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PROCESS SIMULATION OF BENZENE SEPARATION COLUMN OF LINEAR ALKYL BENZENE (LAB)PLANT USING CHEMCAD

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ABSTRACT

CHEMCAD process simulator was used for the analysis of existing benzene separation column in LAB plant(Arab Detergent Company/Beiji-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 & reflux ratio. Also simulated columns profiles for the temperature, vapor & liquid flow rates compositions, were constructed. Four different thermodynamic models options (SRK, TSRK, PR, and ESSO) were used, affecting the results within 1-25% variation for the most cases.

For Benzene Column (32 real stages, feed stage 14), the simulated results show that bottom temperature above 200 ^{o}C the weight fractions of top components, except benzene, increases sharply, where as benzene top weight fraction decreasing sharply. Also, feed temperature above 180 ^{o}C shows same trends. The column profiles remain fairly constant from tray 3 (immediately below condenser) to tray 10 (immediately above feed) and from tray 15 (immediately below feed) to tray 25 (immediately above reboiler). Simulation of the benzene separation 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, multicomponent distillation, LAB, Benzene column.

INTRODUCTION

Process simulation is a computer representation of an individual unit operation, or multiple connected units or an entire chemical 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 currently available modern process simulation software are ASPENPLUS, CHEMCAD, HYSYS & PRO/II. These process simulators have become basic tools in chemical engineering education. Process simulation of existing chemical plants or their individual equipment is an important area of research and development (R & D).[1-3]

CHEMCAD[4] 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 thermo dynamical models like Peng-Robinson (PR), Soave-Redlich-Kwong (SRK), NRTL, UNIQUAC, UNIFAC, mod. 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 benzene separation distillation column diagram constructed using CHEMCAD. Where as Figure (2)

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 existing LAB plant (Arab Detergent Company/Beiji-Iraq) especially one of the major equipment; benzene separation distillation column, using CHEMCAD process simulator.

RESULTS AND DISCUSSIONS

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

Effect of Bottom Temperature

Figures (3) to (7) show the effect of bottom temperature on top temperature, top total flow rate, & top components weight fractions (benzene, C_{10} -paraffin & C_{11}-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 with in 1-10% variation.
2. For bottom temperature between 180 ^{o}C & 200 ^{o}C, the variation of the top temperature is from 104 ^{o}C to 107 ^{o}C, the total top flowrate varies from about 10000 kg/hr to 15000 kg/hr, where as the variation of the top components weight fractions are varied as follows; benzene (from 1 to 0.85), C_{10}-paraffin (from 0 to 0.06), and C_{11}-paraffin (from 0 to 0.06).
3. For bottom temperature above 200 ^{o}C, the rate of change of the variables decreases sharply.

Effect of Feed Temperature

Figures (8) to (12) show the effect of feed temperature on top temperature, top total flow rate, & top components weight fractions (benzene, C10 paraffin, C11 paraffin), at different thermodynamic models. The figures show the following trends:

1. The effect of the thermodynamic models used (SRK, PR, & ESSO) on the general results in within 10% variation, except TSRK model, the variation is higher.
2. For feed temperature between 160^{o}C and 180^{o}C, the variation of the top temperature is within 106 ^{o}C to 107 ^{o}C, the total top flowrate varies from 16800 kg/hr to 17500 kg/hr, where as the variation of top components weight fractions are varied as follows; benzene (from 0.9 to 0.85), C_{10}-paraffin (from 0.0 to 0.06), and C_{11}-paraffin (from 0.0 to 0.06).
3. For feed temperature above 180 ^{o}C, the rates of change of variables are higher.

Effect of Feed Concentration

Feed concentration presentation is very difficult in multicomponent systems. Table (2) shows a comparison between two simulation runs to notice the effect of increasing light components feed weight fractions (benzene) and decreasing heavy components feed weight fractions (C_{10}-paraffin & C_{11}-paraffin). The top temperature decreases from 107^{o}C to 106^{o}C, where as the top total vapor flow rate increases (from about 15900 kg/hr to 19500 kg/hr).

Effect of Reflux Ratio

Figures (13) to (17) show the effect of reflux ratio on top temperature, and top components weight fractions (benzene, C_{10}-paraffin, C_{11}-paraffin), at different thermodynamic models. The figures show the following trends:

1. The effect of the thermodynamic models used (SRK, TSRK,PR, & ESSO) on the general results 5%.
2. For reflux ratio increases between 0.75 to 1.5, the top temperature decreases from 107^{o}C to 107^{o}C, and the total top flowrate decreases from 18400 kg/hr to 17000 kg/hr, where as the variation of top components weight fractions are varied as follows; benzene (from 0.82 to 0.9), C_{10}-paraffin (from 0.07 to 0.045), and C_{11}-paraffin (from 0.075 to 0.045).

Benzene Column Profiles

Figures (18) to (23) show the temperature & composition profiles for

benzene 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. In all cases the profiles are remain fairly constant from tray 2 (immediately below condenser) to tray 10 (immediately above the feed) and from tray 15 (immediately below feed) to tray 25 (immediately above the reboiler).

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. For benzene column (32 real stages, feed stage 14), the simulated results show that bottom temperature above 200 ^{o}C the weight fractions of top components, except benzene, increase sharply, whereas benzene top weight fraction decrease sharply. Also, feed temperature above 180 ^{o}C shows same trends.
3. The benzene column profiles remain fairly constant from tray 3 (immediately below condenser) to tray 10 (immediately above feed) and from tray 15 (immediately below feed) to tray 25 (immediately above reboiler).
4. Simulation of the benzene separation 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. Himmelblau ,D.M. ,Riggs , J.B. , Basic Principles and Calculation in Chemical Engineering ,7th ed. , Prentice Hall, New Jersey, 2004.
4. CHEMCAD User's Guide.
5. Arab Detergent Company; LAB production plant Field data, Beiji-Iraq.

Table (1) Typical Field Data specification of Benzene Column (Arab Detergent Company).[5]

Component	Feed	Top product	Bottom product
Temperature,oC	180	100	225
Pressure , Kpa	400	200	220
Flow rate Kg/hr	75753	15826	59927
HF	0	0	0
Benzene	0.208972	1	0.000095
N-Undecane (C_{10}—paraffin)	0.153242	?	0.193707212
N-Dodecane (C_{11}—paraffin)	0.293817		0.371401825
N-Tridecane (C_{12}—paraffin)	0.18605		0.235177342
N-Tetradecane (C_{13}—paraffin)	0.0793669		0.100324229
N-Undecylbenzene (C_{10}—LAB)	0.0167034	?	0.021114017
N-Dodecylbenzene (C_{11}—LAB)	0.0235897		0.029818716
N-Tridecylbenzene (C_{12}—LAB)	0.018875		0.023859041
N-Tetradecylbenzene (C_{13}—LAB)	0.012431		0.015713429
heavy alkylate (HAB)*	0.0069531		0.008789075
D stripping	***2500mm***		
D rectification	***1400mm***		
Tray spacing	***600mm***		
Tray holes No.	***1942***		
Hole diam d_o	***13mm***		
trays above feed	***12 trays, 13 stages(with condenser)***		
trays below feed	***18 trays, 19 stages(with reboiler)***		
Condenser heat duty Q_C	***11367 MJ/hr***		
Reboiler heat duty Q_r	***18288 MJ/hr***		
Reflux Ratio(R)	***1.1***		

***** Molecular Weight: **366**
Normal boiling: **397 ^oC**
Specific gravity: **0.875**

Table (2) Effect of Feed Concentration: a Comparison Between Two CHEMCAD Simulation Runs of Benzene Column.

Stream No.	1	2	3
Stream Name	feed	top	bottom
Temp C	180.0000*	107.4400	225.0000
Pres kPa	400.0000*	200.0000	220.0000
Enth MJ/h	-85867.	5099.6	-86054.
Vapor mole fraction	0.00000	0.00000	0.00000
Total kmol/h	554.1456	186.5465	367.5991
Total kg/h	75753.0000	15918.4220	59834.5389
Total std L m3/h	97.6383	18.6003	79.0380
Total std V m3/h	12420.42	4181.19	8239.24
Component mass fractions			
HydrogenFluoride	0.000000	0.000000	0.000000
Benzene	0.182570	0.826926	0.011145
N-Decane	0.166443	0.070657	0.191926
N-Undecane	0.307018	0.072185	0.369493
N-Dodecane	0.186050	0.024157	0.229120
N-Tridecane	0.079367	0.005706	0.098964
Decylbenzene	0.016703	0.000161	0.021104
N-Undecylbenzene	0.023590	0.000123	0.029833
N-Dodecylbenzene	0.018875	0.000060	0.023880
Tridecylbenzene	0.012431	0.000022	0.015732
heavy alkylate	0.006953	0.000002	0.008802

Stream No.	1	2	3
Stream Name	feed	top	bottom
Temp C	180.0000*	106.4592	225.0000
Pres kPa	400.0000*	200.0000	220.0000
Enth MJ/h	-74381.	8701.4	-80131.
Vapor mole fraction	0.052732	0.00000	0.00000
Total kmol/h	578.5016	235.0694	343.4324
Total kg/h	75753.0000	19567.6364	56185.3352
Total std L m3/h	96.7491	22.6607	74.0884
Total std V m3/h	12966.33	5268.76	7697.57
Component mass fractions			
HydrogenFluoride	0.000000	0.000000	0.000000
Benzene	0.235373	0.874436	0.012807
N-Decane	0.140042	0.048476	0.171932
N-Undecane	0.280616	0.053106	0.359851
N-Dodecane	0.186050	0.019228	0.244149
N-Tridecane	0.079367	0.004480	0.105448
Decylbenzene	0.016703	0.000120	0.022478
N-Undecylbenzene	0.023590	0.000091	0.031774
N-Dodecylbenzene	0.018875	0.000045	0.025433
Tridecylbenzene	0.012431	0.000016	0.016755
heavy alkylate	0.006953	0.000002	0.009374

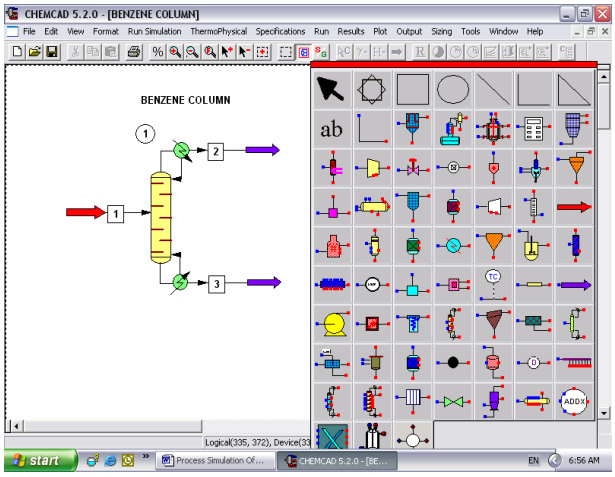
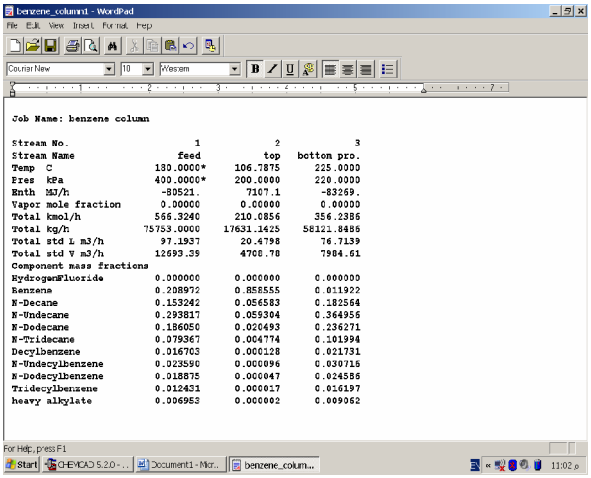


Figure (1) Benzene separation distillation column flowsheet.



benzene_column1 - WordPad

Job Name: benzene column

Stream No.	1	2	3
Stream Name	feed	top	bottom pro.
Temp C	130.0000*	106.7875	225.0000
Pres kPa	400.0000*	200.0000	220.0000
Enth MJ/h	-80521.	7107.1	-83269.
Vapor mole fraction	0.00000	0.00000	0.00000
Total kmol/h	566.3240	210.0856	356.2385
Total kg/h	75753.0000	17631.1425	58121.8485
Total std l m3/h	97.1937	20.4798	76.7139
Total std V m3/h	12693.39	4708.78	7984.61
Component mass fractions			
HydrogenFluoride	0.000000	0.000000	0.000000
Benzene	0.208972	0.858555	0.011922
N-Decane	0.153242	0.056583	0.182564
N-Undecane	0.293817	0.059304	0.364956
N-Dodecane	0.186050	0.020493	0.236271
N-Tridecane	0.079367	0.004774	0.101994
Decylbenzene	0.016703	0.000128	0.021731
N-Undecylbenzene	0.023590	0.000096	0.030715
N-Dodecylbenzene	0.018875	0.000047	0.024556
Tridecylbenzene	0.012431	0.000017	0.016197
heavy alkylate	0.006953	0.000002	0.009062

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

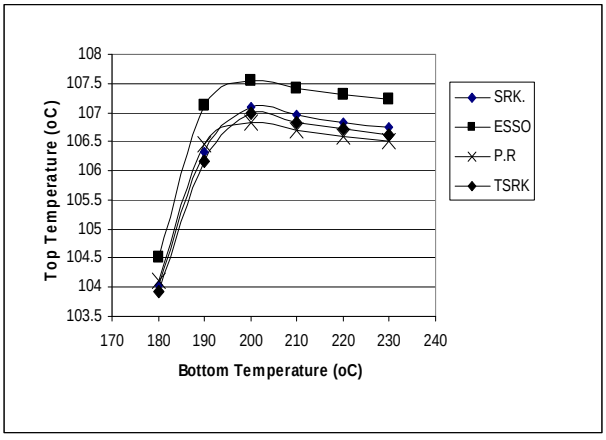


Figure (3) Effect of Bottom Temperature on Top Temperature
P_{Top}=200 Kpa, R=1.1, & T_{Feed} = 180 ^{o}C

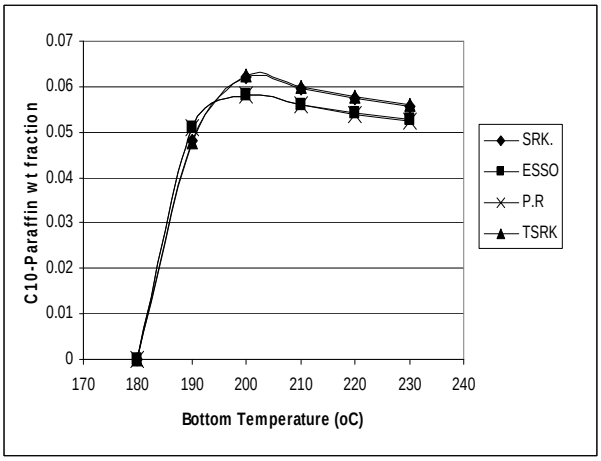


Figure (6) Effect of Bottom Temperature on wt. fraction of C_{10}-Paraffin
P_{Top}=200 Kpa, R=1.1, & T_{Feed}

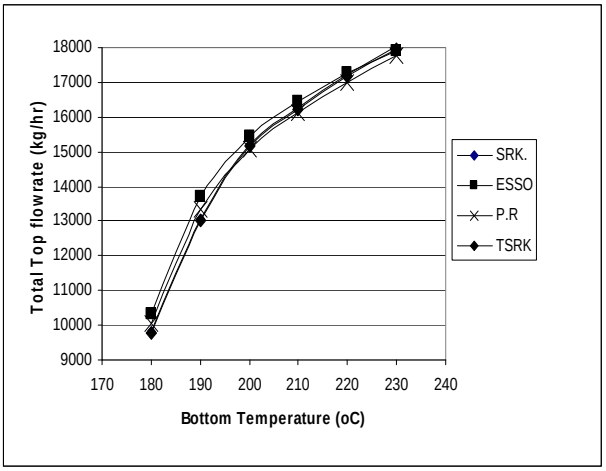


Figure (4) Effect of Bottom Temperature on Total Top vapor Flowrate
P_{Top}=200 Kpa, R=1.1, & T_{Feed} = 180 ^{o}C

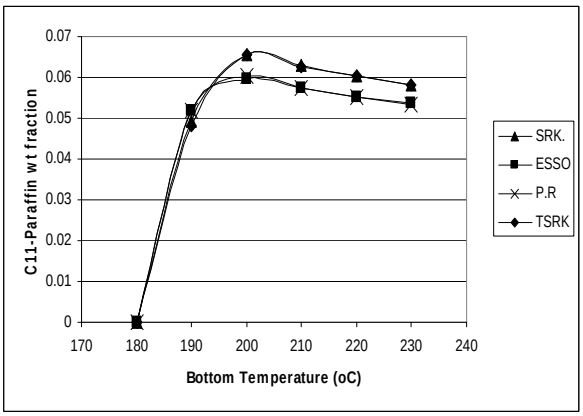


Figure (7) Effect of Bottom Temperature on wt. fraction of C_{11}-Paraffi
P_{Top}=200 Kpa, R=1.1, & T_{Feed} =

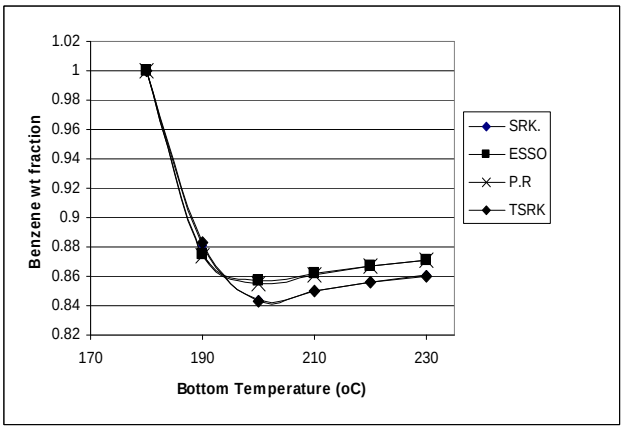


Figure (5) Effect of Bottom Temperature on Benzene wt. fraction
P_{Top}=200 Kpa, R=1.1, & T_{Feed} = 180 ^{o}C

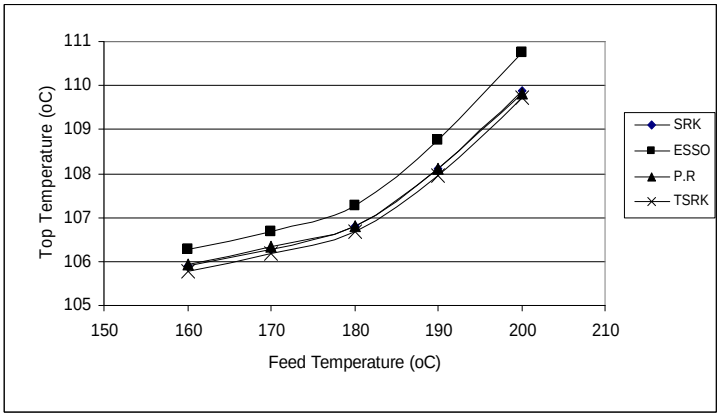


Figure (8) Effect of Feed Temperature on Top Temperature
P_{Top}=200 Kpa, R=1.1,&T_{Bottom}= 225 ^{o}C

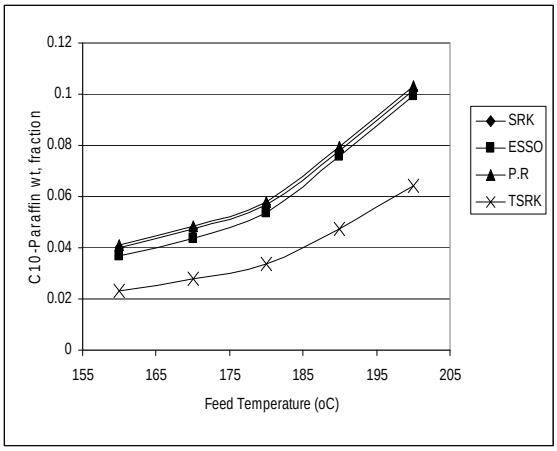


Figure (11) Effect of Feed Temperature on C10-paraffin wt fraction
P_{Top}=200 Kpa,R=1.1,&T_{Bottom} = 225 ^{o}C

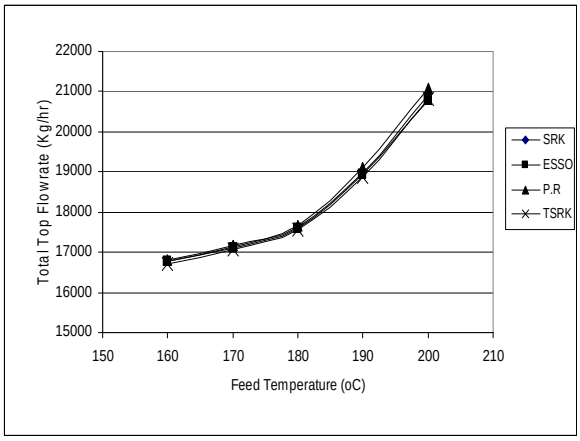


Figure (9) Effect of Feed Temperature on Total Top Flowrate
P_{Top}=200 Kpa,R=1.1,&T_{Bottom} = 225 ^{o}C

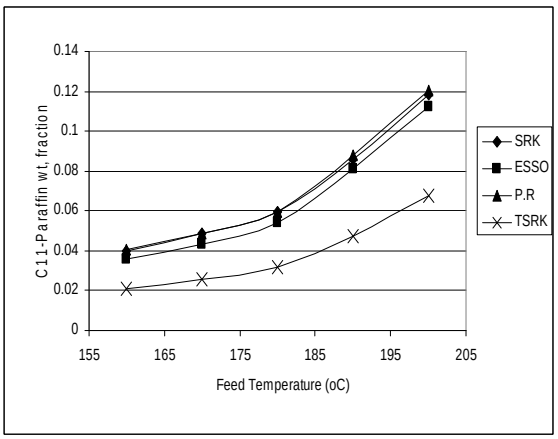


Figure (12) Effect of Feed Temperature on C11-paraffin wt fraction
P_{Top}=200 Kpa,R=1.1,&T_{Bottom} = 225 ^{o}C

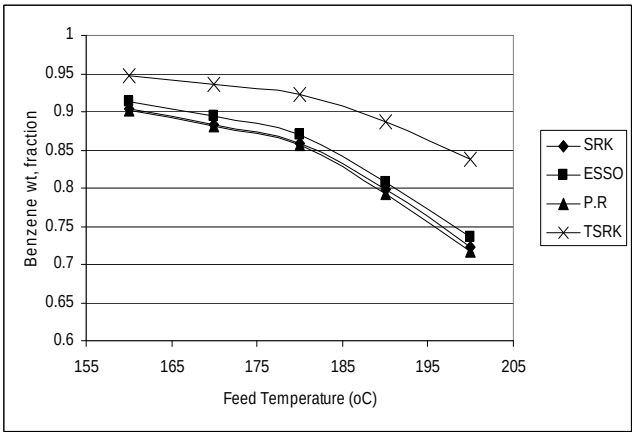


Figure (10) Effect of Feed Temperature on *Benzene wt fraction*
P_{Top}=200 Kpa, R=1.1,&$T_{Bottomad}$= 225 ^{o}C

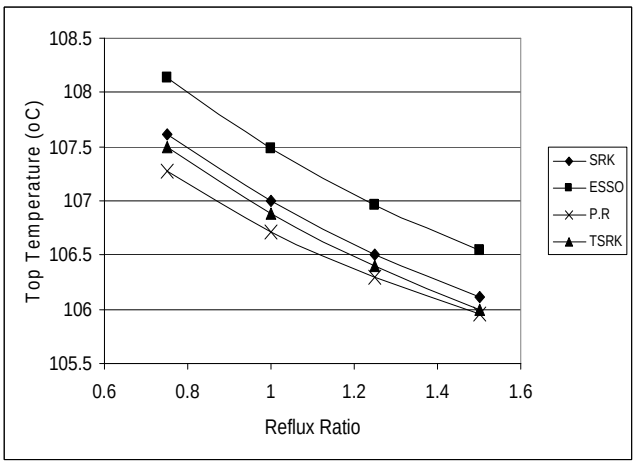


Figure (13) Effect of Reflux Ratio on Top Temperature
P_{Top}=200 Kpa, T_{Bottom} = 225 ^{o}C,
T_{Feed} = 180 ^{o}C

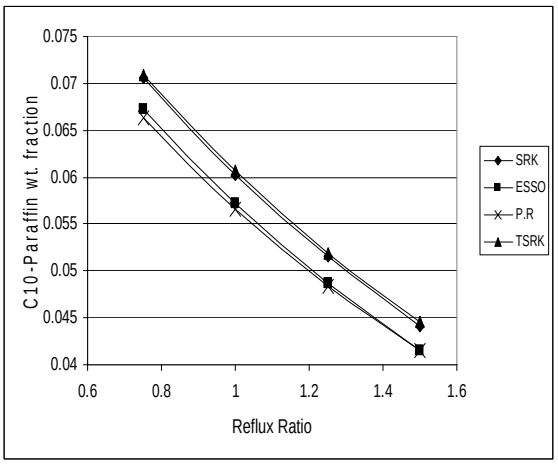


Figure (16) Effect of Reflux Ratio on C10-Paraffin wt. fraction
P_{Top}=200 Kpa, T_{Bottom} = 225 °C, T_{Feed} = 180 °C

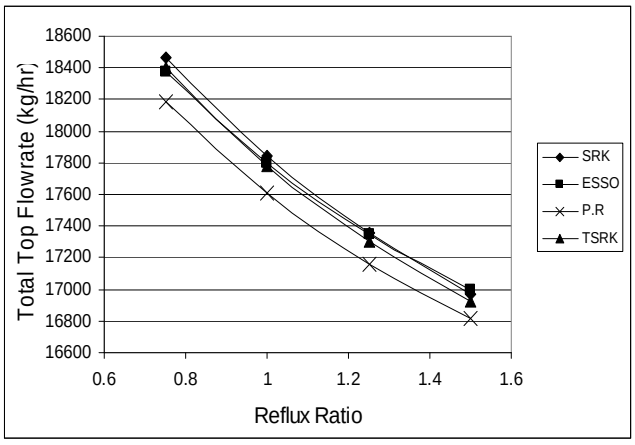


Figure (14) Effect of Reflux Ratio on Total Top Flowrate , P_{Top}=200 Kpa, T_{Bottom} = 225 °C, T_{Feed} = 180 °C

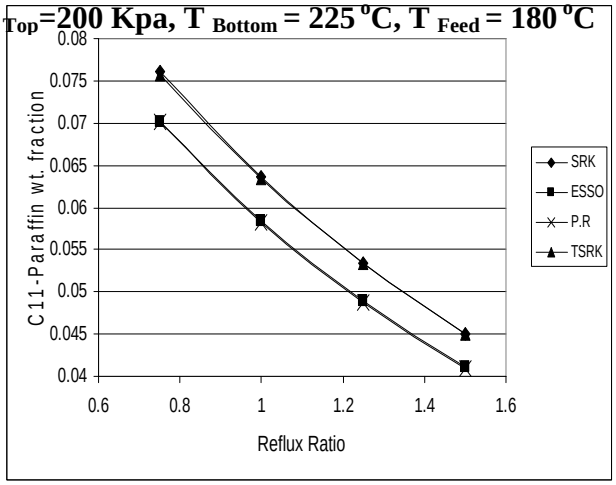


Figure (17) Effect of Reflux Ratio on C11-Paraffin wt. fraction
P_{Top}=200 Kpa, T_{Bottom} = 225 °C, T_{Feed} = 180 °C

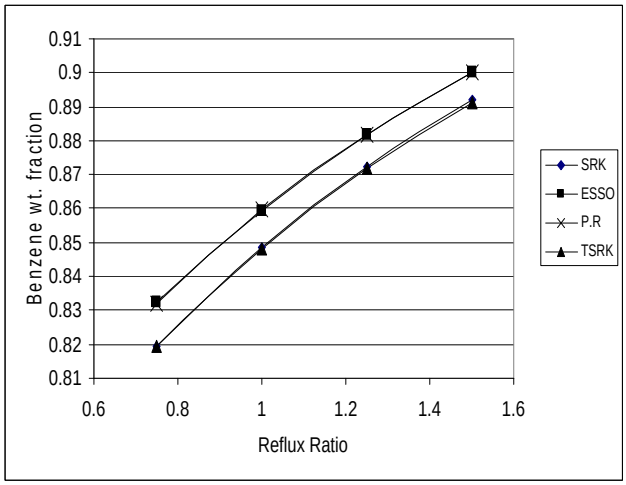


Figure (15) Effect of Reflux Ratio on Benzene wt. fraction
P_{Top}=200 Kpa, T_{Bottom} = 225 °C, T_{Feed} = 180 °C

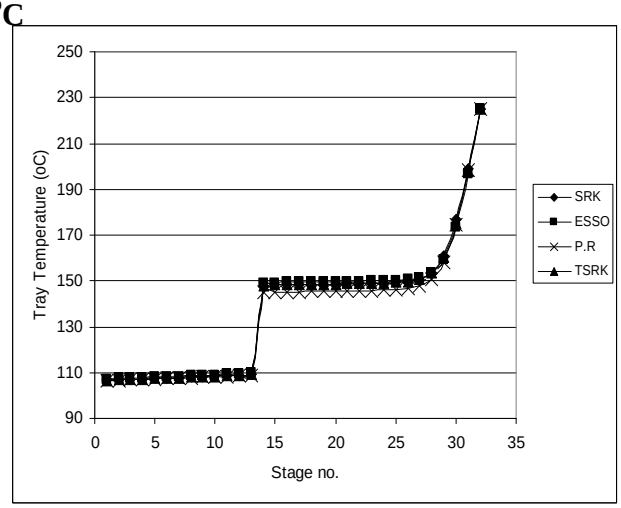


Figure (18) Benzene Tower Temperature Profile
P_{Top}=200 Kpa, T_{Feed} = 180 °C,
T_{Bottom}=225 °C, R=1.1

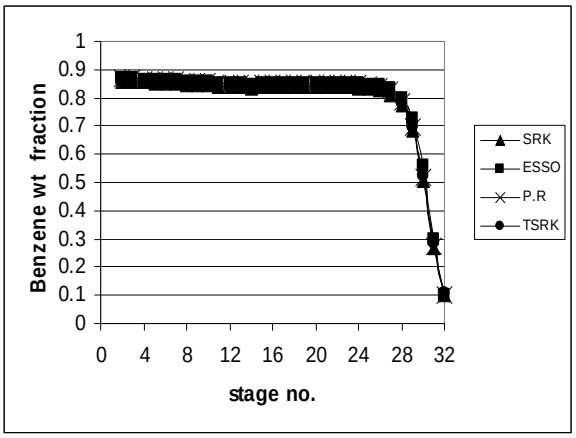


Figure (21) Tray Vapor Profile of Benzene wt fraction
P_{Top}=200 Kpa, T_{Feed} = 180 °C, T_{Bottom}=225 °C, R=1.1

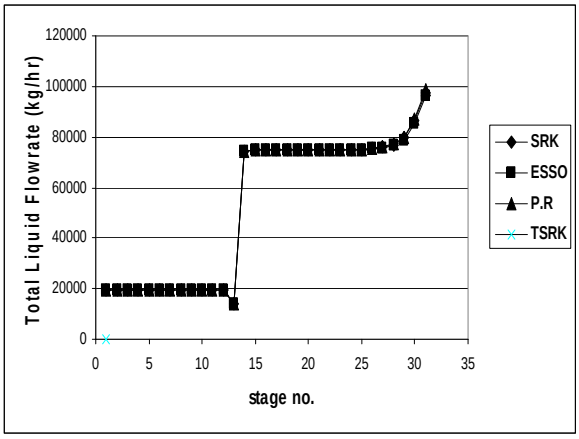


Figure (19) Benzene Column Total Liquid Flowrate Profile, P_{Top}=200 Kpa, T_{Feed} = 180 °C, T_{Bottom}=225 °C, R=1.1

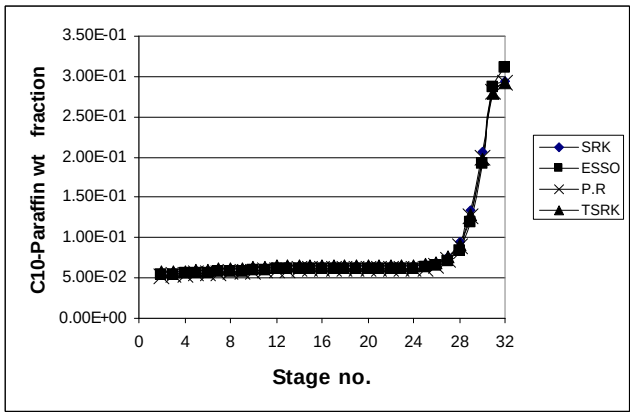


Figure (22) Tray Vapor Profile of C_{10}-Paraffin wt fraction
P_{Top}=200 Kpa, T_{Feed} = 180 °C, T_{Bottom}=225 °C, R=1.1

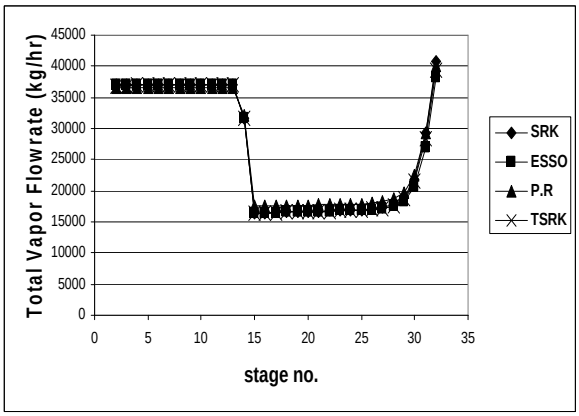


Figure (20) Benzene Column Total Vapor Flowrate Tower Profile, P_{Top}=200 Kpa, T_{Feed} = 180 °C, T_{Bottom}=225 °C, R=1.1

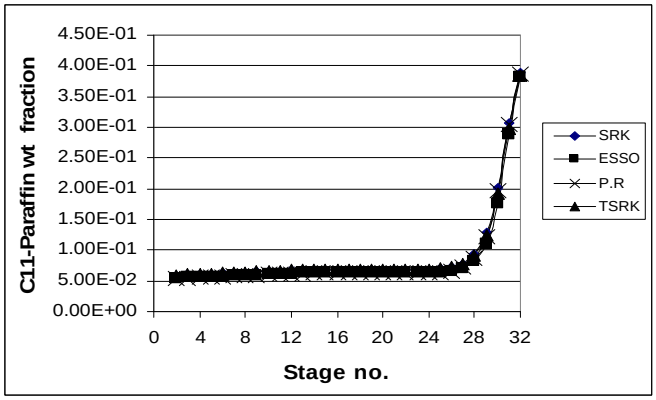


Figure (23) Tray Vapor Profile of C_{11}-Paraffin wt fraction
P_{Top}=200 Kpa,T_{Feed} =180 °C, T_{Bottom}=225 °C, R=1.1

دراسة في المحاكاة النظرية لتحليل عمود فصل البنزين لمصنع انتاج الالكيل بنزين المستقيم باستخدام البرنامج الجاهز CHEMCAD

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الخلاصة

استعمل البرنامج الجاهز CHEMCAD للتحليل الهندسي لعمود فصل البنزين لمصنع انتاج الالكيل بنزين المستقيم للشركة العربية في بيجي. رسمت منحنيات اداء عمود الانتزاع للمتغيرات : موديل ديناميك الحرارة، درجة حرارة اعلى واسفل العمود ، درجة حرارة وتركيز المواد الداخلة ونسبة الاسترجاع. ورسمت ايضا المخططات الداخلية للعمود لتغير درجة الحرارة ومعدل تدفق الاطوار والتركيز.

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

تبين من نتائج المحاكاة ان تاثير درجة حرارة اسفل العمود اعلى من 200 ^{o}C ، للنسبة الوزنية للمواد في اعلى العمود تزداد بحدة عدا نسبة البنزين التي تقل بحدة. ولوحظ نفس التصرف تقريبا لدرجة حرارة المواد الداخلة اعلى من 180 ^{o}C . وتبين من خلال المخططات الداخلية للعمود لتغير درجة الحرارة ، ومعدل تدفق الاطوار والتركيز انها ثابتة نسبيا بين الصينية رقم 3 (اسفل قليلا من المكثف) الى الصينية رقم 10 (اعلى قليلا من المواد الداخلة) ومن الصينية رقم 15 (اسفل قليلا من المواد الداخلة) الى الصينية رقم 25 (اعلى بقليل من المبخر).

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

الكلمات الدالة: المحاكاة، برنامج CHEMCAD ، تقطير متعدد الاطوار ، الالكيل بنزين المستقيم، عمود البنزين.