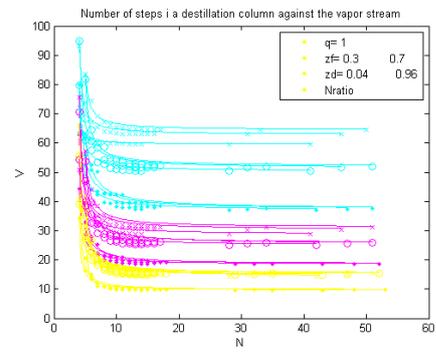
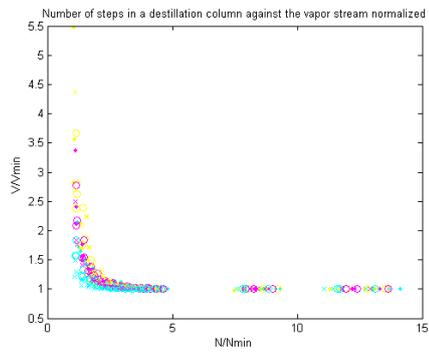


Figure A.11: Simulated data of n-butane-propene

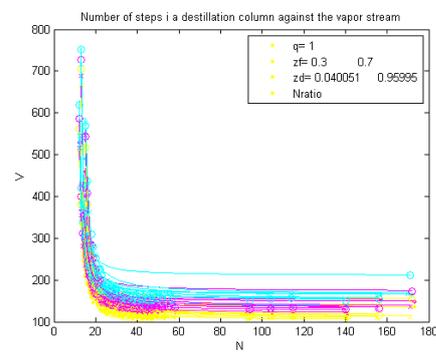
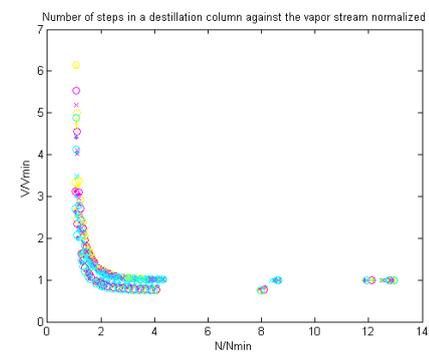


Figure A.12: Simulated data of n-decane-nonane-fitted

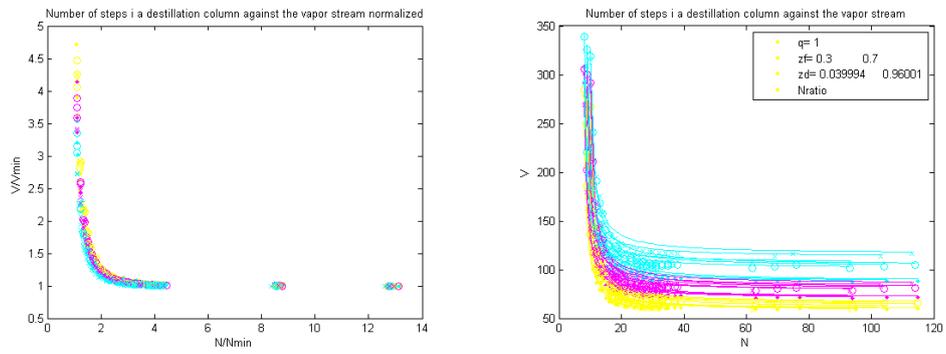


Figure A.13: Simulated data of n-heptanen-hexane

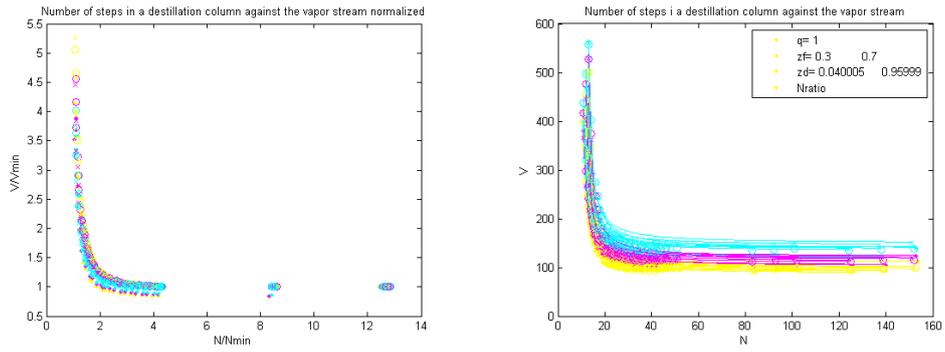


Figure A.14: Simulated data of n-nonanen-octane

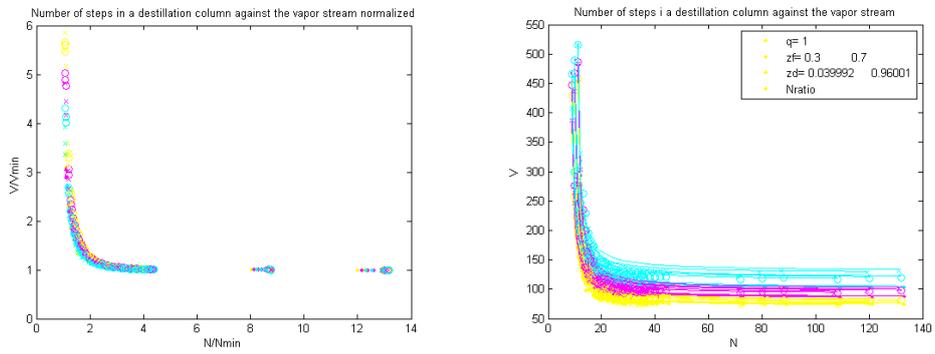


Figure A.15: Simulated data of n-octanen-heptane

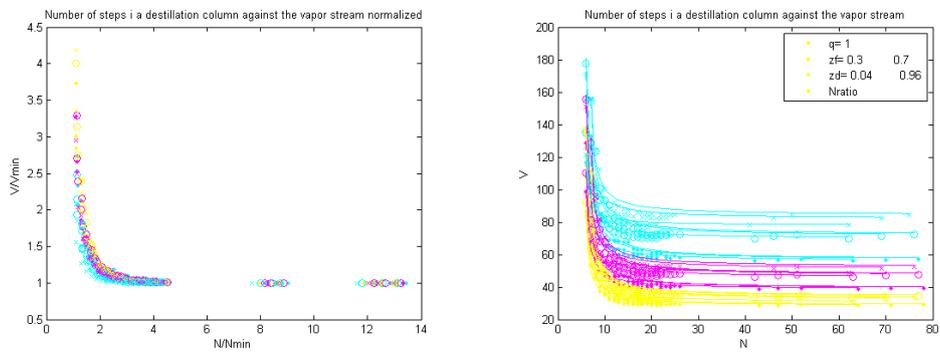


Figure A.16: Simulated data of pentanebutane

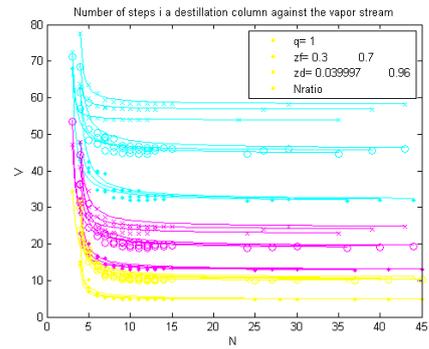
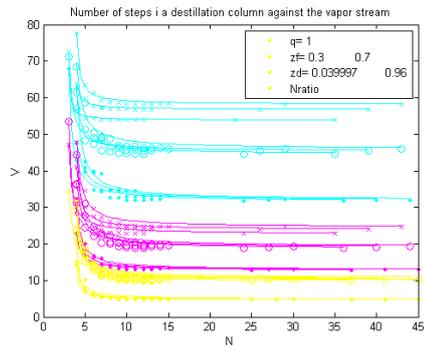


Figure A.17: Simulated data of pentanebutane

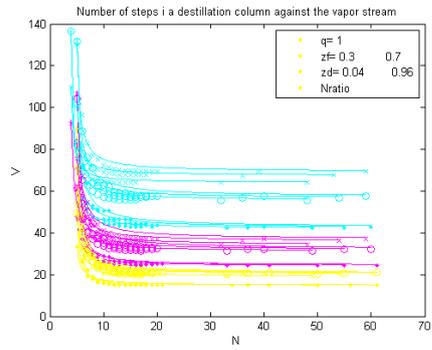
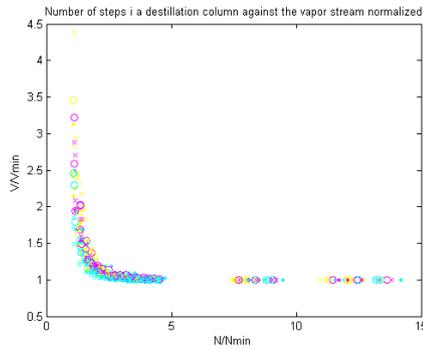


Figure A.18: Simulated data of p-xylenebenzene

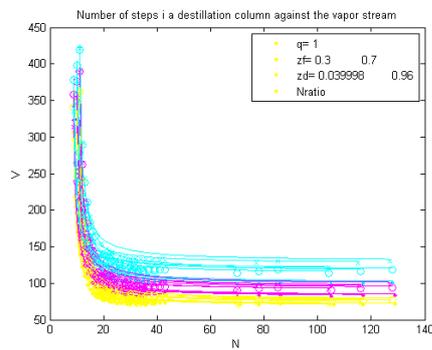
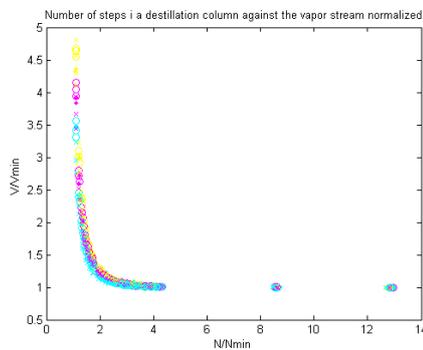


Figure A.19: Simulated data of p-xylenebenzene

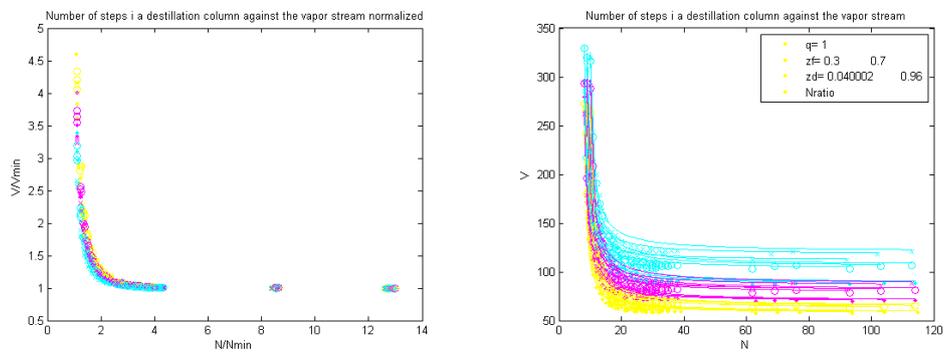


Figure A.20: Simulated data of toluenebenzene

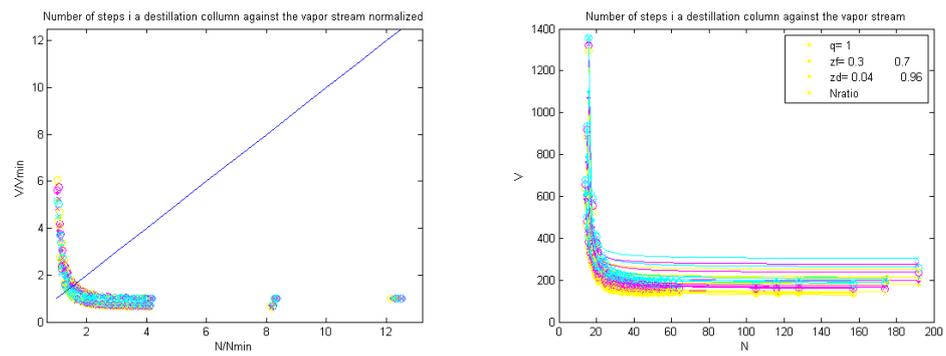


Figure A.21: Simulated data of xylenolphenolfitted

B Matlab scripts

Some of the matlab script that is used in the simulation is found in the following subchapters. The rest of the matlab script that is used will be given on request.

B.1 main

Main.m changes z_f , z_d , q and N , either in the document or by using other subscripts. All the changes and the corresponding V values are stored in the data matrix. After all the simulations have been run, is the data matrix stored as a matlab datafile. Main.m also performs the curve fitting of the results to equation ??.

```
%% Main.m
% Summary:
% UniSim is used to simulate a distillation column. Number of
% steps, minimum number of steps, and  $V$  is calculated by UniSim. This script
% systematically changes the following parameters in UniSim
%            $q$            - quality of feed
%            $z_f$           - composition of feed
%            $z_d_{heavy}$  - Heavy fraction of distillate
%            $N$            - Number of trays
% author:      Tor Anders Marvik and Jonas Kaasa
% organization: Department of Chemical Engineering, NTNU, Norway
% contact:     torandma@stud.ntnu.no
% license:
% requires:    matlab, UniSim and SCP scrips
% since:      2012.02.24
% version:    1.0
%
%
% started     February 2012
% changed:
% note:      Bla-bla.
%
%Input:      Data from UniSim and scrips that connects with UniSim
%Output:     alfa    - Relative volatility
%            $q$        - quality of feed
%            $F_f$       - Molar flow feed [kmol/h]
%            $z_f$       - Molar fraction feed [Heavy Light]
%            $F_d$       - Molar flow distillate [kmol/h]
%            $z_d$       - Molar fraction distillate [Heavy Light]
%            $V$         - Vapor flow from reboiler [kmol/h]
%            $V_{min}$     - Minimum vapour flow [kmol/h]
%            $N$         - Number of stages in rigorous column model
%            $N_{min}$     -  $N_{min}$  from shortcut column (Fenske)
%
```

```

%
% Guide to use the script
% 1. Open the UniSim simulation
% 2. Copy the UPC scripts on to the script folder in UniSim
% 3. Specify the path to the script folder in UniSim, line 57 in main.m
% 4. Manually change the components and the fluid package in UniSim. The
%     choice of fluid package have to be discussed for each case.
% 5. Run the matlab script
% 6. UniSim stops if the parameters specified is infeasible. Do not
%     fulfill the mass balance
%%

clc
clear all
close all

global script_folder %makes script_folder global
script_folder='D:\Skole\4aar\New folder\UPC scripts'; %the directory
%containing the UPC scripts

addpath([pwd, '\q_feed']) %add the folder q_feed to search path
serv = actxserver('UniSimDesign.Application'); %connects to UniSim ActiveX
%server
hyCase = serv.ActiveDocument; %UniSim model
col=hyCase.Flowsheet.Operations.Item('T-100'); %rigorous column in UniSim
specs=col.ColumnFlowsheet.Specifications; %specs in column
stream=hyCase.Flowsheet.MaterialStreams; %stream path
shortcut=hyCase.Flowsheet.Operations.Item('T-101'); %shortcut column path
EnergyStreams=hyCase.Flowsheet.EnergyStreams; %energy stream path

data=[]; %Matrix to save created data
%data=[q,Ff,zf,Fd,zd,tray,V(i),N(i),l,l,massflow,rhoL,rhoV,Duty_reboiler,
% Duty_condenser,T1R,T2R,T1C,T2C];

color=['y';'m';'c';'r';'g';'b';'w';'k']; %for color in plot

symbol=['.', 'o', 'x', '+', '*']; %for symbol in plot
count_symbol=0;
count=0; %keeps track of the series in the data file

%-----Loop that changes zf-----
zf_matrix=[0.7:-0.2:0.3;0.3:0.2:0.7]'; %[zf_heavy, zf_light]
for j=1:length(zf_matrix) %systematic change of feed composition
    zf_change(zf_matrix(j,:),script_folder,hyCase); %change feed
%composition in UniSim [heavy light]
    count_symbol=count_symbol+1;

%-----Loop that changes q-----
count_color=0;
for q=0:0.5:1

```

```

q_feed(q,100,hyCase);           %iterate on temperatur to reach q, 100°C=To
count_color=count_color+1;

%-----Loop that changes zd-----
zd_heavy=[0.01,0.02,0.04];      %fraction of heavy component in distillate
for zd_heavy_teller=1:length(zd_heavy)
specs.Item('Comp Fraction').goalValue=zd_heavy(zd_heavy_teller); %set heavy
                                %fraction distillate

%Retrive molar flow and compositions from column streams
zf= stream.Item('F1').componentMolarFractionValue;      %mole fraction feed
                                %stream [heavy light]
Ff=stream.Item('F1').molarFlow.value*3600; %molar flow feed stream [kmol/h]
zd= stream.Item('D1').componentMolarFractionValue;      %mole fraction
                                %distillate[heavy light]
Fd=stream.Item('D1').molarFlow.value*3600; %molar flow distillate[kmol/h]
zb= stream.Item('B1').componentMolarFractionValue;      %mole fraction bottom
                                %[heavy light]
Fb=stream.Item('B1').molarFlow.value*3600; %molar flow bottom [kmol/h]
EnergyReboiler=EnergyStreams.Item('E_btm1').heatFlowValue*3600; %energy
                                %reboiler [kJ/h]
%-----Data from rigourous UniSim simulation, not changing with stage-----
hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B21').CellValue=zd(1);
                                %fraction of heavy component in distillate in shortcut column
hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B20').CellValue=zb(2);
                                %fraction of light component in bottom in shortcut column
Nmin=hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B6').CellValue;
                                %Nmin from shortcut model, via spreadsheet
%-----
Nratio=[1 1.1 1.2 1.3 1.4 1.5 1.6 1.8 1.9 2 2.1 2.2 2.4 2.6 2.8 3 3.2...
        3.4 3.6 3.8 4 8 12]; %ratio between N and Nmin, 11 elements long

count=count +1;

for i=1:length(Nratio);

    N(i)=ceil(Nratio(i)*Nmin); %set number of stages. Does not include
                                %reboiler
    Nr_Ns=((zf(1)/zf(2))*(zb(2)/zd(1))^2*(Fb/Fd))^(0.206); %Ratio between
                                %rectifying and stripping stages in column
    tray=round((N(i)+1)/(1+1/Nr_Ns)); %set the feed tray
    stage_change(N(i),script_folder,hyCase); %change N in rigorous model
    feedstagechange(tray,script_folder,hyCase); %change feed tray
    V(i)=...
        col.ColumnFlowsheet.MaterialStreams.Item('boilup').molarFlowValue...
        *3600; %from sub flowsheet, vapor to reboiler [kmol/h]

%-----data importing for the cost estimation-----

massflow = ...

```

```

col.ColumnFlowsheet.MaterialStreams.Item('boilup').massFlowValue;
                                %massflow boilup[kg/s]
rhoL=...
hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B33').CellValue;
                                %density liquid boilup stream [kg/m3]
rhoV=...
hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B34').CellValue;
                                %density vapor boilup stream [kg/m3]
Duty_reboiler=...
hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B36').CellValue;
                                %Energy reboiler [kJ/h]
Duty_condenser=...
hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B37').CellValue;
                                %Energy condenser [kJ/h]

T1R=hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B40').CellValue;
                                %temperature in to reboiler [°C]
T2R=hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B41').CellValue;
                                %temperature out of reboiler [°C]
T1C=hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B38').CellValue;
                                %temperature in to condenser [°C]
T2C=hyCase.Flowsheet.operations.Item('SPRDSHT-1').Cell('B39').CellValue;
                                %temperature out of condenser [°C]

data=[data;q,Ff,zf,Fd,zd,tray,V(i),N(i),1,1,massflow,rhoL,rhoV,...
      Duty_reboiler,Duty_condenser,T1R,T2R,T1C,T2C,count]; %values stored
                                %in data file

%-----Plots-----
figure(2)
plot(N(i),V(i),[color(count_color) symbol(count_symbol)]) %plot N vs V
xlabel('N')
ylabel('V')
title('Number of steps in a distillation column against the vapor stream')
hold on
legend(['q= ' num2str(q)],...
       ['zf= ', num2str(zf)],['zd= ', num2str(zd)],'Nratio')

end

%-----Calculation of Nmin and V min using curv fittion by least square

V_calc=data((end-length(N)+1):end,9); %store column 9 in data as V_calc
N_calc=data((end-length(N)+1):end,10); %store column 10 in data as N_calc

Nmin=0; %Guess for Nmin, have to below the true Nmin
b=0.1; %Guess for b
Vmin=V_calc(end); %sets Vmin equal to last V_calc
[x,error,flag] = fminsearch('least_square',[Nmin,b],[],N_calc,V_calc,Vmin);
%minimizes the function least_square. Nmin and b are output. N_calc, V_calc
%and Vmin are input

```

```

Nmin=x(1);
b=x(2);

data(end-length(N)+1:end,11)=data(end-length(N)+1:end,9)./Vmin; %calculate
                                %ratio between V/Vmin
data(end-length(N)+1:end,12)=data(end-length(N)+1:end,10)./Nmin; %calculate
                                %ratio between N/Nmin

figure(3) %plot the ratios N/Nmin vs V/Vmin
V_Vmin=data(end-length(N)+1:end,11);
N_Nmin=data(end-length(N)+1:end,12);
xlabel('N/Nmin')
ylabel('V/Vmin ')
title...
('Number of steps in a distillation column vs the vapor stream normalized')

plot(N_Nmin,V_Vmin,[color(count_color) symbol(count_symbol)])
hold on

figure(2)
N_space=linspace(min(N),max(N));
plot(N_space,b./(N_space-Nmin)+Vmin,[color(count_color),'-'])

end
end
end

save('data\toluenebenzeneData.mat','data'); %store the datamatrix as a
                                           %.mat file

'Success!' %end of simulation

```

B.2 Stage change

This script changes the number of stages in the column in UniSim. The m-script shows how the changes in matlab were implemented in UniSim by UPC scripts.

```

function []=stage_change(N,script_folder,hyCase)

% Summary:      Changes the number of stages in rigorous column
% author:      Tor Anders Marvik
% contact:     ?????
% changed:     25 feb 2012
% Input:       N, script folder to unisim with the
%              script\change_stage.SCP
% Output:     None

```

```

% Assumes:      nothing

fid = fopen([script_folder, '\change_stage.SCP'], 'r+');      %opens the UPC
                                                         %script change_stage.SCP
                                                         %and enables writing
fseek(fid, 148, 'bof');                                     %find symbol 148
fwrite(fid, num2str(N, '%10.14e\n'));      %writes the number of stages before
                                                         %symbol 148
fclose(fid);                                              %closes change_stage.SCP

hyCase.Application.PlayScript([script_folder, '\change_stage.SCP']); %plays
                                                         %change_stage.SCP in UniSim

end

```

B.3 curve fitting developed

Curve fitting the developed curve to the simulation series using the least square method.

```

% Summary:      Least square method for curve fitting
% author:      Tor Anders Marvik
% contact:     ????
% changed:     25 feb 2012
% Input:      Nmin (x(1)), b (x(2)), N, V, Vend
% Output:     None
% Assumes:     nothing

function error=least_square(x,N,V,Vend)

error=0;                                               %Initial error
Nmin=x(1);                                           %Guess sent from main
b=x(2);                                              %Guess sent from main
error = sum((b./ (N-Nmin)+Vend)-V).^2);             %equation that the curve is
                                                         %fitted to

end

```

B.4 curve fitting Gilliland

Curve fitting the simulation series to the Molokanov equation 3.12 in a Gilliland plot.

B.4.1 Main gilliland script

```
% Summary:      Curve fit simulation series to Molokonov equation in
%              Gilliland plot
% author:       Tor Anders Marvik
% contact:      ?????
% changed:      20 March feb 2012
% Input:        data files from simulation
% Output:       None
% Assumes:      nothing

clear all
clc
hold on
close all

load([pwd, '\data\ferdigkjørt\n-butanepropeneData']) ;

%give the plot different colors and symbols
color=['y';'m';'c';'r';'g';'b';'w';'k'];           %for color in plot
symbol=['.','o','x','+','*'];                     %for symbol in plot

count_color=1;
count_symbol=1;
k=1;

lengde(1)=1;

figure(4)
hold on

xlabel('(V-Vmin)/V')
ylabel('(N-Nmin)/(N+1)')

for i=1:size(data,1)                               %loop that finds the size of each series
    if data(i,22)~=k
        k=k+1;
        lengde(k)=i;
    end
end
lengde(28)=size(data,1)+1;

i=1;
for count_zd=1:3                                   %changes zf
    for count_color=1:3                             %changes q
        for count_symbol=1:3                       %changes zd
```

```

figure(4)
N=data(lengde(i):lengde(i+1)-1,10);
V=data(lengde(i):lengde(i+1)-1,9);
Vmin=1;
Nmin=1;
[min,error,flag] = fminsearch('gilliland_Vmin_Nmin',[Nmin...,
    Vmin] , [],N,V);          %find minimum value of the function in
                                %gilliland_Vmin_Nmin

Nmin=min(1);
Vmin=min(2);
xaxis=1-Vmin./V;
yaxis=((N-Nmin)./(N+1));
plot(xaxis,yaxis,[color(count_color)... %plot simulation series
    symbol(count_symbol),'-'])      %in Gilliland plot

data(lengde(i):lengde(i+1)-1,23)=Vmin; %New Vmin in data(:,23)
data(lengde(i):lengde(i+1)-1,24)=Nmin; %New Nmin in data(:,23)
data(lengde(i):lengde(i+1)-1,25)=V./Vmin; %New V/Vmin data(:,23)
data(lengde(i):lengde(i+1)-1,26)=N./Nmin; %New N/Nmin data(:,23)

figure(2)                                %gilliland with curve fitting
xlabel(' (V-Vmin)/V')
ylabel(' (N-Nmin)/(N+1) ')

hold on
[x_curv,y_curv]=plot_gilliland(data(lengde(i)... %calculate axis
    :lengde(i+1)-1,:));
plot(x_curv,y_curv,[color(count_color)... %plot curve fit
    symbol(count_symbol),'-'])
xlim([0,1])
i=i+1;
end
end
end

figure(4)                                %Plot of the the molokanov equation
x=linspace(0,1);
y=1-exp(((1+54.4.*x)./(11+117.2.*x)).*((x-1)./sqrt(x)));
plot(x,y,'k')

figure(2)                                %gilliland with curve fitting
x=linspace(0,1);
y=1-exp(((1+54.4.*x)./(11+117.2.*x)).*((x-1)./sqrt(x)));
plot(x,y,'k')

```

B.4.2 Gilliland function

```

% Summary:      Curve fit to Molokonov equation using least square method
% author:      Tor Anders Marvik
% contact:     ????
% changed:    25 feb 2012
% Input:      min, N, V
% Output:     None
% Assumes:    nothing

function error=gilliland_Vmin_Nmin(min,N,V)

Nmin=min(1);
Vmin=min(2);

x=1-Vmin./V;                                %gilliland x axis
y=( (N-Nmin) ./ (N+1) );                    %gilliland y axis

m=1-exp( ((1+54.4.*x) ./ (11+117.2.*x)) .*... %Molokonov equation
        ((x-1) ./ sqrt(x)) );

error=sum((m-y).^2);                          %calculates the difference

```

B.4.3 Gilliland plot

```

% Summary:      Plot the Molokonov curve fit in a Gilliland plot
% author:      Tor Anders Marvik
% contact:     ????
% changed:    10 March 2012
% Input:      data
% Output:     x_curv, y_curv
% Assumes:    nothing

function [x_curv,y_curv]=plot_gilliland(data)
N_Nmin=data(:,12);                          %N/Nmin
V_Vmin=data(:,11) ;                          %V/Vmin
N=data(:,10);
V=data(:,9);
Nmin=N./N_Nmin;                              %calculate Nmin
Vmin=V./V_Vmin;                              %calculate Vmin

y_curv=(N-Nmin) ./ (N+1);
x_curv=(V-Vmin) ./ V;

```

B.5 Analysis

Plot the average $\frac{V}{V_{min}}$ values against $\frac{N}{N_{min}}$. The plot is discretized to give smooth curves.

B.5.1 Analysis

```
% Summary:      Find the average curve fit for the simulation cases
% author:       Tor Anders Marvik
% contact:      ????
% changed:      26 feb 2012
% Input:        None
% Output:       None
% Assumes:      nothing

clear all
close all
clc

hold on
figure(4)

xlabel('N/Nmin')
ylabel('V/Vmin')
hold on

N_Nmin=linspace(1,5); %discretize from 1 to 5
load([pwd, '\data\Ferdigkjørt\toluenebenzeneData.mat']);%loads the .mat file
[b]=plot_curvfit(data); %curve fits the data

V_Vmin_average=b./(N_Nmin-1)+1; %find the average V/Vmin value
plot(N_Nmin,V_Vmin_average, 'r') %plot the average V/Vmin value

%-----

load([pwd, '\data\Ferdigkjørt\1-butanol2-propanolData.mat']) ;
[b]=plot_curvfit(data);

V_Vmin_average=b./(N_Nmin-1)+1;
plot(N_Nmin,V_Vmin_average, 'c')

%-----

load([pwd, '\data\Ferdigkjørt\c4chloridec3chlorideData.mat']) ;
[b]=plot_curvfit(data);
```

```

V_Vmin_average=b./(N_Nmin-1)+1;
plot(N_Nmin,V_Vmin_average,'g')

%-----

load([pwd,'\data\Ferdigkjørt\glycoleglycolData.mat']) ;
[b]=plot_curvfit(data);

V_Vmin_average=b./(N_Nmin-1)+1;
plot(N_Nmin,V_Vmin_average,'b')

%-----

load([pwd,'\data\Ferdigkjørt\n-heptanen-hexaneData.mat']) ;
[b]=plot_curvfit(data);

V_Vmin_average=b./(N_Nmin-1)+1;
plot(N_Nmin,V_Vmin_average,'k')

%-----

load([pwd,'\data\Ferdigkjørt\m-cresolphenolData.mat']) ;
[b]=plot_curvfit(data);

V_Vmin_average=b./(N_Nmin-1)+1;
plot(N_Nmin,V_Vmin_average,'m')
%-----

axis([1,3,1,5]); %sets the axis to 1-3 in x-direction and
                 %1-5 in y-direction

legend('Toluene and Benzene','1-butanol and 2-propanol',...
'c4chloride and c3chloride','Glycole and Glycol',...
'n-heptanen and Hexane','m-cresol and PhenolData')

```

B.5.2 Plot curve

```

clear

Nmin=7;
Vmin=200;

```

```

N= [8 9 11 13 15 16 19 22 26 29 58];
V=[138.0300 96.5994 72.1627 61.8815 56.9952 56.2987 53.2823 52.3745 51.8653 51.7354 51.5799];
b=100;
c=10;

[x,error,flag] = fminsearch('least_sqaure',[Nmin,Vmin,b],[],N,V);

Nmin=x(1);
Vmin=x(2);
b=x(3);
%c=x(4);
plot(N,V,'o')
hold on

N_curv=[8:0.1:40];

%for i=1:length(N_curv)
%V_curv(i)=b*exp(c/(N_curv(i)-Nmin))+Vmin;
%end

V_curv=(b./(N_curv-Nmin)+Vmin);
plot(N_curv,V_curv)
plot([Nmin,Nmin],[0,max(V_curv)],'r')
plot([0,max(N)],[Vmin,Vmin],'r')

Vmin
Nmin

```

B.5.3 Last square function

```

function error=least_square_data(x,N,V)

% Summary:      Find the average curve fit for the simulation cases
% author:      Tor Anders Marvik
% contact:     ????
% changed:     25 feb 2012
% Input:      b (x(1)), N, V
% Output:     None
% Assumes:    nothing

error=0;
b=x(1);

error = sum((b./(N-1)+1)-V).^2;

```

end

C Average N/N_{min} when fixed capital cost is considered

The figure below shows the average N/N_{min} for different components when the properties for the components is changing. It is just the fixed capital cost that is considered. The different properties for the point in the figures below is shown in figure D.1

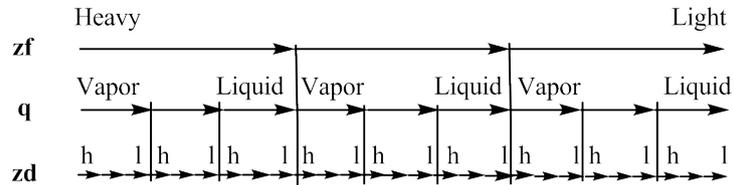
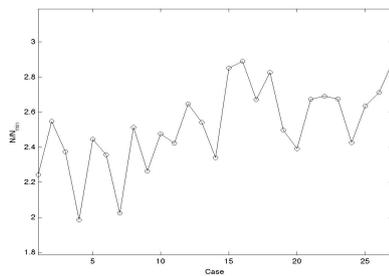
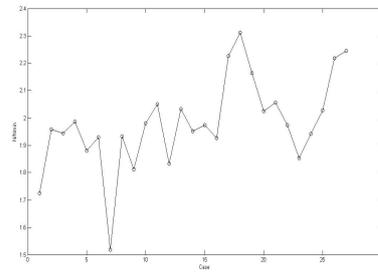


Figure C.1: Properties for the different points for the figures below

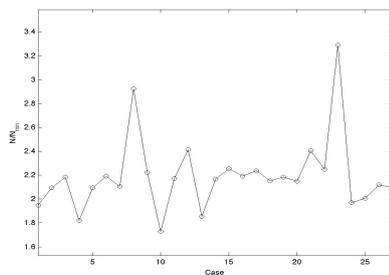


(a) Cost method from Turton

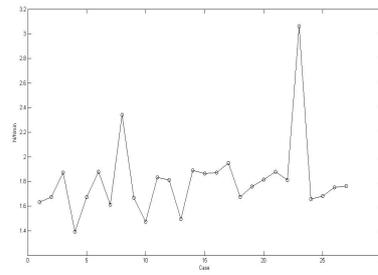


(b) Cost method from Sinnott

Figure C.2: 1-Butanol and 2-Propanol



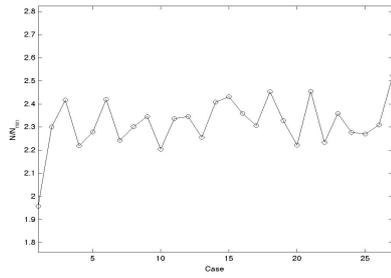
(a) Cost method from Turton



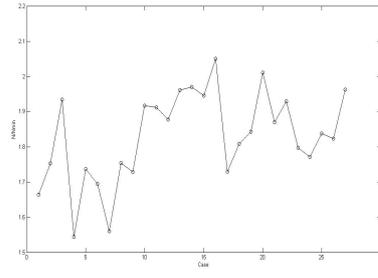
(b) Cost method from Sinnott

Figure C.3: 26-xylenol and phenol

In the case for separate 26-Xylenol and Phenol high pressure steam used instead of low pressure steam. Since the inlet temperature that is being heated in the reboiler has a higher temperature then the temperature in the low pressure steam.

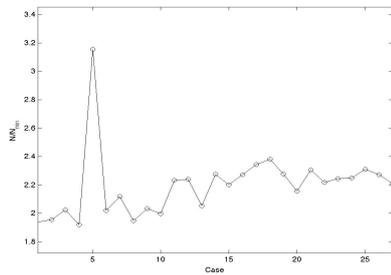


(a) Cost method from Turton

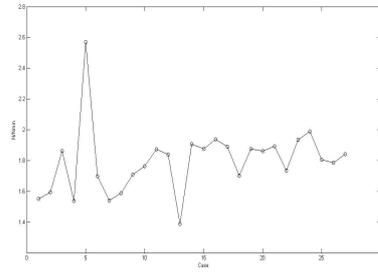


(b) Cost method from Sinnott

Figure C.4: C4-Chloride and C3-Chloride

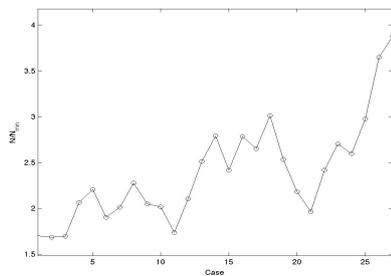


(a) Cost method from Turton

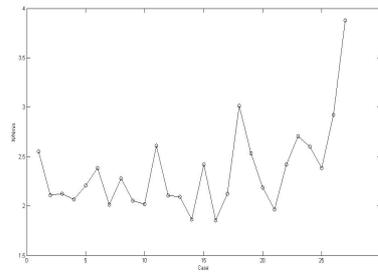


(b) Cost method from Sinnott

Figure C.5: Ethanol and Merhanol



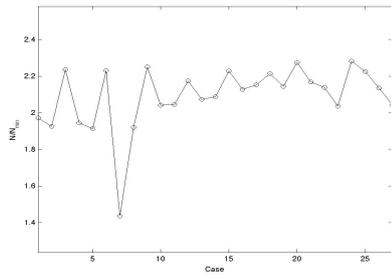
(a) Cost method from Turton



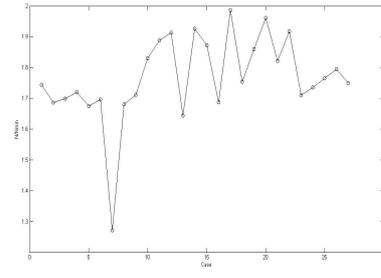
(b) Cost method from Sinnott

Figure C.6: Glycerol and Ethyl Glycol

For the case when Glycerol and Ethyl Glycol is being separate the inlet temperature in the reboiler is higher the the temperature for high pressure steam. Then it is been assumed that the inlet temperature for the steam in the reboiler is 40 °C higher then the outlet temperature for the steam.



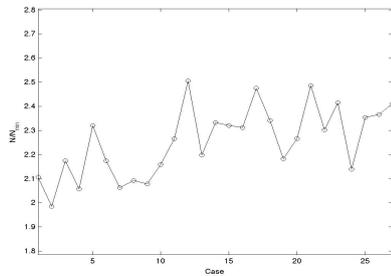
(a) Cost method from Turton



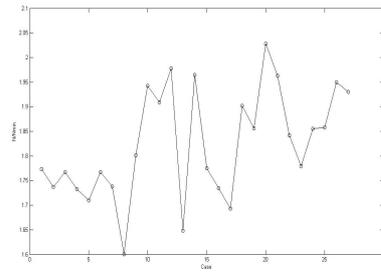
(b) Cost method from Sinnott

Figure C.7: n-Decanen and n-Nonane

In the case for separate n-Decane and n-Nonane medium pressure steam used instead of low pressure steam since the inlet temperature that is being heated in the reboiler is higher then the temperature for the low pressure steam.

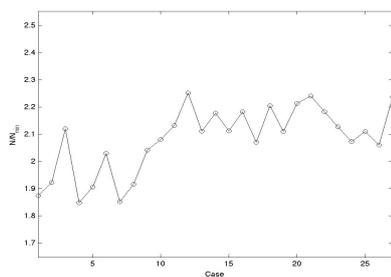


(a) Cost method from Turton

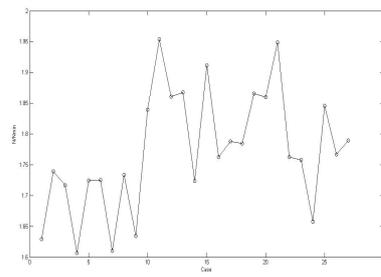


(b) Cost method from Sinnott

Figure C.8: n-Heptane and n-Hexane



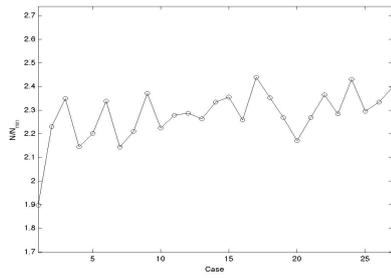
(a) Cost method from Turton



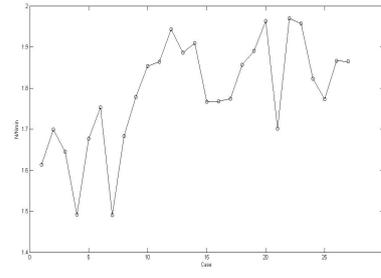
(b) Cost method from Sinnott

Figure C.9: n-Nonanen and n-Octane

In the case for separate n-Nonane and n-Octane medium pressure steam used instead of low pressure steam since the inlet temperature that is being heated in the reboiler is higher then the temperature for the low pressure steam.

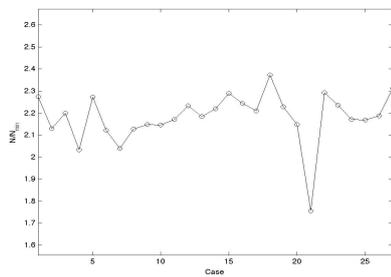


(a) Cost method from Turton

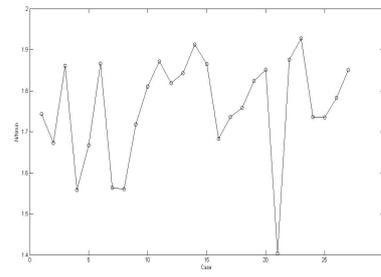


(b) Cost method from Sinnott

Figure C.10: n-Octane and n-Heptane



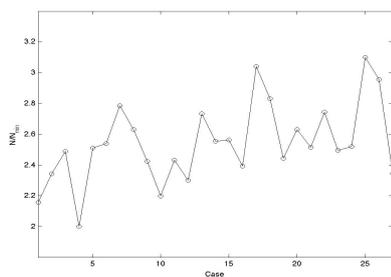
(a) Cost method from Turton



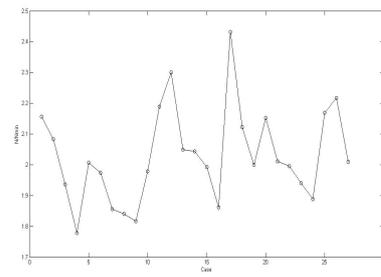
(b) Cost method from Sinnott

Figure C.11: m-Cresol and Phenol

In the case for separate m-Cresol and Phenol high pressure steam used instead of low pressure steam. Since the inlet temperature that is being heated in the reboiler has a higher temperature than the temperature in the low pressure steam.

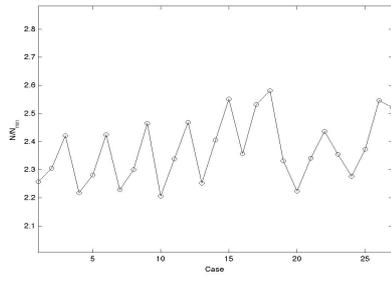


(a) Cost method from Turton

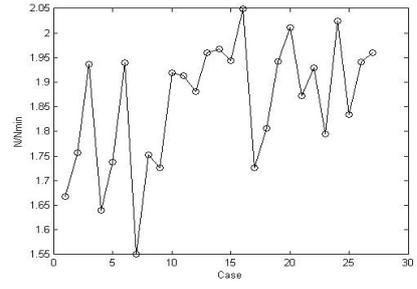


(b) Cost method from Sinnott

Figure C.12: p-Xylene and Benzene

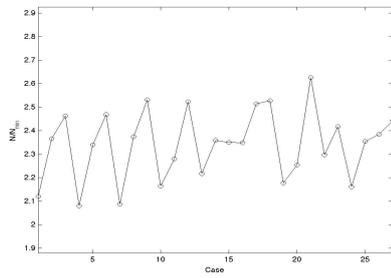


(a) Cost method from Turton

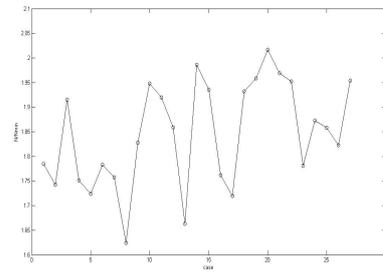


(b) Cost method from Sinnott

Figure C.13: p-Xylene and Toluene



(a) Cost method from Turton



(b) Cost method from Sinnott

Figure C.14: Toluene and Benzene

D Average N/N_{min} after cost calculation

The figure below shows the average N_{ratio} for different components when the overall cost is considered. In the different points in the figure below the properties for the components is changing and properties for the different point

The different properties for the point in the figures below is shown in figure D.1

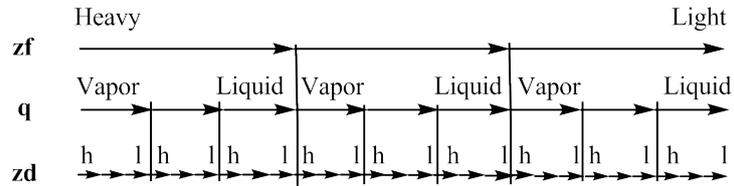
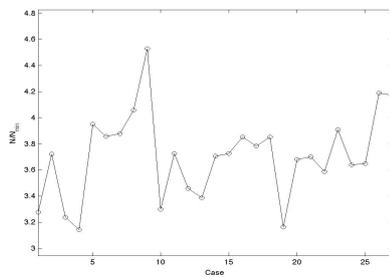
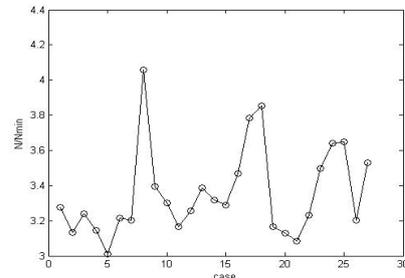


Figure D.1: Properties for the different points for the figures below

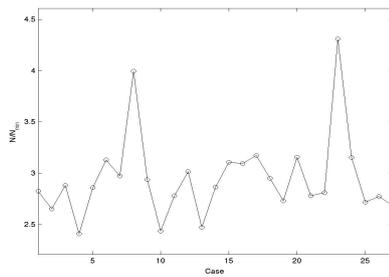


(a) Cost method from Turton

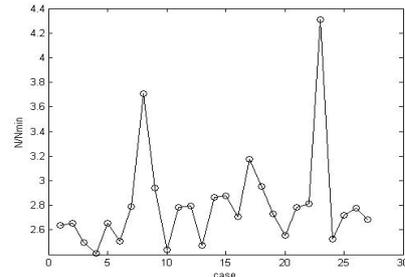


(b) Cost method from Sinnott

Figure D.2: 1-Butanol and 2-Propanol



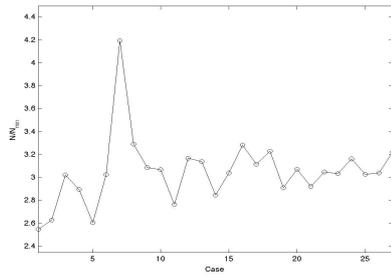
(a) Cost method from Turton



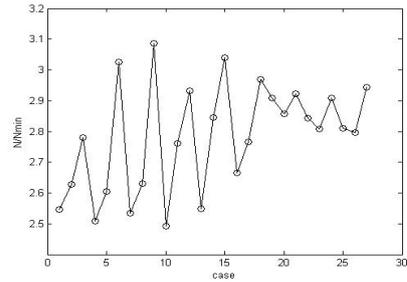
(b) Cost method from Sinnott

Figure D.3: 26-xylenol and phenol

In the case for separate 26-Xylenol and Phenol high pressure steam used instead of low pressure steam. Since the inlet temperature that is being heated in the reboiler has a higher temperature then the temperature in the low pressure steam.

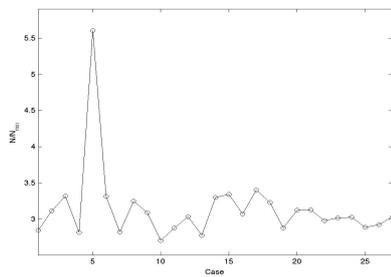


(a) Cost method from Turton

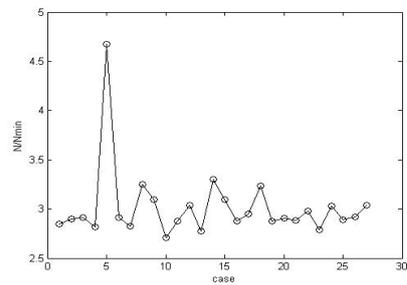


(b) Cost method from Sinnott

Figure D.4: C4-Chloride and C3-Chloride

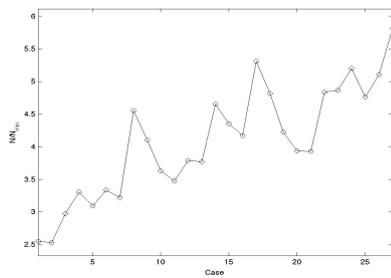


(a) Cost method from Turton

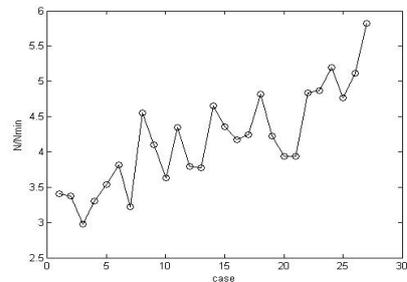


(b) Cost method from Sinnott

Figure D.5: Ethanol and Merhanol



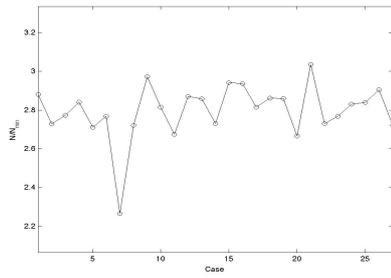
(a) Cost method Turton



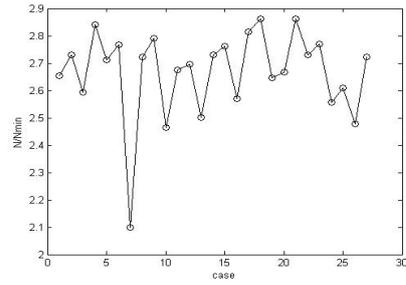
(b) Cost method from Sinnott

Figure D.6: Glycerol and Ethylene Glycol

For the case when Glycerol and Ethylene Glycol is being separate the inlet temperature in the reboiler is higher the the temperature for high pressure steam. Then it is been assumed that the inlet temperature for the steam in the reboiler is 40 °C higher then the outlet temperature for the steam.



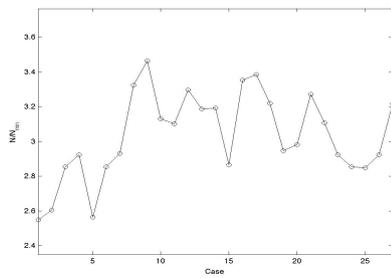
(a) Cost method from Turton



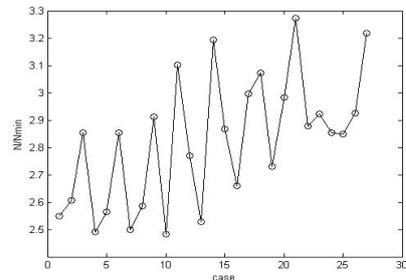
(b) Cost method from Sinnott

Figure D.7: n-Decanen and n-Nonane

In the case for separate n-Decane and n-Nonane medium pressure steam used instead of low pressure steam since the inlet temperature that is being heated in the reboiler is higher then the temperature for the low pressure steam.

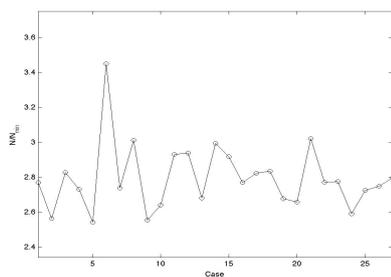


(a) Cost method from Turton

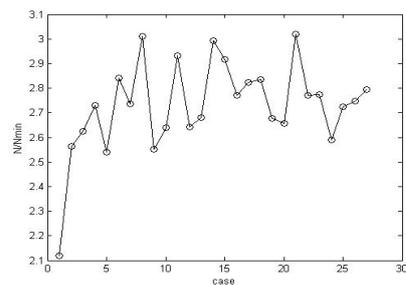


(b) Cost method from Sinnott

Figure D.8: n-Heptane and n-Hexane



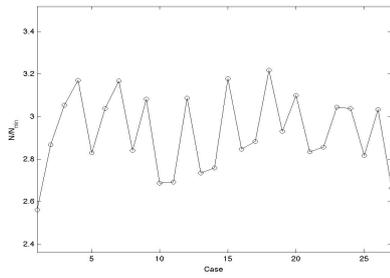
(a) Cost method from Turton



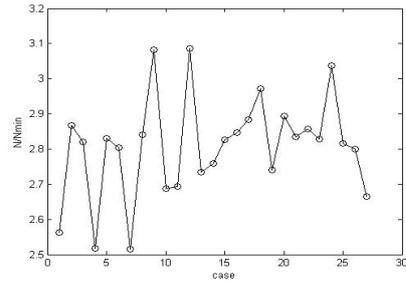
(b) Cost method from Sinnott

Figure D.9: n-Nonanen and n-Octane

In the case for separate n-Nonane and n-Octane medium pressure steam used instead of low pressure steam since the inlet temperature that is being heated in the reboiler is higher then the temperature for the low pressure steam.

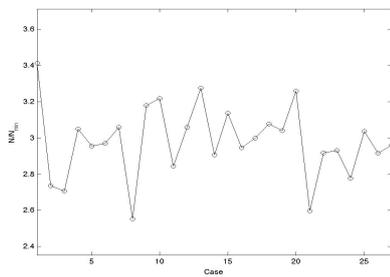


(a) Cost method from Turton

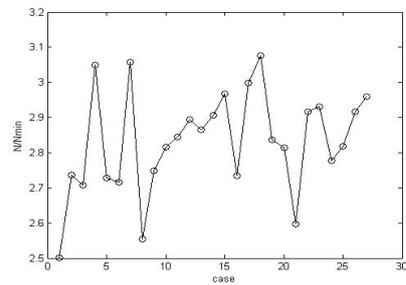


(b) Cost method from Sinnott

Figure D.10: n-Octane and n-Heptane



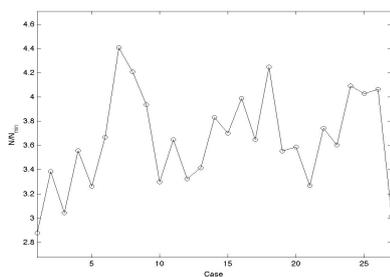
(a) Cost method from turton



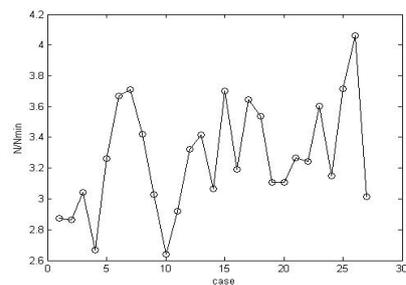
(b) Cost method from Sinnott

Figure D.11: m-Cresol and Phenol

In the case for separate m-Cresol and Phenol high pressure steam used instead of low pressure steam. Since the inlet temperature that is being heated in the reboiler has a higher temperature then the temperature in the low pressure steam.

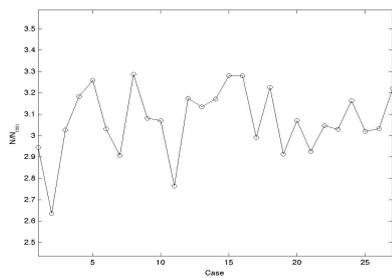


(a) Cost method from Turton

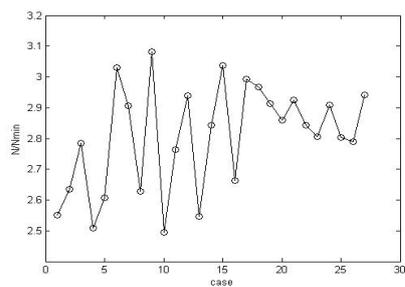


(b) Cost method from Sinnott

Figure D.12: p-Xylene and Benzene

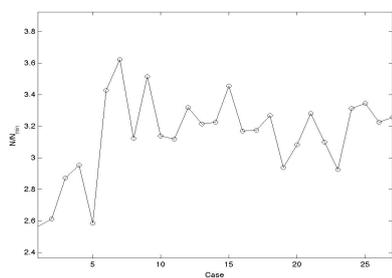


(a) Cost method from Turton

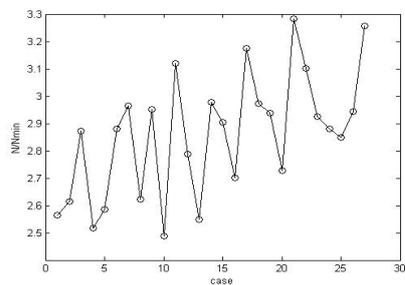


(b) Cost method from Sinnott

Figure D.13: p-Xylene and Toluene



(a) Cost method from Turton



(b) Cost method from Sinnott

Figure D.14: Toluene and Benzene

E Calculation example

E.1 Calculation of column diameter

Constants from simulation and assumptions

$$l_t = 0.9m$$

$$\rho_L = 874.7425kg/m^3$$

$$\rho_V = 3.1040kg/m^3$$

$$V_g = 1.5776kg/s$$

$$u_w = (-0.171l_t^2 + 0.27l_t - 0.047) \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \quad (E.1)$$

$$u_w = (-0.171 \cdot 0.9m^2 + 0.27 \cdot 0.9m - 0.047) \sqrt{\frac{874.7425kg/m^3 - 3.1040kg/m^3}{3.1040kg/m^3}}$$

$$u_w = 0.9634 m/s$$

$$D = \sqrt{\frac{4V_g}{\pi\rho_V u_w}} \quad (E.2)$$

$$D = \sqrt{\frac{4 \cdot 1.5776kg/s}{\pi \cdot 3.1040kg/m^3 \cdot 2.5385m/s}}$$

$$D = 0.8196 m$$

E.2 Calculation of shell weight

The calculate the wall thickness equation in Sinnott [12] is used and given below

$$P = 10bar$$

$$P = 1N/mm^2$$

$$SE = 103.42 \frac{N}{mm^2}$$

D is the diameter in column and calculated above. L is the tray spacing and assumed to be 0.9 m

$$\rho = 8030kg/m^2$$

$$t = \frac{P_i D_i}{(2SE - 1.2P_i)} \quad (E.3)$$

$$t = 3.9856mm$$

$$M = pt_w \rho DL \quad (E.4)$$

$$M = 1.3349 \cdot 10^3 kg$$

E.3 Calculation of area

In the example the reboiler area is calculated. Constants from simulation and assumptions

$$T_{in,reboiler} = 108.8316^{\circ}C$$

$$T_{ut,reboiler} = 109.7654^{\circ}C$$

$$T_{in,steam} = 159^{\circ}C$$

$$Q = 5.7587 \cdot 10^5 W$$

$$U = 1000 W/m^2$$

$$T_{out,steam} = T_{ut,reboiler} + 20^{\circ}C = 129.7654^{\circ}C$$

$$Q = UA\Delta T_{lm} \quad (E.5)$$

$$A = \frac{Q}{U \cdot \Delta T_{lm}} \quad (E.6)$$

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} \quad (E.7)$$

$$\Delta T_1 = T_{out,steam} - T_{in,reboiler} \quad (E.8)$$

$$\Delta T_2 = T_{in,steam} - T_{out,reboiler} \quad (E.9)$$

$$\Delta T_{lm} = 33.0339^{\circ}C$$

$$A = 17.4327 m^2$$

E.4 Cost calculation of capital cost when Turton is used

E.4.1 Calculation of purchased equipment cost

In the example the purchased equipment cost for the reboiler is shown. Parameters for calculated the cost for the reboiler is given below and found in Turton [13]

$$K_1 = 4.4646$$

$$K_2 = -0.5277$$

$$K_3 = 0.3955$$

A is the area calculated above and is equal to 17.4327

$$\log(C_p^0) = K_1 + K_2 \log(A) + K_3 \log(A)^2 \quad (E.10)$$

$$C_p^0 = 1.7896 \cdot 10^4 US\$$$

In the example the bare module cost for the reboiler is shown. Parameters for calculated the bare module cost for the reboiler is given below and found in Turton [13]

$$B_1 = 1.63$$

$$B_2 = 1.66$$

$F_M = 2.7$ which is the material factor and is given for stainless steel

$$F_p = 1$$

C_p^0 is the purchased cost and given above

$$C_{BM} = C_p^0 F_{BM} \quad (\text{E.11})$$

$$F_{BM} = B_1 + B_2 F_M F_p \quad (\text{E.12})$$

$$C_{BM} = 1.6039 \cdot 10^5 \text{ US\$}$$

To find the total capital cost the two equations below is used.

$$C_{TM} = 1.18 C_{BM,i} \quad (\text{E.13})$$

$$C_{GR} = C_{TM} + 0.50 C_{BM,i}^0 \quad (\text{E.14})$$

$C_{BM,i}^0$ is found when the material is carbon steel and the column operate with ambient pressure.

$$C_{BM,i}^0 = C_p^0 (B_1 + B_2 F_M F_p) \quad (\text{E.15})$$

B_1 , B_2 and F_p are equal to the value given above and F_M are equal to one.

$$\begin{aligned} C_{BM,i}^0 &= 8.6335 \cdot 10^4 \\ C_{GR} &= 1.18 C_{BM,i} + 0.50 C_{BM,i}^0 \\ C_{GR} &= 2.3224 \cdot 10^5 \end{aligned} \quad (\text{E.16})$$

This gives the value in USGC basis in 2001.

E.5 Cost calculation when Sinnott is used

In the example the cost for the reboiler is shown. The cost equation used below is found in Sinnott

$$a=25000$$

$$b=340$$

$$n=0.9$$

S is the area in the reboiler and is calculated above and is equal to 17.4327

$$C_e = a + bS^n \quad (\text{E.17})$$

$$C_e = 2.7486 \cdot 10^4 \text{ US\$}$$

C_e gives the cost in carbon steel, to get the cost in stainless steel, C_e is multiplied with 1.3

$$C_e = 3.5732 \cdot 10^4 \text{ US\$}$$

To find the fixed capital cost the new C_e value is multiplied with 6.

$$C_e = 2.1439 \cdot 10^5 \text{ US\$ in USGC basis for 2006}$$