PROCESS SIMULATION ANALYSIS OF HF STRIPPING COLUMN OF LINEAR ALKYL BENZENE (LAB) PLANT

Dr. Zaid A. Abdel-Rahman
Lecturer

Omar S. Latif
Assistant Lecturer

Chemical Eng. Dept.-University of Tikrit

ABSTRACT

CHEMCAD process simulator was used for the analysis of existing HF stripping column in LAB plant(Arab Detergent Company/Baji-Iraq).

Simulated column performance curves were constructed. The variables considered in this study are the thermodynamic model option, top and bottom temperatures, feed temperature, & feed composition. Also simulated columns profiles for the temperature, vapor and liquid flow rates and compositions, were constructed, using different thermodynamic models options. Four different thermodynamic models 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 5% of paraffin (C10 & C11) presents at the top stream which may cause a problem in the LAB production plant. The major variations were noticed for the total top vapor flow rate with bottom temperature and with feed composition. The column profiles maintain fairly constants from tray 5 (immediately below feed) through tray 18 (immediately above reboiler). These trays can be removed without severely affected the column profile. Simulation of the HF stripping column in LAB production plant using CHEMCAD simulator, confirms the real plant operation data. The study gives evidence about a successful simulation with CHEMCAD.

KEYWORDS

Process simulation, CHEMCAD Simulator, multicomponents distillation, LAB, HF stripper.

ABBREVIATIONS

ESSO	Empirical K-value model uses the Maxwell-Bonnell vapor pressure equation to calculate K-values, used for heavy hydrocarbon materials effectively at pressures below 7 bar. This model can be used to model vacuum towers.
NRTL	Non-Random Two-Liquid Equation based on activity coefficient Equilibrium thermodynamic model recommended for Polar (Highly Non-Ideal Solutions)
PR	Peng-Robinson thermodynamic model to calculate K-values, based on equation of state recommended for most hydrocarbon systems
SRK	Soave-Redlich-Kwong thermodynamic model to calculate K-values , based on equation of state recommended for most hydrocarbon systems
TSRK	Extended Soave-Redlich-Kwong thermodynamic model to calculate K-values based on equation of state recommended for Methanol system; particularly with light gases.
UNIFAC	UNIQUAC Functional-Group Activity Coefficient Equilibrium thermodynamic model recommended for Polar (Highly Non-Ideal Solutions) , used where data is absent.
UNIQUAC	Activity Coefficient Equilibrium thermodynamic model recommended for Polar (Highly Non-Ideal Solutions)

INTRODUCTION

Process simulation is a computer representation of an individual unit operation, or multiple connected units or an entire plant. It is applicable in different fields of the process engineering; analysis of existing processes (rating), synthesis of new processes (design), and operator training (process dynamic startup & shutdown). The authors of many chemical engineering textbooks added a chapter dealing with process simulation & process simulation softwares (Process Simulators).[1-6] Currently available modern process Simulators are shown in Table (1). Major sections of typical process simulator are:

1. Unit operation (block) model library.
2. Physical properties & thermodynamic model selection.
3. General flowsheeting , steady state material and energy balance , recycle processes , and dynamic processes .

The process simulation softwares (Process Simulators) consist of standard chemical engineering relationships and models. These are material balance, energy balance, kinetics relationships, equilibrium relationships and dynamic & control relationships. Typically, steady state simulation involves the solution of algebraic equations, while dynamic simulation involves the solution of ordinary differential equations. The disadvantage of commercial simulators are that they do not provide the simulator's source code; the user must rely on closed black box for the unit operation process.

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 existing LAB plant (Arab Detergent Company/Beiji-Iraq) especially one of the major equipment; HF-stripper column, using the process simulation software (CHEMCAD).

CHEMCAD PROCESS SIMULATOR

CHEMCAD[7] is a process simulation programmed for quick calculation and simulation of chemical processes normally occurring in chemical, petrochemical, pharmaceutical and environmental technology. Being an alternative to long-lasting manually done calculations CHEMCAD provides time saving calculations and simulations of small batch processes as well as large scale continuous chemical plants. The data base included contains more than 1800 components, with more than 6000 binary data from the DECHEMA data bank. Other sources for vapor-liquid equilibrium, in combination with mixing rules and more than 20 thermodynamic models like Peng-Robinson (PR) , Soave-Redlich-Kwong (SRK), NRTL, UNIQUAC, UNIFAC, Henry, etc., provide the ideal means to easily model processes. The database can be quickly and easily extended to include customers' own components and own measured data. 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. In most cases the user need not be concerned with the details of the internal calculation, this is done automatically by CHEMCAD. The following six basic steps are used to run a flowsheet simulation in CHEMCAD:

1. Creating a flowsheet.
2. Selecting components & engineering units.

3. Selecting thermodynamics options.
4. Defining the feed streams.
5. Input equipment parameters.
6. Running the simulation & Reviewing the results.

Figure (1) shows the HF Stripper distillation column diagram constructed using CHEMCAD. Where as Figure (2) gives a typical simulation results in a wordpad file.

RESULTS AND DISCUSSIONS

HF stripping column in LAB production plant has been simulated utilizing plant field data presented in Table(2), using CHEMCAD simulator.

1- Effect of Bottom Temperature

Figures (3) to (7) show the effect of bottom temperature on top temperature, top total vapor flow rate, & top components weight fractions (benzene, C10 paraffin, C11 paraffin), at different thermodynamic models. The figures show that the effect of the thermodynamic models used (SRK, TSRK, PR, and ESSO) on the general results is within about 5% variation, except the top components weight fractions of C10 paraffin & C11 paraffin, the variation is within 25% . SRK & TSRK thermodynamic options give the average values.

Top temperature can be replacing bottom temperature of figures (2) to (5) giving same behavior. The bottom temperature increase of 30 °C (from 170 °C to 200 °C) cause, the top temperature increase of 3 °C (from 139 °C to 142 °C).

The major variation of the total top vapor flow rate has been noticed, from about 7000 kg/hr to 19000 kg/hr with the 30 °C difference of bottom temperature, figure (4. Where as the variation of the top components weight

fractions are small (0.9-0.925 for benzene, figure (5) , and approximately constant at about 0.025 for both C10 paraffin & C11 paraffin, figure (6) & (7)).

The results obtained from simulation using CHEMCAD. show that about 5% of paraffin (C10 & C11), Figures (6) & (7), presents at top stream which may cause a problem in the LAB production plant.

2- Effect of Feed Temperature

Figures (8) to (12) show the effect of feed temperature on top temperature, top total vapor flow rate, & top components weight fractions (benzene, C10 paraffin, C11 paraffin), at different thermodynamic models. 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 top components weight fractions of C10 paraffin & C11 paraffin, the variation is within 25% . SRK & TSRK thermodynamic options give the average values.

The feed temperature increase of 20 °C (from 90 °C to 110 °C) cause, the top temperature increase of 3 °C (from 138 °C to 141 °C). The variation of the total top vapor flow rate, the top components weight fractions are small. The variations are within 1%.

3- Effect of Feed Concentration

Feed concentration presentation is very difficult in multicomponents systems. Table (3) show a comparison between two simulation runs to notice the effect of decreasing light components feed weight fractions (benzene) and increasing heavy components feed weight fractions (C10 paraffin & C11 paraffin). The top temperature decreases (from 139.7 °C to 135.6 °C), where as the top total vapor flow rate decreases (from about 10000 kg/hr to 3500 kg/hr).

4- HF Stripper Column Profiles

Figures (13) to (18) show the temperature & composition profiles for HF-stripper 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 top total vapor flowrate profile, figure (15), the variation is within 15%. In all cases the profiles remain fairly constant from tray 5 (immediately below feed) through tray 18 (immediately above reboiler). In fact, these trays can be removed without severely affected the column performance.

CONCLUSIONS

The following conclusions can be drawn from the present work:

1. 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 (C10 & C11) presents at the top stream which may cause a problem in the LAB production plant.
3. The major variations were noticed for the total top vapor flow rate with bottom temperature and with feed composition.
4. The column profiles maintain fairly constants from tray 5 (immediately below feed) through tray 18 (immediately above reboiler). These trays can be removed without severely affected the column profile.
5. Simulation of the HF stripping column in LAB production plant using CHEMCAD simulator, confirms the real plant operation data. The study gives evidence about a successful simulation with CHEMCAD.

REFERANCES

1. 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. Biegler, L. T., Grossmann, I. E., and Westerberg, Systematic Methods of Chemical Process Design, Prentice Hall, New Jersey, 1997.
4. Sinnot, R. K., Coulson ,J. M., Richardson ,J. F. , Chemical Engineering : An Introduction to Design , Vol.(6) , 2nd. Ed. , Butterworth Heinemann, Oxford, 1993.
5. Himmelblau ,D.M. ,Riggs , J.B. , Basic Principles and Calculation in Chemical Engineering ,7th ed. , Prentice Hall, New Jersey, 2004.
6. Seider, W.D., Seader, J.D., Lewin, D.R., Product and Process Design Principles, Synthesis, Analysis and Evaluation, 2nd, ed., John Wiley and Sons, Inc., New York, 2004.
7. CHEMCAD User's Guide.
8. Arab Detergent Company; LAB production plant Field data, Beiji-Iraq.

Table (1) Current Modern Process Simulation Softwares (Process Simulator)[1]

Process Simulator	Source
ASPENPLUS	Aspen Technology Corp., Cambridge , MA
CHEMCAD	Chemstations , Houston , TX
HYSYS	Hyprotech , Calgary , Alberta
PRO/II	Simulation Sciences , Fullerton , CA

Table (2) Typical Field Data specification of HF- stripper (Arab Detergent Company).[8]

Component	Feed	Top product	Bottom product
Temperature,oC	102	135	175
Pressure , Kpa	420	340	360
Flow rate Kg/hr	87585	11670	75915
HF	0.00333406131	0.025	0
Benzene	0.2893438698	0.975	0.183838
N-Undecane (C_{10}—paraffin)	0.138489129	?	0.159799
N-Dodecane (C_{11}—paraffin)	0.2630186368	?	0.303491
N-Tridecane (C_{12}—paraffin)	0.1657250937	?	0.191226
N-Tetradecane (C_{13}—paraffin)	0.07050733071	?	0.081357
N-Undecylbenzene (C_{10}—LAB)	0.01479858229		0.017076
N-Dodecylbenzene (C_{11}—LAB)	0.02089618633		0.024112
N-Tridecylbenzene (C_{12}—LAB)	0.01671867888		0.019291
N-Tetradecylbenzene (C_{13}—LAB)	0.01101028361		0.012705
heavy alkylate (HAB)*	0.00615814763		0.007106
Column Diameter(D)	2000 mm		
No of trays	20 sieves tray		
No of stages	21 stages (with reboiler)		
Trays pacing	600 mm		
No. of holes	1260		
Hole diam d_o	13 mm		
Reboiler heat duty Q_r	21356 MJ/hr		

* Molecular Weight: *366*
Normal boiling: *397 °C*
Specific gravity: *0.875*

Table (3) Effect of Feed Concentration; a Comparison Between Two CHEMCAD Runs of HF-Stripper Column.

Stream No.	1	2	3
Stream Name	Feed	top product	bottom produ
Temp C	102.0000*	139.7164	175.0000
Pres kPa	420.0000*	340.0000	360.0000
Enth MJ/h	-95817.	6110.5	-83492.
Vapor mole fraction	0.00000	1.0000	0.00000
Total kmol/h	715.2811	135.3644	579.9168
Total kg/h	87585.0083	10013.9889	77571.0141
Total std L m3/h	110.9508	11.4246	99.5263
Total std V m3/h	16032.06	3034.01	12998.05
Component mass fractions			
HydrogenFluoride	0.003334	0.029161	0.000000
Benzene	0.289344	0.911906	0.208975
N-Decane	0.138489	0.024208	0.153242
N-Undecane	0.263019	0.024452	0.293816
N-Dodecane	0.165725	0.008291	0.186049
N-Tridecane	0.070507	0.001882	0.079367
Decylbenzene	0.014799	0.000044	0.016703
N-Undecylbenzene	0.020896	0.000032	0.023590
N-Dodecylbenzene	0.016719	0.000016	0.018875
Tridecylbenzene	0.011010	0.000006	0.012431
heavy alkylate	0.006158	0.000001	0.006953

Stream No.	1	2	3
Stream Name	Feed	top product	bottom produ
Temp C	102.0000*	135.6126	175.0000
Pres kPa	420.0000*	340.0000	360.0000
Enth MJ/h	-1.0892E+005	-798.04	-91192.
Vapor mole fraction	0.00000	1.0000	0.00000
Total kmol/h	686.1460	54.0737	632.0723
Total kg/h	87586.0147	3495.4158	84090.5894
Total std L m3/h	112.0347	3.9784	108.0563
Total std V m3/h	15379.04	1211.99	14167.05
Component mass fractions			
HydrogenFluoride	0.003334	0.083542	0.000000
Benzene	0.234161	0.845922	0.208732
N-Decane	0.171260	0.031883	0.177054
N-Undecane	0.285434	0.027978	0.296135
N-Dodecane	0.165723	0.008637	0.172253
N-Tridecane	0.070507	0.001938	0.073357
Decylbenzene	0.014798	0.000045	0.015412
N-Undecylbenzene	0.020896	0.000032	0.021763
N-Dodecylbenzene	0.016718	0.000016	0.017413
Tridecylbenzene	0.011010	0.000006	0.011468
heavy alkylate	0.006158	0.000001	0.006414

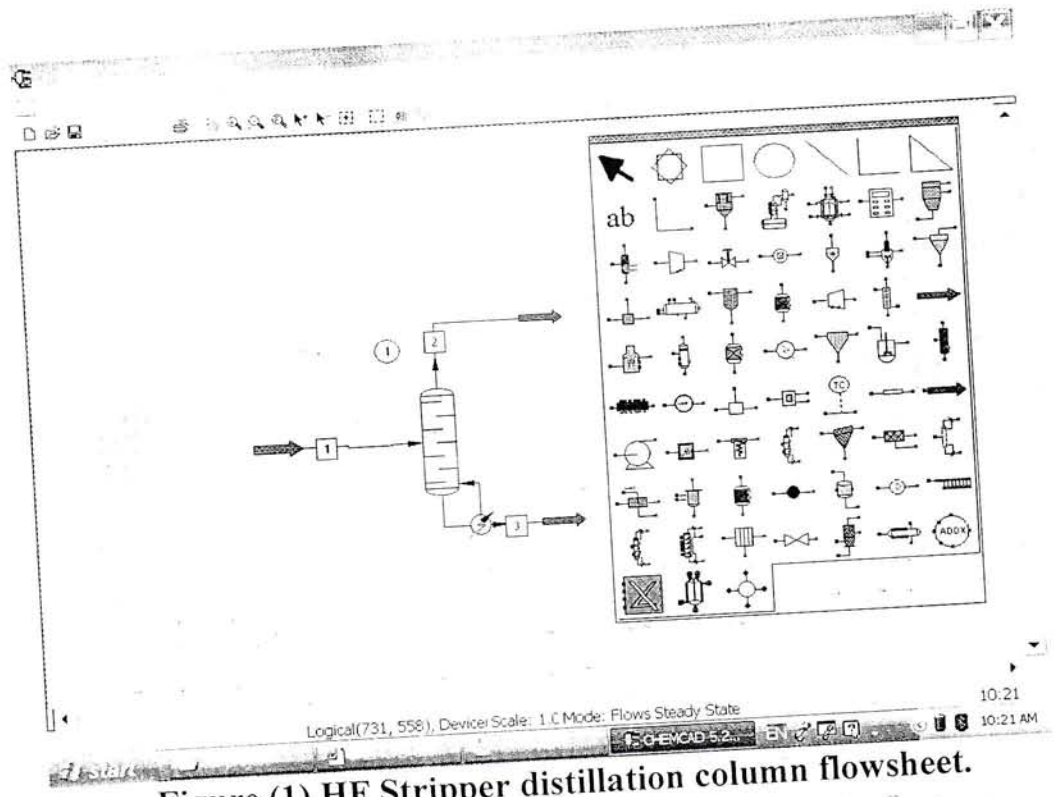

Figure (1) HF Stripper distillation column flowsheet.

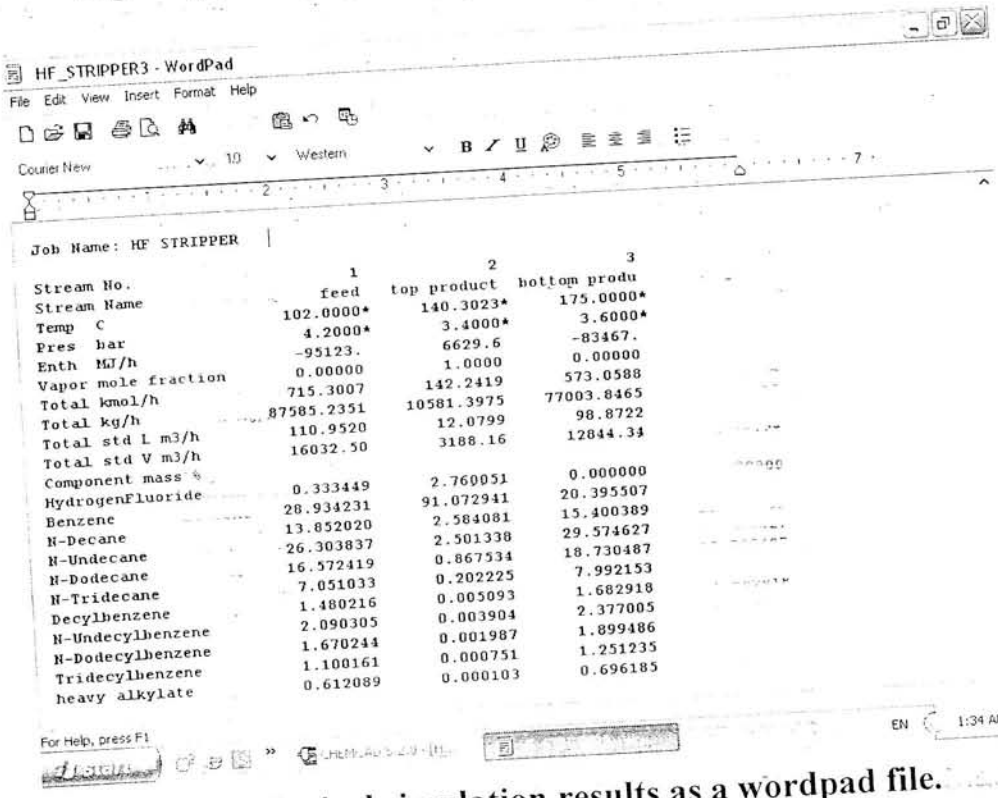

Figure (2) Typical simulation results as a wordpad file.

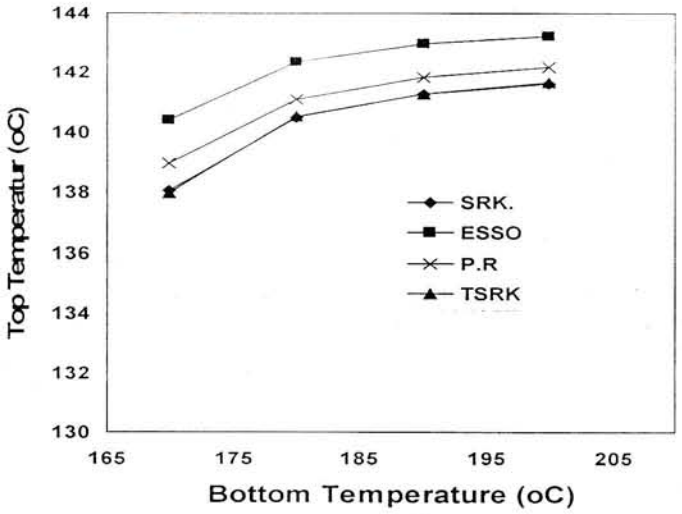

Figure (3) Effect of Bottom Temperature on Top Temperature

P_{Top}=340 Kpa, & T_{Feed} = 102 °C

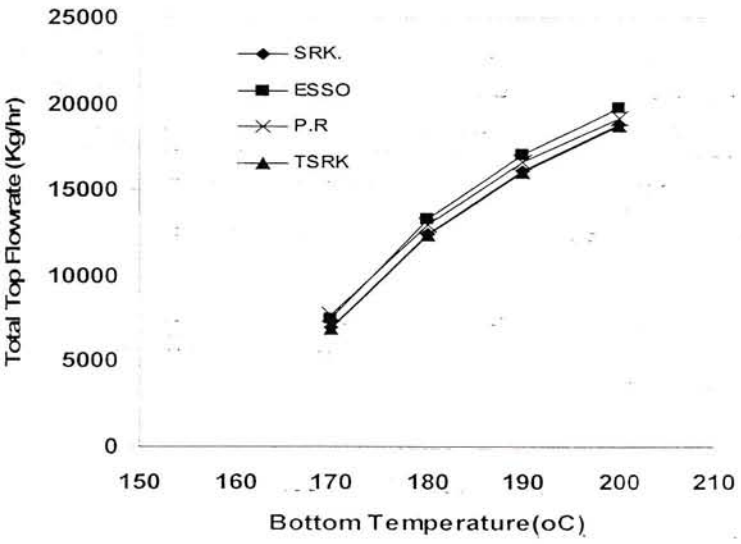

Figure (4) Effect of Bottom Temperature on Total Top vapor Flowrate
P_{Top}=340 Kpa, & T_{Feed} = 102 °C

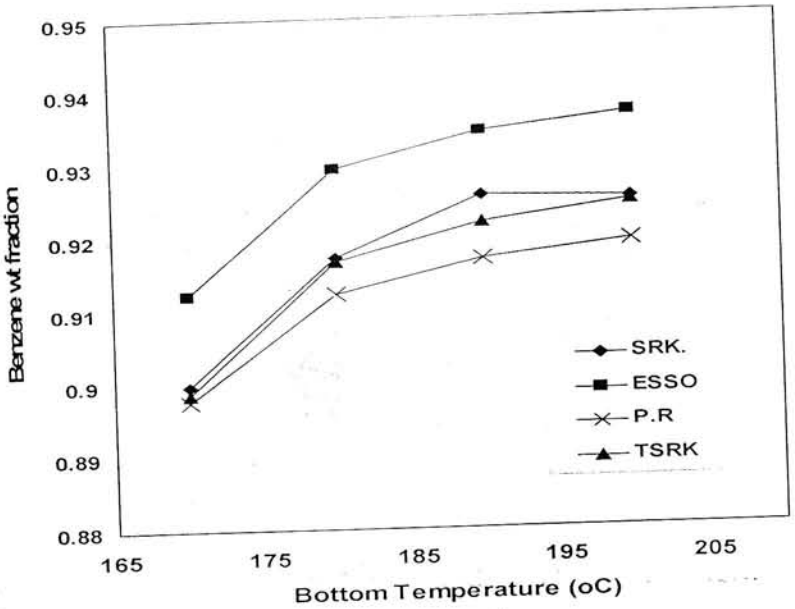

Figure (5) Effect of Bottom Temperature on Benzene wt. fraction
P_{Top}=340 Kpa, & T_{Feed}= 102 °C

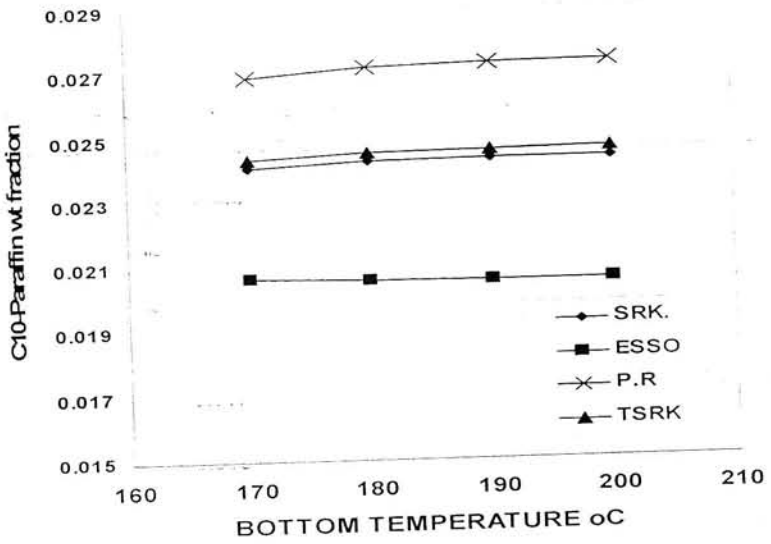

Figure (6) Effect of Bottom Temperature on wt. fraction of C_{10}-Paraffin
P_{Top}=340 Kpa, & T_{Feed}= 102 °C

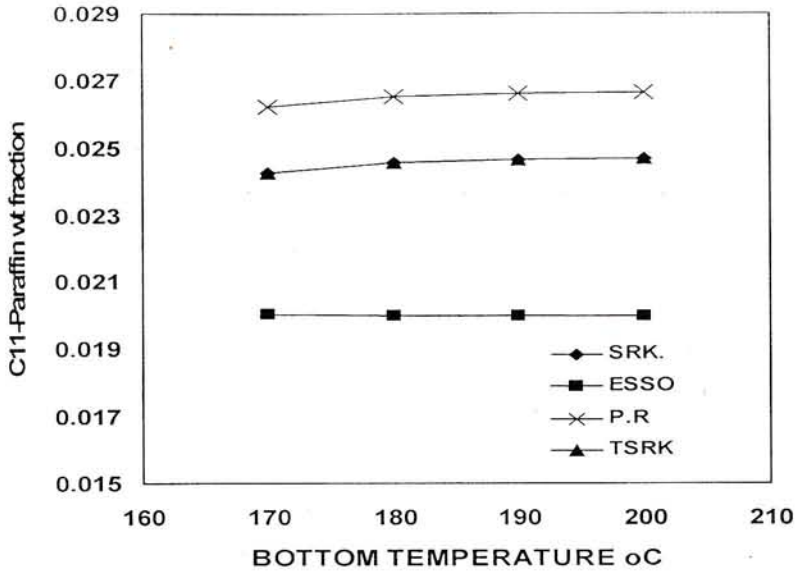

Figure (7) Effect of Bottom Temperature on wt. fraction of C_{11}-Paraffi
P_{Top}=340 Kpa, & T_{Feed} = 102 °C

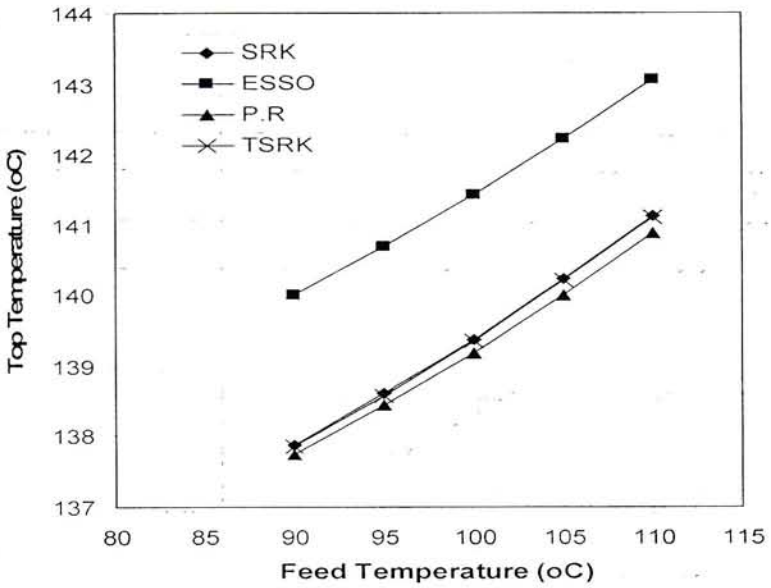

Figure (8) Effect of Feed Temperature on Top Temperature
P_{Top}=340 Kpa, & T_{Bottom} = 175 °C

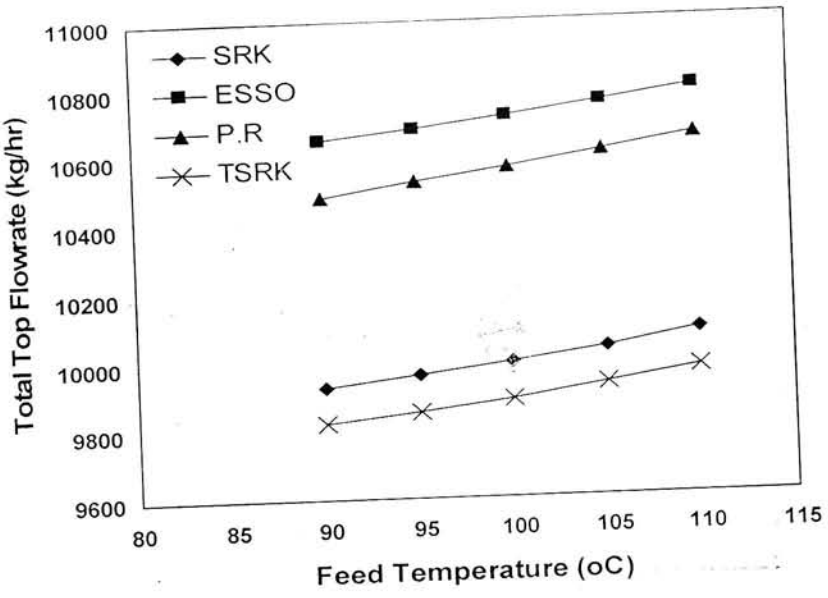

Figure (9) Effect of Feed Temperature on Total Top Flowrate
P_{Top}=340 Kpa, & T_{Bottom} = 175 °C

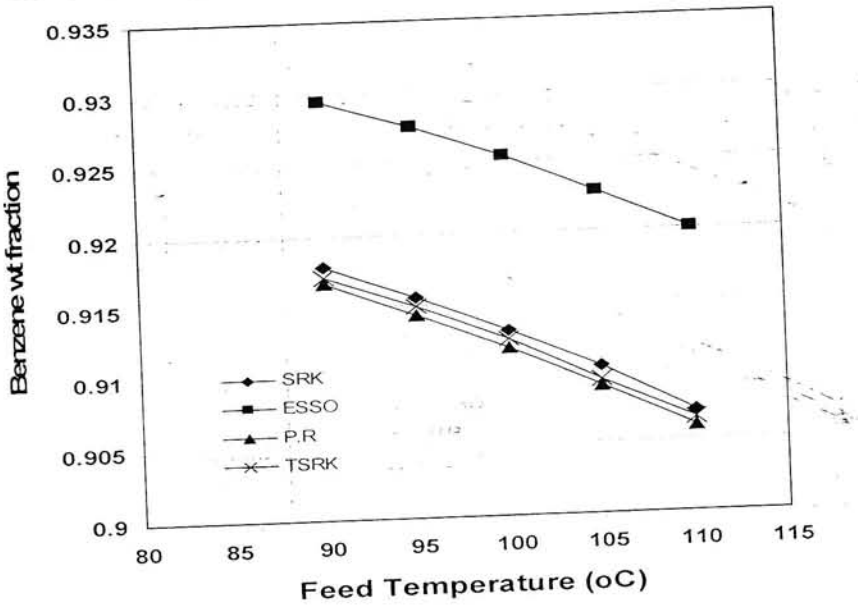

Figure (10) Effect of Feed Temperature on *Benzene wt fraction*
P_{Top}=340 Kpa, & T_{Bottom} = 175 °C

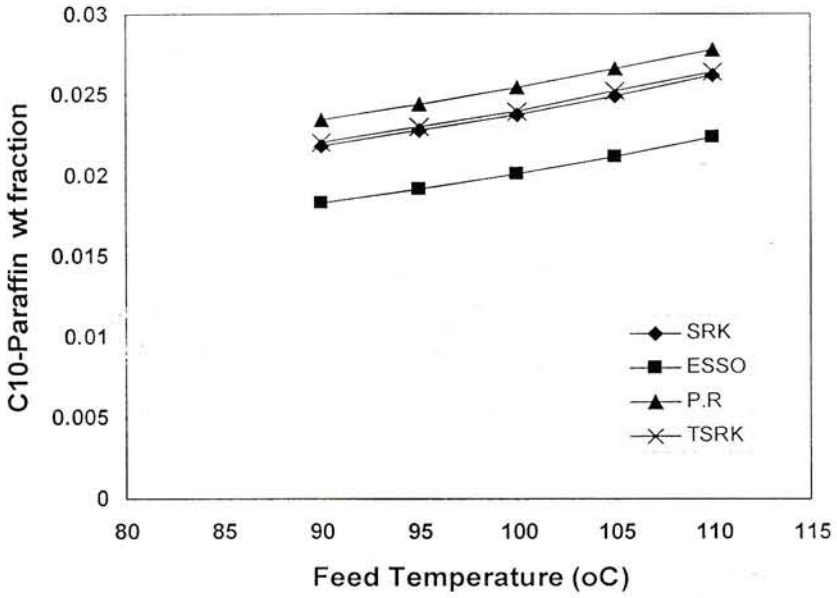

Figure (11) Effect of Feed Temperature on *C10-paraffin wt fraction*
P_{Top}=340 Kpa, & T_{Bottom} = 175 °C

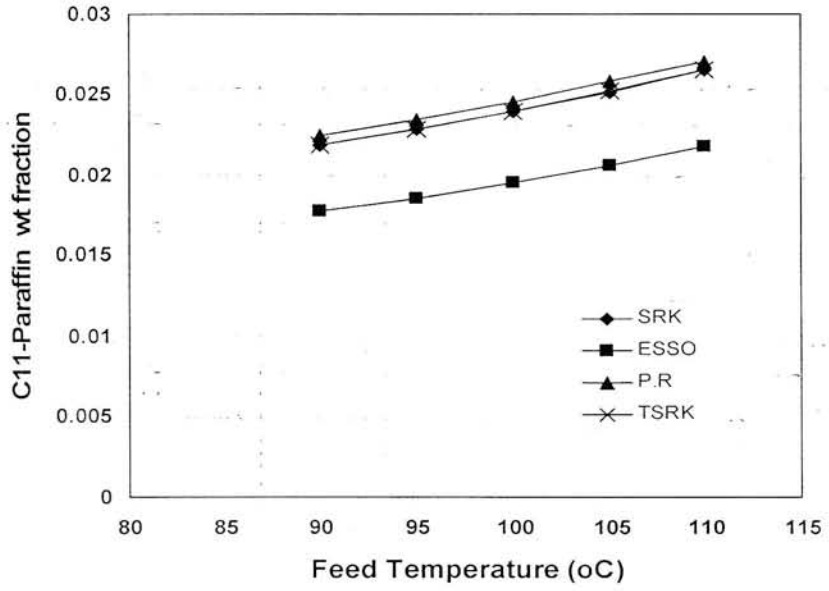

Figure (12) Effect of Feed Temperature on *C11-paraffin wt fraction*
P_{Top}=340 Kpa, & T_{Bottom} = 175 °C

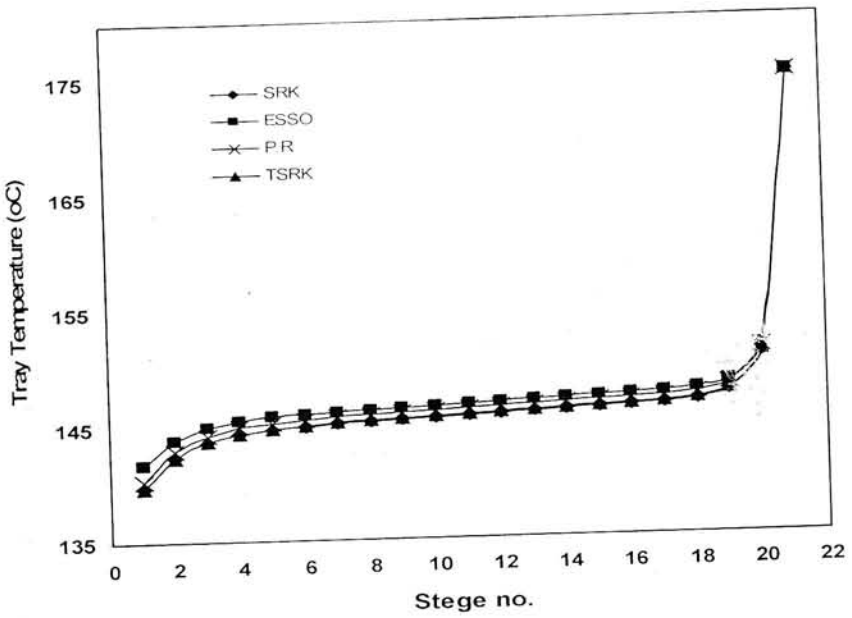

Figure (13) HF Stripper Tower Temperature Profile
P_{Top}=340 Kpa, T_{Feed} = 102 °C, & T_{Bottom}=175 °C

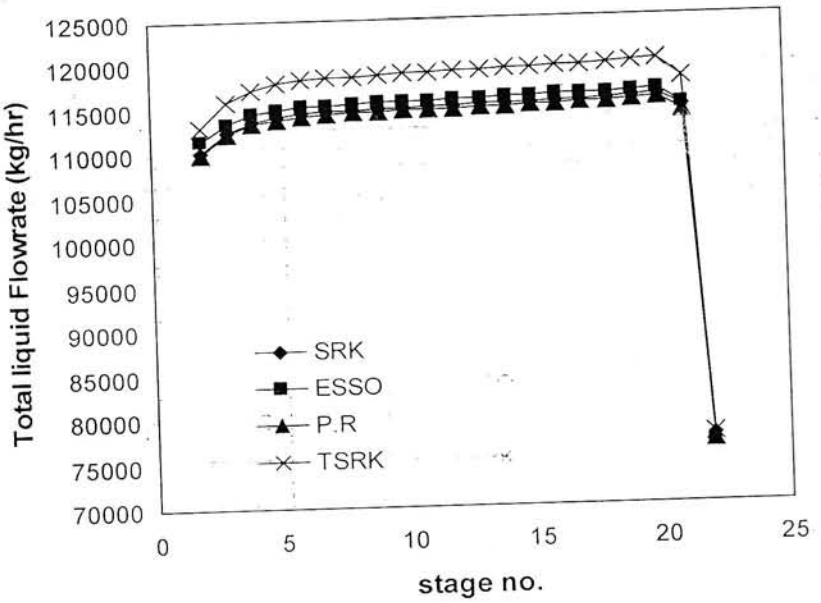

Figure (14) HF Stripper Total Liquid Flowrate Profile
P_{Top}=340 Kpa, T_{Feed} = 102 °C, & T_{Bottom}=175 °C

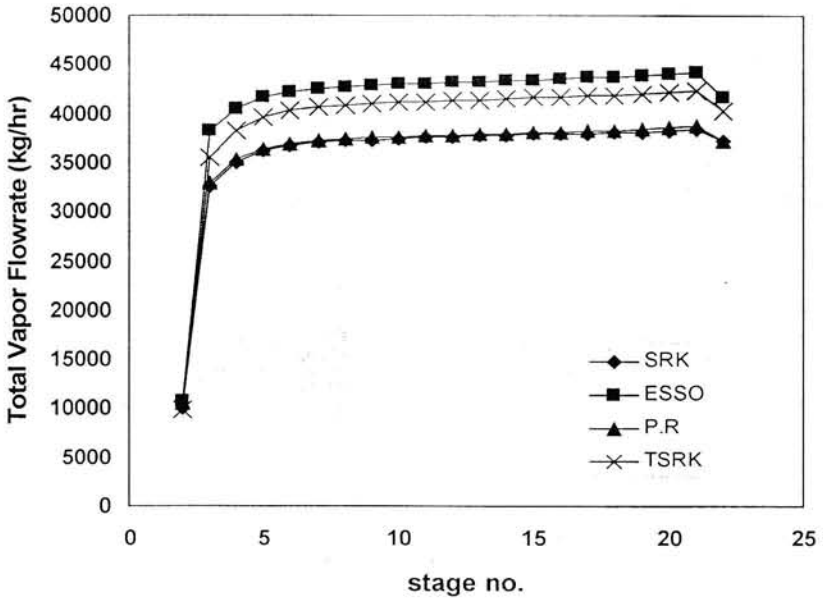

Figure (15) HF Stripper Total Vapor Flowrate Tower Profile
P_{Top}=340 Kpa, T_{Feed} = 102 °C, & T_{Bottom}=175 °C

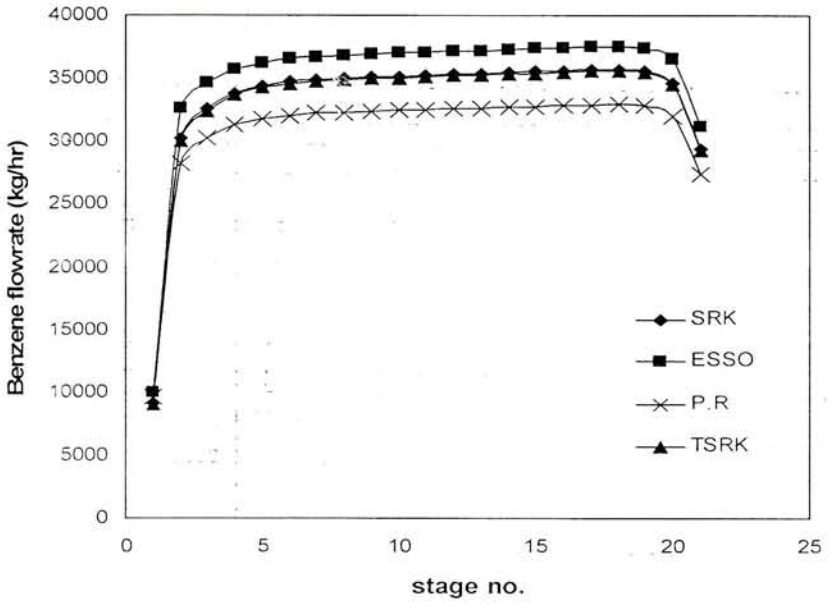

Figure (16) Tray Vapor Profile of Benzene wt fraction
P_{Top}=340 Kpa, T_{Feed} = 102 °C, & T_{Bottom}=175 °C

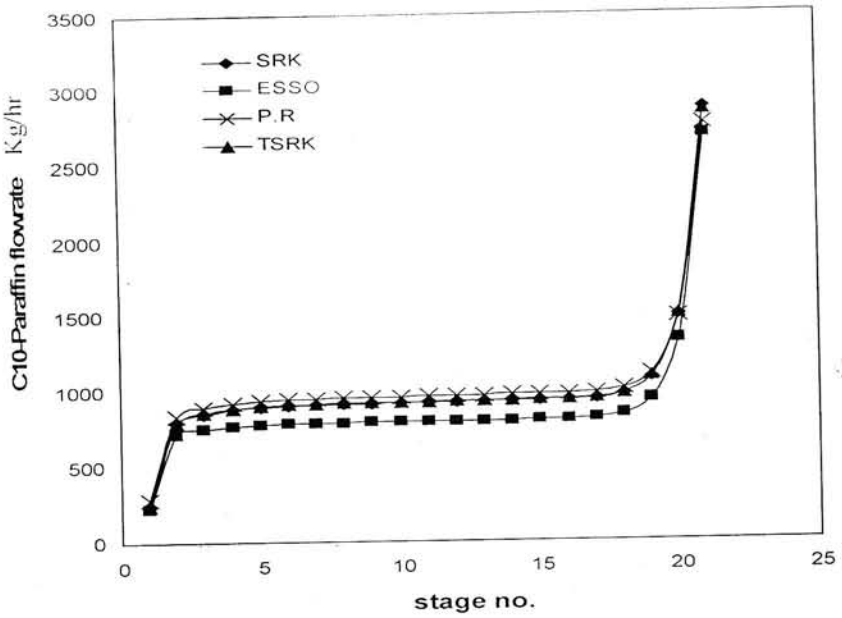

Figure (17) Tray Vapor Profile of C_{10}-Paraffin wt fraction
P_{Top}=340 Kpa, T_{Feed} = 102 °C, & T_{Bottom}=175 °C

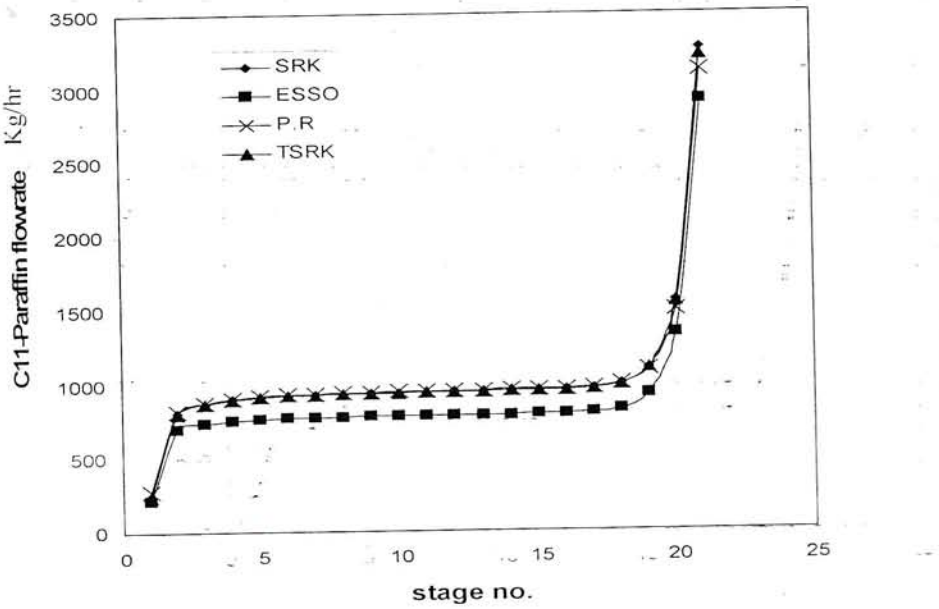

Figure (18) Tray Vapor Profile of C_{11}-Paraffin wt fraction
P_{Top}=340 Kpa, T_{Feed} = 102 °C, & T_{Bottom}=175 °C

دراسة في المحاكاة النظرية لتحليل عمود انتزاع حامض الهيدروفلوريك لمصنع انتاج الالكيل بنزين المستقيم

د.زيد عدنان عبدالرحمن عمر سعيد لطيف
مدرس مدرس مساعد
قسم الهندسة الكيمياوية-كلية الهندسة-جامعة تكريت

الخلاصة

استعمل البرنامج الجاهز CHEMCAD للتحليل الهندسي لعمود انتزاع حامض الهيدروفلوريك لمصنع إنتاج الالكيل بنزين المستقيم للشركة العربية في بيجي. رسمت منحنيات أداء عمود الانتزاع للمتغيرات : موديل ديناميك الحرارة، درجة حرارة أعلى وأسفل العمود ، درجة حرارة وتركيز المواد الداخلة ونسبة الاسترجاع. ورسمت أيضا المخططات الداخلية للعمود لتغير درجة الحرارة ، ومعدل تدفق الاطوار والتركيز.

استعمل أربعة موديلات لديناميك الحرارة وهي (SRK, TSRK, PR, & ESSO) وكان تاثيرها على النتائج بحدود 1-25% لمعظم الحالات.

تبين من نتائج المحاكاة ان هنالك ٥% من البارافين في مجرى العلوي والذي قد يسبب مشكلة في المصنع. وتم ملاحظة اكبر تغير في معدل تدفق البخار في أعلى العمود مع تغير درجة حرارة أسفل العمود ودرجة حرارة وتركيز المواد الداخلة. وتبين أيضا بان المخططات الداخلية للعمود لتغير درجة الحرارة ، ومعدل تدفق الأطوار والتركيز أنها ثابتة نسبيا بين الصينية رقم 5 (أسفل قليلا من مدخل المواد) إلى الصينية رقم 18 (أعلى قليلا من المبخر). وهذه الصواني يمكن حذفها من دون التأثير على أداء العمود. وأخيرا تبين من خلال الدراسة الحالية إمكانية استخدام البرنامج الجاهز CHEMCAD بنجاح في المحاكاة النظرية لعمود انتزاع حامض الهيدروفلوريك المستخدم.

الكلمات الدالة

المحاكاة، برنامج CHEMCAD ، تقطير متعدد الأطوار ، الالكيل بنزين المستقيم، انتزاع حامض الهيدروفلوريك.