PARAFFIN SEPARATION VACUUM DISTILLATION COLUMN ANALYSIS IN LINEAR ALKYL BENZENE (LAB) CHEMICAL PLANT USING CHEMCAD SIMULATOR

Zaid A. Abdel-Rahman Omar S. Latif Lecturer Ass. Lecturer Chem. Eng. Dept.- University of Tikrit

ABSTRACT

Simulated column performance curves were constructed for existing paraffin separation vacuum distillation column in LAB plant (Arab Detergent Company/Baiji-Iraq). The variables considered in this study are the thermodynamic model option, top vacuum pressure, top and bottom temperatures, feed temperature, feed composition & reflux ratio. Also simulated columns profiles for the temperature, vapor & liquid flow rates composition were constructed. Four different thermodynamic model options (SRK, TSRK, PR, and ESSO) were used, affecting the results within 1-25% variation for the most cases.

The simulated results show that about 2% to 8 % of paraffin (C_{10} , C_{11} , C_{12} , & C_{13}) present at the bottom stream which may cause a problem in the LAB plant. The major variations were noticed for the top temperature & the paraffin weight fractions at bottom section with top vacuum pressure. The bottom temperature above 240 °C is not recommended because the total bottom flow rate decreases sharply, where as the weight fraction of paraffins decrease slightly. The study gives evidence about a successful simulation with CHEMCAD

KEYWORDS

Process simulation, CHEMCAD Simulator, multicomponent distillation, LAB, paraffin column, vacuum pressure

INTRODUCTION

Process simulation has become a core element of chemical engineering education, and the simulation of existing chemical plants (either an individual unit operation, or multiple connected units or an entire plant) is an important area of research and development (R & D). The currently available modern process simulation software are ASPENPLUS, CHEMCAD, HYSYS & PRO/II.^[1]

A typical process simulator has six main feature as illustrated in the left-hand column of Figure (1) and seven input steps to setting up a process simulation problem as shown on the right hand side of the same figure. The interaction between the elements and steps and the general flow of information is shown by the lines on the diagram.^[2]

CHEMCAD simulator has the most features of the typical process simulator mentioned. It is a very easy program to learn, and the best way to master it is by using it. The input procedure is simple and straightforward. It is designed to be intuitive for a chemical engineer familiar with the Windows environment. In most cases the user need not be concerned with the details of the internal calculation, this is done automatically by CHEMCAD. It provides about 50 unit operations (columns, reactors, heat exchanger, compressor, valve, pump, cyclone, etc.), models 20 thermodynamic (Peng-Robinson (PR), Soave-Redlich-Kwong (SRK), NTRL, UNIFAC, etc.), 1900 chemical components, and 6000 binary data from the DECHEMA data bank. The database can be quickly and easily extended to include customers' own components and own measured data. Incremental methods like Lyderson-Joback are available to estimate critical data, formation enthalpy and heat for capacity values. Methods the prediction of pseudo components from boiling analyses and regressions of measured data are also available. All data can be shown and plotted numerically and graphically.

The calculation method for distillation in CHEMCAD is done to a high standard in accordance with the matrix method. A quick convergence and short simulation time is therefore guaranteed. It offers a shortcut method and two basic types of rigorous methods, inside-out and simultaneous corrections. The inside-out method comes in two forms, TOWR and TOWER PLUS. TOWR represents standard column configurations while TOWER PLUS allows for complex

columns with heat exchangers, pump rounds and side strippers. The simultaneous corrections method, SCDS, is typically preferred for super fractionators and chemical columns requiring substantial robustness.^[3]

Figure (2) shows the paraffin separation vacuum distillation column diagram constructed using CHEMCAD. Where as Figure (3) gives a typical simulation results in a wordpad file.

To take advantage of the existing chemical plants in Iraq for engineering process analysis research & development, Linear Alkyl Benzene (LAB) plant (Arab Detergent Company/Beiji-Iraq) which contain cumulative field data of plant operation, was used as a case study using process simulation. The purpose of the present study is the analysis of one of the major equipment of the plant; paraffin separation vacuum distillation column, using CHEMCAD process simulator.

RESULTS AND DISCUSSIONS

Paraffin separation column in LAB plant has been simulated utilizing plant field data presented in Table (1), using CHEMCAD simulator.

Effect of top vacuum pressure

Figures (4) to (9) show the effect of top vacuum pressure on top temperature,

bottom total flow rate, & bottom components weight fractions (C_{10} paraffin, C_{11} -paraffin, C_{12} -paraffin, & C_{13} -paraffin), at different thermodynamic models. The figures show the following trends:

- The effect of the thermodynamic models used (SRK, TSRK, PR, and ESSO) on the general results is within 5-15 % variation.
- 2. For top pressure increase from 3 kPa to 11 kPa, the top temperature increases from about 70 °C to 110 °C, the total bottom flow rate increases from 6100 kg/hr to 6500 kg/hr, and variation of the the bottom components weight fractions vary as 0.0002-0.0007, C₁₀-paraffin C₁₁paraffin 0.002-0.007, C₁₂ -paraffin 0.007-0.023, & C₁₃-paraffin 0.015-0.05.
- **3.** The problem of the presence of 2-8% paraffin in bottom section of the column was noticed.

Effect of Bottom Temperature

Figures (10) to (15) show the effect of bottom temperature on top temperature, bottom total flow rate, & bottom components weight fractions (C_{10} -paraffin, C_{11} -paraffin, C_{12} -paraffin, & C_{13} -paraffin), at different thermodynamic models. The figures show the following trends:

- The effect of the thermodynamic models used (SRK, TSRK, PR, and ESSO) on the general results is within 5-15 % variation.
- For bottom temperature increase between 210 °C & 240 °C, the top temperature slightly increases from about 93 °C to 93.5 °C, where as the total bottom flow rate decreases from 7000 kg/hr to 6000 kg/hr.
- For bottom temperature increase from 240 °C to 260 °C, the top temperature increases from about 93.5 °C to 95 °C, where as the total bottom flow rate decreases from 6000 kg/hr to 2000 kg/hr.
- 4. For bottom temperature increase between 210 °C & 240 °C, the bottom components weight fractions of C_{10} paraffin, C_{11} -paraffin, C_{12} -paraffin, & C_{13} -paraffin decrease sharply (high rate of decrease). Where as they decrease slightly (low rate of decrease) for bottom temperature above 240 °C.

Effect of Feed Temperature

Figures (16) to (21) show the effect of bottom temperature on top temperature, bottom total flow rate, & bottom components weight fractions (C_{10} -

paraffin, C_{11} -paraffin, C_{12} -paraffin, & C_{13} -paraffin), at different thermodynamic models. The figures show the following trends:

- 1. The effect of the thermodynamic models used (SRK, TSRK, PR, and ESSO) on the general results is within 5-25 % variation.
- 2. For feed temperature between 160 °C & 200 °C, the variation of the top temperature is very small and can be regarded constant. Where as the total bottom flow rate increases slightly from 6250 kg/hr to 6350 kg/hr.
- 3. For feed temperature between 160 °C & 200 °C, the variation of the bottom component weight fractions vary as C_{10} -paraffin 0.006-0.002, C_{11} -paraffin 0.006-0.017, C_{12} -paraffin 0.017-0.013, & C_{13} -paraffin 0.03-0.05.
- Feed concentration presentation is very difficult in multicomponent systems. Table (2) show a comparison between two simulation runs to notice the effect of increasing light components feed weight fractions (C₁₃-paraffin) and decreasing heavy components feed weight fractions (C₁₀-LAB & C₁₁-LAB). The top temperature remains constant at 93.5 °C, where as the total bottom flow rate decreases (from about 7300 kg/hr to 6300 kg/hr).

Effect of Reflux Ratio

Figures (22) to (27) show the effect of reflux ratio on top temperature, and bottom components weight fractions (benzene, C_{10} -paraffin, C_{11} -paraffin), at different thermodynamic models. The figures show the following trends:

- The effect of the thermodynamic models used (SRK, TSRK, PR, and ESSO) on the general results is within 5-10 % variation.
- 2. For reflux ratio from 0.3 to 1.2, the variation of the top temperature is very small and can be regarded constant. Where as the the total bottom flow rate varies between about 6250 kg/hr to 6400 kg/hr, with the minimum value at reflux ratio of 0.5.
- 3. For reflux ratio from 0.3 to 1.2, the variation of the bottom component weight fractions vary as C_{10} -paraffin 0.001-0.005 (maximum value at R=0.5), C_{11} -paraffin 0.001-0.005(maximum value at R=0.5), C_{12} -paraffin 0.008-0.016(maximum value at R=0.5), & C_{13} -paraffin 0.03-0.06(minimum value at R=0.5).

Paraffin Column Profiles

Figures (28) to (33) show the temperature & composition profiles for paraffin column. The figures show that the effect of the thermodynamic models used (SRK, TSRK, PR, and ESSO) on the general results is within 5% variation, except the vapor component weight fractions, the variations are within 10-25% & higher.

Comparison of Results of Paraffin Column

The comparison of the simulated results with plant Paraffin column parameters is shown in Table (3). The deviation of simulated top temperature and the total top flow rate from the actual value is less than 11%, which can be attributed to the uncertainty or the difference of feed concentration. The high deviations of simulated bottom weight fractions of paraffin with the plant values can be noticed.

CONCLUSIONS

The following conclusions can be drawn from the present work:

 Four different thermodynamic models options (SRK, TSRK, PR, and ESSO) were used, affecting the results within 1-25% variation for the most cases.

- 2. The simulated results show that about 5% of paraffin (C_{10} , C_{11} , C_{12} , & C_{13}) present at the bottom stream which may cause a problem in the LAB plant.
- 3.The major variations were noticed for the top temperature & the paraffin weight fractions at bottom section with top vacuum pressure.
- 4.The simulated results show that bottom temperature above 240 °C is not recommended because the total bottom flow rate decreases sharply, where as the weight fractions of paraffins decrease slightly.
- 5.Simulation of the paraffin separation column in LAB production plant using CHEMCAD simulator, confirms the real plant operation data. The study gives evidence about an acceptable simulation with CHEMCAD.

REFERANCES

Peters,M.S. and Timmerhaus,
 K.D., West, R.E., Plant Design &
 Economics for Chemical
 Engineers,5thed., McGraw-Hill, New
 York, 2003.

2. Turton, R., Bailie, R.C, Whiting, W.B. and Shaeiwitz, J.A., Analysis, Synthesis, and Design of Chemical Processes, 2nd ed., Prentice Hall, New Jersey, 2003.

3. CHEMCAD User's Guide.

4. Arab Detergent Company; LAB production plant Field data, Beiji-Iraq.

Component	Feed	Top product	Bottom
			product
Temperature, ^o C	178	93	232
Pressure , Kpa	200	7	20
Flow rate Kg/hr	63707	56579	7128
HF	0	0	0
Benzene	0.00009	0.000101	0
N-Undecane (C_{10} —paraffin)	0.19874	0.21201	0.00024
N-Dodecane (C_{11} —paraffin)	0.3808	0.4185	0.00045
N-Tridecane (C_{12} —paraffin)	0.23169	0.24431	0.00029
N-Tetradecane (C ₁₃ —paraffin)	0.09974	0.11202	0.00013
N-Undecylbenzene (<i>C</i> ₁₀ — <i>LAB</i>)	0.01959	0.0085	0.09184
N-Dodecylbenzene (C ₁₁ —LAB)	0.02827	0.00098	0.3671
N-Tridecylbenzene (C_{12} —LAB)	0.02325	0.00231	0.32511
N-Tetradecylbenzene (<i>C</i> ₁₃ — <i>LAB</i>)	0.01416	0.00121	0.15311
heavy alkylate (HAB) [*]	0.002867	0	0.0611
Stripping section diameter D stripping	2800mm		
Rectification section diameter	5600mm		
Tray spacing	600mm		
Number of Tray holes	1942		
Hole diameter d_o	13mm		
trays above feed	15 trays, 16 stages(with condenser)		
trays below feed	21 trays, 22 stages(with reboiler)		
Q_c (condenser heat duty)	31212 MJ/hr		
Q_r (reboiler heat duty)	22363 MJ/hr		
Reflux Ratio(R)	0.5		

 Table (1) Typical Field Data specification of Paraffin Column (Arab Detergent Company).^[4]

* Molecular Weight: <u>366</u> Normal boiling: <u>397 °C</u> Specific gravity: <u>0.875</u>

Stream No.	1	2	3
Stream Name	FEED	top product	bottom produ
Temp C	178.0000*	93.2471	232.0000*
Pres kPa	200.0000*	7.0000	20.0000*
Enth MW	-27.777	-29.792	-1.1530
Vapor mole fraction	0.00000	0.00000	0.00000
Total kmol/h	390.3695	359.6601	30.7094
Total kg/h	63707.0058	56417.0000	7290.0152
Total std L m3/h	84.0950	75.5622	8.5327
Total std V m3/h	8749.60	8061.29	688.31
Component mass fractio	ns		
HydrogenFluoride	0.00000	0.00000	0.00000
Benzene	0.009000	0.010163	0.00000
N-Decane	0.198123	0.223669	0.000426
N-Undecane	0.363047	0.409359	0.004638
N-Dodecane	0.237213	0.265930	0.014976
N-Tridecane	0.083515	0.090862	0.026654
Decylbenzene	0.027710	0.000012	0.242062
N-Undecylbenzene	0.035899	0.00003	0.313691
N-Dodecylbenzene	0.022444	0.00001	0.196129
Tridecylbenzene	0.014782	0.00000	0.129172
heavy alkylate	0.008268	0.00000	0.072251
Stream No.	1	2	3
Stream No. Stream Name	1 FEED	2 top product	3 bottom produ
Stream No. Stream Name Temp C	1 FEED 178.0000*	2 top product 93.6413	3 bottom produ 232.0000*
Stream No. Stream Name Temp C Pres kPa	1 FEED 178.0000* 200.0000*	2 top product 93.6413 7.0000	3 bottom produ 232.0000* 20.0000*
Stream No. Stream Name Temp C Pres kPa Enth MW	1 FEED 178.0000* 200.0000* -28.050	2 top product 93.6413 7.0000 -30.308	3 bottom produ 232.0000* 20.0000* -0.99527
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction	1 FEED 178.0000* 200.0000* -28.050 0.00000	2 top product 93.6413 7.0000 -30.308 0.00000	3 bottom produ 232.0000* 20.0000* -0.99527 0.00000
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519	3 bottom produ 232.0000* -0.99527 0.00000 26.2006
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std V m3/h	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std V m3/h Component mass fractio	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std V m3/h Component mass fractio HydrogenFluoride	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std L m3/h Component mass fractio HydrogenFluoride Benzene	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.009000	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std L m3/h Component mass fractio HydrogenFluoride Benzene N-Decane	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.009000 0.198123	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std L m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Undecane	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.009000 0.198123 0.363047	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000409 0.004603
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std L m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Undecane N-Dodecane	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.099000 0.198123 0.363047 0.237213	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000 0.000409 0.004603 0.015204
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total kg/h Total std L m3/h Total std L m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Undecane N-Dodecane N-Tridecane	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.099000 0.198123 0.363047 0.237213 0.099212	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490 0.106526	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000 0.000409 0.004603 0.015204 0.032324
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total std L m3/h Total std L m3/h Total std V m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Decane N-Dodecane N-Tridecane Decylbenzene	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.099000 0.198123 0.363047 0.237213 0.099212 0.019862	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490 0.106526 0.000010	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000 0.000409 0.004603 0.015204 0.032324 0.201406
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total std L m3/h Total std L m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Decane N-Dodecane N-Tridecane Decylbenzene N-Undecylbenzene	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.198123 0.363047 0.237213 0.099212 0.019862 0.028050	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490 0.106526 0.000010 0.000003	3 bottom produ 232.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000 0.000409 0.004603 0.015204 0.032324 0.201406 0.284542
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total std L m3/h Total std L m3/h Total std V m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Decane N-Dodecane N-Tridecane Decylbenzene N-Undecylbenzene N-Dodecylbenzene	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.099000 0.198123 0.363047 0.237213 0.099212 0.019862 0.028050 0.022444	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490 0.106526 0.000010 0.000003 0.000001	3 bottom produ 232.0000* 20.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000409 0.004603 0.015204 0.032324 0.201406 0.284542 0.227683
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total std L m3/h Total std L m3/h Total std V m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Decane N-Dodecane N-Dodecane N-Tridecane Decylbenzene N-Undecylbenzene Tridecylbenzene	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.198123 0.363047 0.237213 0.099212 0.019862 0.028050 0.022444 0.014782	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490 0.106526 0.000010 0.000003 0.000001 0.000001	3 bottom produ 232.0000* 20.0000* -0.99527 0.00000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000 0.000409 0.004603 0.015204 0.032324 0.201406 0.284542 0.227683 0.149954
Stream No. Stream Name Temp C Pres kPa Enth MW Vapor mole fraction Total kmol/h Total std L m3/h Total std L m3/h Total std V m3/h Component mass fractio HydrogenFluoride Benzene N-Decane N-Decane N-Dodecane N-Undecane N-Tridecane Decylbenzene N-Undecylbenzene N-Dodecylbenzene Tridecylbenzene heavy alkylate	1 FEED 178.0000* 200.0000* -28.050 0.00000 391.3524 63707.0058 84.2496 8771.64 ns 0.000000 0.198123 0.363047 0.237213 0.099212 0.019862 0.028050 0.022444 0.014782 0.008268	2 top product 93.6413 7.0000 -30.308 0.00000 365.1519 57427.3101 76.8935 8184.39 0.000000 0.009984 0.219743 0.402243 0.261490 0.106526 0.000010 0.000003 0.000001 0.000000	3 bottom produ 232.0000* 20.0000 20.0000 26.2006 6279.6967 7.3561 587.25 0.000000 0.000000 0.000000 0.000409 0.004603 0.015204 0.032324 0.201406 0.284542 0.227683 0.149954 0.083875

Table (2) Effect of Feed Concentration: a Comparison BetweenTwo CHEMCAD Simulation Runs of Paraffin Column.

Table(3) Comparison between simulated and plant data of Paraffin Column at; $T_{e} = -178 \ {}^{\circ}C \ P_{e} = -7 \ K_{P2} \ T_{e} = -232 \ {}^{\circ}C \ \& \ B = 0.5$

$\Gamma_{\text{feed}} = 1/8 \text{ C}, P_{\text{top}} = 7 \text{ Kpa}, \Gamma_{\text{bottom}} = 252 \text{ C} \approx R = 0.5$					
Variable	Plant	Simulated	%Deviation		
Top temperature (_o C)	93	93.6	- 0.645%		
Total Top Flowrate (kg/hr)	7128	6350	- 10.91 %		
C10-paraffin wt fraction in bottom	0.00024	0.0004	+ 66.67%		
C11-paraffin wt fraction in bottom	0.00045	0.005	+ 1011%		
C12-paraffin wt fraction in bottom	0.00029	0.015	+ 5072%		
C13-paraffin wt fraction in bottom	0.00013	0.032	+24515%		



Figure (1) The Structure of a Typical Process Simulator.^[2]



Figure (2) Paraffin separation distillation column (SCDS) flowsheet.

		51		
ounerfriew + 10	· Western	- 8 /		1
		1		
	See side	7		a
Job Mame: parrarrin c	DIUMI			
Stream No.	1	2	3	
Stream Name	FEED	top product	bottom produ	
Temp C	178.0000*	109.5906	232.0000*	
Fres kPa	200.0000*	7.0000	20.0000+	
Enth MW	-28,455	-30.086	-1.0015	
Vapor mole fraction	0.00000	0.00000	0.00000	
Total kmol/h	387.5388	361.1365	26.4023	
Total kg/h	63707.0200	57377.6913	6329,3216	
Total std L m3/h	84.3593	76.9460	7.4134	
Total std V m3/h	8686.16	8094.39	591.77	
Component mass fracti	ons			
RydrogenFluoride	0.000000	0.000000.	0.000000	
Senzene	0.000091	0.000101	0.000000	
N-Decane	0.199904	0.221905	0.000461	
-Undecane	0.366311	0.406182	0.004862	
-Dodecane	0.239345	0.264039	0.015493	
N-Tridecane	0.100104	0.107753	0.030757	
Decylbenzene	0.020040	0.000014	0.201583	
N-Undecylbenzene	0.028302	0.000004	0.284839	
S-Dodecylbenzene	0.022646	0.000001	0.227926	
Tridecylbenzene	0.014914	0.000000	0.150115	
heavy alkylate	0.008342	0.000000	0.083965	
r Help, press Fit				I I I I I I I I I I I I I I I I I I I
Start CHENCAD 5.2.0	Document2 - Mo	📖 💽 parraffin_	colum	📓 = 🛒 🖲 🗐 🚺 11:04,

Figure (3) Typical simulation results as a wordpad file.



Figure (4) Effect of top vacuum pressure on top temperature, T_{bottom} =232 °C, T $_{Feed}$ =178 °C ΔP =13 Kpa, R=0.5



Figure (5) Effect of top vacuum pressure on total bottom flowrate, T $_{bottom}$ =232 °C, T $_{Feed}$ =178 °C ΔP =13 Kpa, R=0.5



Figure (6) Effect of top vacuum pressure on wt fraction of C₁₀-Paraffin, T _{bottom} =232 °C, T _{Feed} =178 °C Δ P =13 Kpa, R=0.5



Figure (7) Effect of top vacuum pressure on wt fraction of C₁₁-Paraffin, T $_{bottom}$ =232 °C, T $_{Feed}$ =178 °C ΔP =13 Kpa, R=0.5



Figure (8) Effect of top vacuum pressure on wt fraction of C₁₂-Paraffin, T $_{bottom}$ =232 °C, T $_{Feed}$ =178 °C ΔP =13 Kpa, R=0.5



Figure (9) Effect of top vacuum pressure on wt fraction of C₁₃-Paraffin, T $_{bottom}$ =232 °C, T $_{Feed}$ =178 °C ΔP =13 Kpa, R=0.5



Figure (10) Effect of Bottom Temperature on Top Temperature, T $_{Feed}$ =178 °C P $_{Top}$ =7, Kpa ΔP =13 Kpa, R=0.5



Figure (11) Effect of Bottom Temperature on Total Top vapor Flowrate, T $_{Feed}$ =178 °C P $_{Top}$ =7, Kpa, ΔP =13 Kpa, R=0.5



Figure (12) Effect of Bottom Temperature on wt. fraction of C_{10} -Paraffin, T _{Feed} =178 °C P_{Top} =7, Kpa, ΔP =13 Kpa, R=0.5



Figure (13) Effect of Bottom Temperature on wt. fraction of C_{11} -Paraffin, T _{Feed} =178 °C P_{Top} =7, Kpa, ΔP =13 Kpa, R=0.5



Figure (14) Effect of Bottom Temperature on wt. fraction of C₁₂-Paraffin, T $_{Feed}$ =178 °C P $_{Top}$ =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (15) Effect of Bottom Temperature on wt. fraction of C₁₃-Paraffin, T _{Feed} =178 °C P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5

15





Figure (18) Effect of Feed Temperature on *C10-paraffin wt* fraction, $T_{Bottom} = 232$ °C $P_{Top} = 7$ Kpa, $\Delta P = 13$ Kpa, R=0.5



Figure (19) Effect of Feed Temperature on C11-paraffin wt fraction, $T_{Bottom} = 232$ °C $P_{Top} = 7$ Kpa, $\Delta P = 13$ Kpa, R=0.5



Figure (20) Effect of Feed Temperature on C12-paraffin wt fraction, T_{Bottom} =232 °C P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (21) Effect of Feed Temperature on *C13-paraffin wt* fraction, T_{Bottom} =232 °C P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5





Figure (22) Effect of Reflux Ratio on top temperature , T_{Feed} =178 °C, Figure (25) Effect of Reflux Ratio on C11-Paraffin wt. fraction, $T_{Bottom} = 232 \text{ }^{\circ}\text{C}, P_{Top} = 7 \text{ Kpa}, \Delta P = 13 \text{ Kpa}$



Figure (23) Effect of Reflux Ratio on total bottom flowrate , T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa



Figure (24) Effect of Reflux Ratio on C10-Paraffin wt. fraction, T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa

 $T_{\text{Feed}} = 178 \text{ }^{\circ}\text{C}, T_{\text{Bottom}} = 232 \text{ }^{\circ}\text{C}, P_{\text{Top}} = 7 \text{ Kpa}, \Delta P = 13 \text{ Kpa}$



Figure (26) Effect of Reflux Ratio on C12-Paraffin wt. fraction $T_{\text{Feed}} = 178 \text{ }^{\circ}\text{C}, T_{\text{Bottom}} = 232 \text{ }^{\circ}\text{C}, P_{\text{Top}} = 7 \text{ Kpa}, \Delta P = 13 \text{ Kpa}$



Figure (27) Effect of Reflux Ratio on C13-Paraffin wt. fraction T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa



Figure (28) Paraffin Tower Temperature Profile T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (29) Paraffin Column Total Vapor Flowrate Tower Profile, T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (30) Tray Vapor Profile of C_{10} -Paraffin wt fraction T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (31) Tray Vapor Profile of C₁₁-Paraffin wt fraction T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (32) Tray Vapor Profile of C₁₂-Paraffin wt fraction T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5



Figure (33) Tray Vapor Profile of C₁₃-Paraffin wt fraction T_{Feed} =178 °C, T_{Bottom} =232 °C, P_{Top} =7 Kpa, ΔP =13 Kpa, R=0.5

تحليل عمود التقطير الفراغي لفصل البارافين لمصنع انتاج الالكيل بنزين المستقيم باستعمال برنامج المحاكاة الجاهز CHEMCAD

> د.زيد عدنان عبد الرحمن عمر سعيد لطيف مدرس قسم الهندسة الكيمياوية-كلية الهندسة-جامعة تكريت

الخلاصة

استعمل البرنامج الجاهز CHEMCAD للتحليل الهندسي لعمود فصل البارافين لمصنع انتاج الالكيل بنزين المستقيم للشركة العربية في بيجي. رسمت منحنيات اداء عمود الانتزاع للمتغيرات : نوع موديل ديناميك الحرارة وضغط اعلى العمود ودرجة حرارة وتركيز المواد الداخلة ونسبة الاسترجاع. ورسمت ايضا المخططات الداخلية للعمود لتغير درجة الحرارة ومعدل تدفق الاطوار والتركيز. استخدمت اربعة موديلات لديناميك الحرارة ايضا المخططات الداخلية للعمود لتغير درجة الحرارة ومعدل تدفق الاطوار والتركيز. استخدمت اربعة موديلات لديناميك الحرارة وسنت الداخلية العمود العمود ودرجة حرارة ومعدل تدفق الاطوار والتركيز. استخدمت اربعة موديلات لديناميك الحرارة ومعدل تدفق الاطوار والتركيز. استخدمت اربعة موديلات لديناميك الحرارة وهي (SRK, TSRK, PR, & ESSO) وكان تاثيرها على النتائج بحدود 1–25% لمعظم الحالات. تبين من نتائج المحاكاة ان هنالك نسبة حوالي 2% من البارافين في المجرى السفلي والذي قد يسبب مشكلة في المصنع. وتم ملاحظة اكبر تغير في درجة حرارة اعلى العمود والي 2% من البارافين في المحرى السفلي والذي قد الحالات. تبين من نتائج المحاكاة ان هنالك نسبة حوالي 2% الى 8% من البارافين في المجرى السفلي والذي قد الحالات. تبين من نتائج المحاكاة ان هنالك نسبة حوالي 2% الى 8% من البارافين في المجرى السفلي والذي قد الحالات. تبين من نتائج المحاكاة ان هنالك نسبة حوالي 2% الى 8% من البارافين في المجرى السفلي والذي قد الحالات. تبين من نتائج المحاكاة ان هنالك نسبة حوالي 2% الى 8% من البارافين في المجرى السفلي والذي قد الحالات. تبين من نتائج المحاكاة ان هنالك نسبة حوالي 2% الى 8% من البارافين في المجرى السفلي والذي قد يسبب مشكلة في المصنع. وتم ملاحظة اكبر تغير في درجة حرارة اعلى العمود ونسبة البارافينات اسفل العمود مع الضاراخي في المود مع مال الفراغي في المود من من 20 20 عدل المود مع الصنون مالمود مع الضراغي في المحرى المود. ان درجة حرارة اسفل العمود اعلى من 20 200 عبر المود مع مالادفق الضعود يقل بحدة بينما النسبة الوزنية للبارافين تقل بصورة طفيفة.

واخيرا تبين من خلال الدراسة الحالية سهولة استخدام البرنامج الجاهز CHEMCAD بنجاح في المحاكاة النظرية لعمود فصل البارافين المستخدم.

الكلمات الدالة

المحاكاة، برنامج CHEMCAD ، تقطير متعدد الاطوار ، الالكيل بنزين المستقيم، عمود البارافين ، الضغط الفراغي.