SIMULATION OF CUMENE MANUFACTURING

Submitted By
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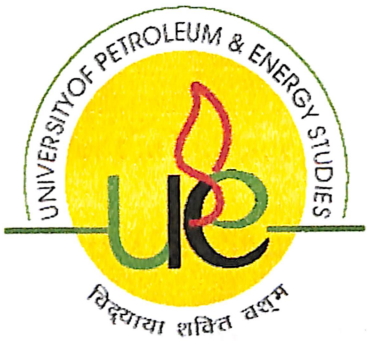
Master of Technology in Refining & Petro Chemical Engineering
(2008-10)



College of Engineering
University of Petroleum & Energy Studies
Dehradun
May, 2010

SIMULATION OF CUMENE MANUFACTURING

A thesis submitted in partial fulfilment of the requirements for the Degree of

Master of Technology

(Refining & Petrochemical Engineering)

By

(Y.Ram Rakesh)

Under the guidance of

Mr. B. Uma Shankar

(Assistant professor)

Approved

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College of Engineering

University of Petroleum & Energy Studies

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May, 2010

CERTIFICATE

This is to certify that the work contained in this thesis titled "SIMULATION OF CUMENE MANUFACTURING" has been carried out by **Mr.B.Uma shankar**. under my/our supervision and has not been submitted elsewhere for a degree.

Mr. B. Uma shankar.
(Assistant professor)
Date :

ACKNOWLEDGEMENT

I wish to acknowledge my sincere thanks to **Prof.Dr.Srihari**, Dean, College of Engineering Studies, for his timely support and help.

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Y.RAM RAKESH

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ABSTRACT

Objective of this project is to use Aspen plus as a simulation tool to simulate a flow sheet for the Manufacturing of Cumene with benzene and propylene as the raw materials. The simulation of various equipments such as Plug Flow Reactor, Distillation Column, Heaters and Flash Column are default with in this project.

The project presents improvement of conversion by varying the distillate to feed ratio of the Distillation Columns using Design Specs.

Sensitivity analysis has been performed in which the reflux ratio of the distillation columns has been varied and a graph between the reflux ratio and mole fraction of the cumene has been plotted and the optimum reflux ratio is found for best separation. Sensitivity analysis is also been performed for the plug flow reactor by varying the length of the tube and a graph is plotted between the length of the tubes and the mole fraction the cumene and the optimum length of the tube is determined.

The Project presents a case of optimization, in which the reboiler duty is optimized to get a minimum objective function. The project also deals with choice of proper thermo package. Calculator option is used to find out the total profit of the plant.

The Product Cumene Recovery is increased up to 98.05% with the use of Design spec. Sensitivity, Optimization when compared to Base case. Also Product Purity increased approximately to 85.5 % with the use of above techniques.

INTRODUCTION

Cumene is the common name for **isopropylbenzene**, an organic compound that is an aromatic hydrocarbon. It is a constituent of crude oil and refined fuels. It is a flammable colorless liquid that has a boiling point of 152 °C. Cumene is produced by reacting propylene and benzene over an acid catalyst. Cumene may be used to increase the octane in gasoline, but its primary use is as a feedstock for manufacturing phenol and acetone. The Chemical formula for cumene is C_6H_5-C_3H_7.

The unit, to which I am assigned, converts the benzene and propylene into styrene, producing around 156322.67 Rs/hr.

PROPERTI

Appearance: Clear, colorless liquid.
Odor: Sharp penetrating aromatic odor.
Solubility: Insoluble in water.
Specific Gravity: 0.864 .
pH: No information found.
% Volatiles by volume @ 21C (70F): 100
Boiling Point: 152C (306F)
Melting Point:-96C (-141F)
Vapor Density (Air=1): 4.1
Vapor Pressure (mm Hg):8 @ 20C (68F)
Evaporation Rate : No information found.
Molecular Weight: 120.20.

Effects of cumene:

Danger!! Harmful or fatal if swallowed. Flammable liquid and vapor. Harmful if inhaled or absorbed through skin. Causes irritation to skin, eyes and respiratory tract, affects central nervous system.

USES

Around 98% of cumene is used to produce phenol and its co-product acetone. However, the outlook for cumene is largely dependent on the performance of phenol's derivatives which have resulted in healthy growth rates for cumene.

- It is also used as an important raw material in the manufacture of pesticide intermediates such as Para Cumidine.
- It finds application in the manufacture of cumene hydroperoxide, dicumyl peroxide which are used as Initiators in polymerisation process, grafting of vinyl monomers onto polymer backbone, curing of resins and rubber etc.
- It finds application as a good solvent for flats and resins.
- It is used as thinner for paints, enamels and lacquers used as a component in aviation gasolines which enables to improve the octane rating of internal combustion engines.

PROCESS DESCRIPTION

Process flow diagram for the production of cumene is shown below. The raw materials are benzene and propylene (which has small amounts of propane). Benzene and propylene are fed from separate storage tanks namely benz and propy through pump1 and pump2 respectively. These two raw materials are then fed into the mixer for the mixing purpose then the mixture M-out is to be heated by the heater. The heater outlet is then fed into the plug flow reactor. The process feed to the reactor consists of 75% excess benzene. In the reactor, benzene and propylene react in an isothermal, exothermic reaction to form cumene. The PFR out consists of the mixture of cumene, p-diisopropylbenzene (p-DIP),benzene and propylene are obtained. Then the mixture is

cooled in the cooler and the cool-outlet is fed into the rad frac column1 where the top product contains of large amount of benzene and small fractions of propylene and propane which are further fed to the flash column where the top product are natural gas and the fuel gas by-product of the process goes out as the fuel gases and the bottoms contains large amounts of benzene which is recycled to the pump1. The bottom product from the Rad Frac1 consists of large amounts of cumene and small amounts of p-DIP is fed into the Rad Frac2 where the top product is the desired product Cumene and a very small amount of the p-diisoproplbenzene is produced.

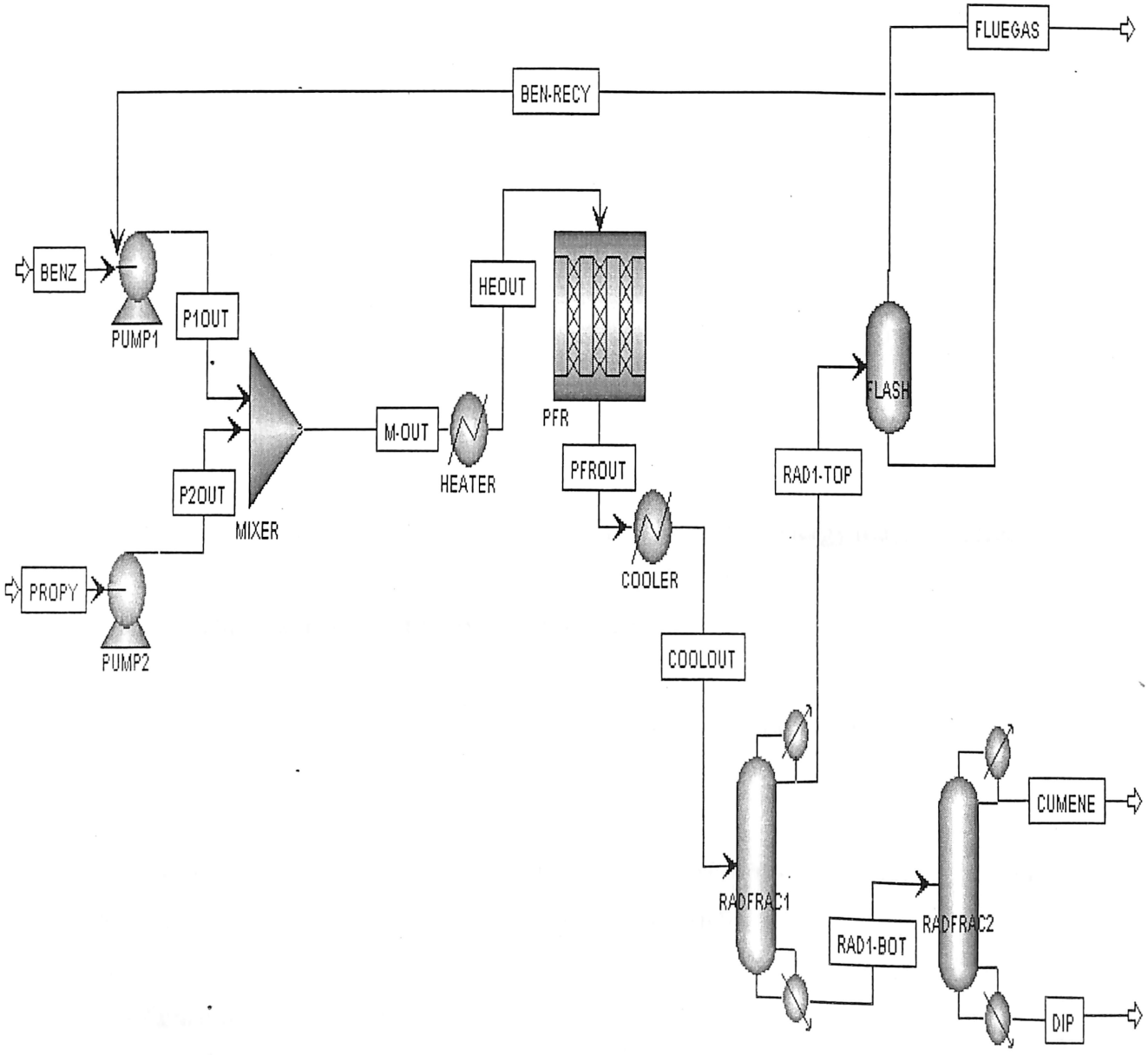
Cumene Production Reactions:

The reactions for cumene production from benzene and propylene are as follows:

$$\underset{propylene}{C_3H_6} + \underset{benzene}{C_6H_6} \rightarrow \underset{cumene}{C_9H_{12}}$$

$$\underset{propylene}{C_3H_6} + \underset{cumene}{C_9H_{12}} \rightarrow \underset{p-diisopropyl\ benzene}{C_{12}H_{18}}$$

PROCESS FLOW SHEET FOR CUMENE PRODUCTION



OPERATING CONDITIONS

Feed Streams:

Benz: Benzene, pure liquid, 25°C and 101.3 kPa.

Propy: Propylene with 4.5 wt% propane impurity, saturated liquid at 25°C.

Effluent Streams

Fuel Gas: Fuel gas stream, credit may be taken for LHV of fuel.

Cumene: Cumene product, assumed pure.

Equipment

Pump1: The pump increases pressure of the benzene feed from 101.3kPa to about 3400 kPa. Pump operation may be assumed isothermal and the cost of energy may be neglected.

Pump2: The pump increases the pressure of the propylene feed to about 3400 kPa. Pump operation may be assumed isothermal and the cost of energy may be neglected.

Mixer: The mixer is used to mix the two feed streams.

Heater: The heater desubcools, vaporizes, and superheats the mixed feed up to 400°C and a pressure of 3200kPa.

Plug Flow Reactor: The reactor type is reactor with specified tempature and is constant at inlet temperature to achieve the desired reaction.

***Configuration of reactor*:**

Length = 6 m.

Diameter = 4 in.

Number of tubes = 800.

The following reaction occurs:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{cumene}}{C_9H_{12}}$$

There are no side reactions.

Cooler: Cooler is operated at 120 ^{0}C temperature and a pressure of 1 atm.

Flash Vessel: The flash is operated at a temperature of 20^{0}C and a pressure of 1 bar. Here the large amounts of benzene are recycled as bottom product and fuel gases as the top product.

Rad Frac Column1: Column is operated with condenser pressure of 1bar and a temperature of -25.7^{0}C. Reboiler pressure is 1 bar and a temperature of 101.5^{0}C. The column is operated at a temperature is 120^{0}C and a pressure of 1.01bar. The no of stages are 10. In this column separation occurs and where propylene and benzene are separated as top product and cumene and p-diisopropylbenzene as the bottom product.

Rad Frac Column2: Column is operated with condenser pressure of 1bar and a temperature of 105.9^{0}C. Reboiler pressure is1 bar and a temperature of 148.6^{0}C. The column is operated at a temperature is 143^{0}C and a pressure of 1.01bar. The no of stages are 11. In this column separation occurs and where the desired product cumene is collected as the top product and p-diisopropylbenzene is the bottom product.

KINETICS:

The reactions for cumene production from benzene and propylene are as follows:

Reaction1:

$$\underset{propylene}{C_3H_6} + \underset{benzene}{C_6H_6} \rightarrow \underset{cumene}{C_9H_{12}}$$

Reaction2:

$$\underset{propylene}{C_3H_6} + \underset{cumene}{C_9H_{12}} \rightarrow \underset{p-diisopropyl\ benzene}{C_{12}H_{18}}$$

Power law is used to define the kinetics.

The kinetics are calculated from the expression as below:

Kinetic factor = $k\ (T/T_0)^{\wedge n} * e^{(-E/R)(1/T - 1/T0)}$

The units of reaction rate are K mol/m^3sec.; the activation energy is in cal/mol.

Therefore, the values for the k and E are taken as

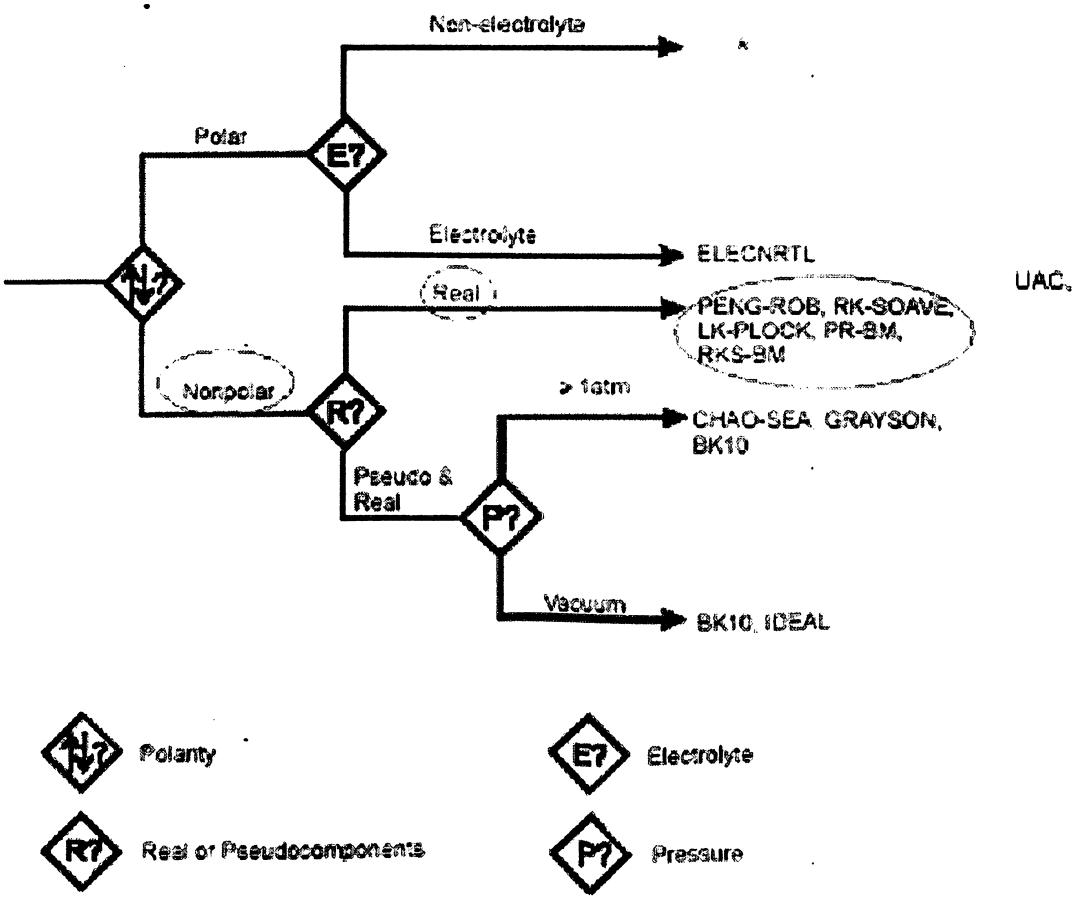
k = 3435431 and E = 24900 cal/mol (For Reaction # 1)

k =284871452 and E = 35080 cal/mol (For Reaction # 2).

THERMODYNAMIC PACKAGE PROPERTY METHOD SELECTION:

Choice of thermodynamic package is an important area of concern for a Simulation engineer. An incorrect choice would undermine the accuracy of model and hence the decisions based on the model could prove to be costly.

Thermodynamic Packages that can be used RK-SOAVE, PENG-ROB WILSON, NRTL,UNIQUAC.



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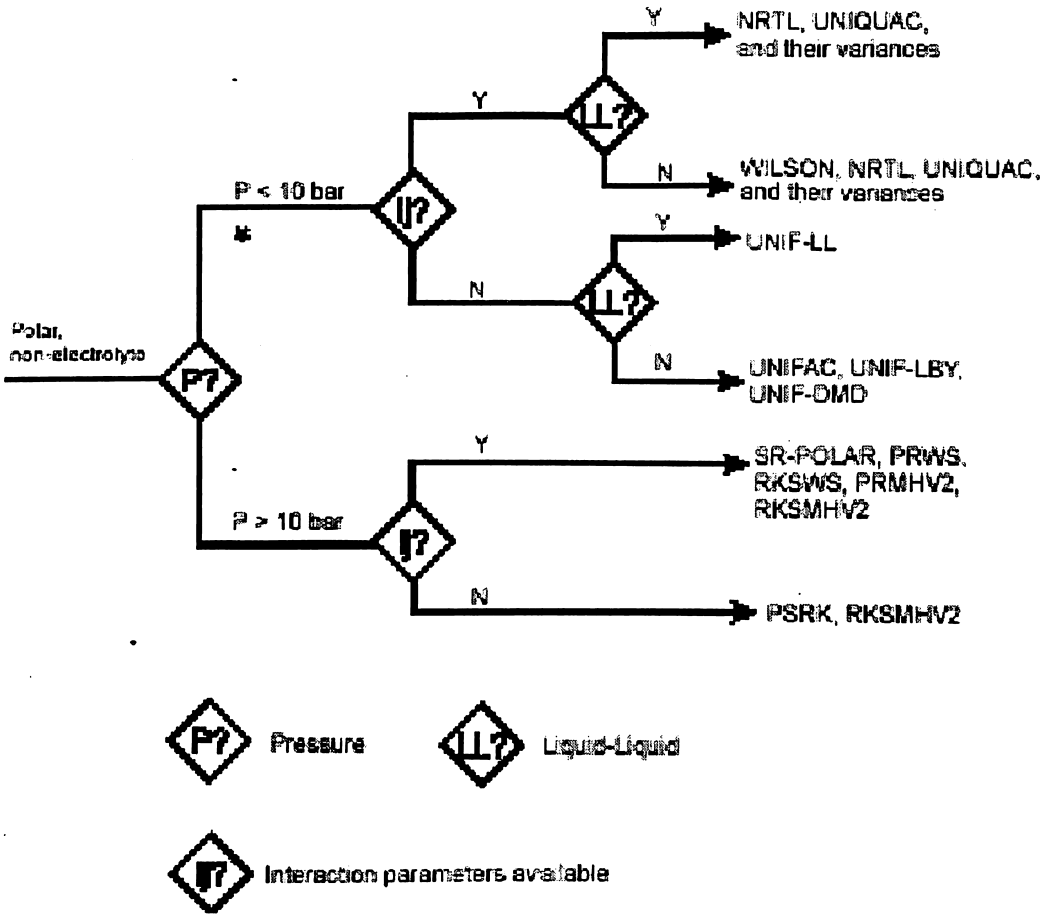
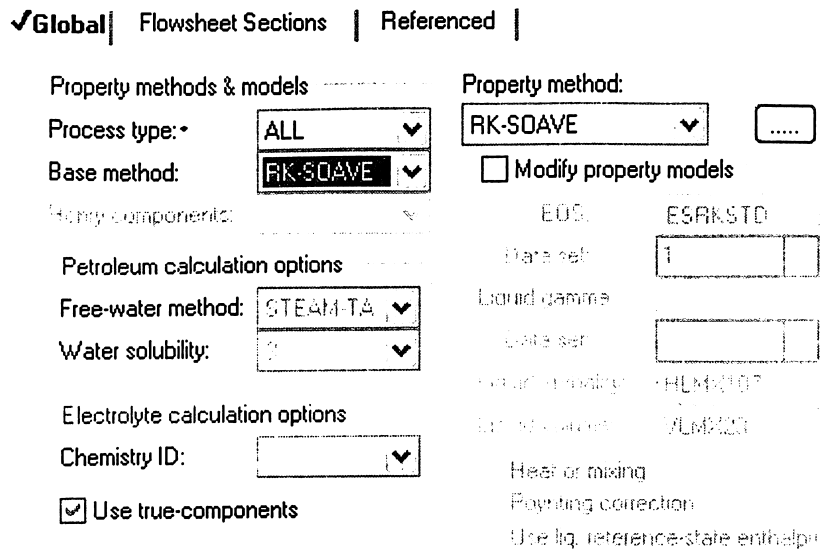
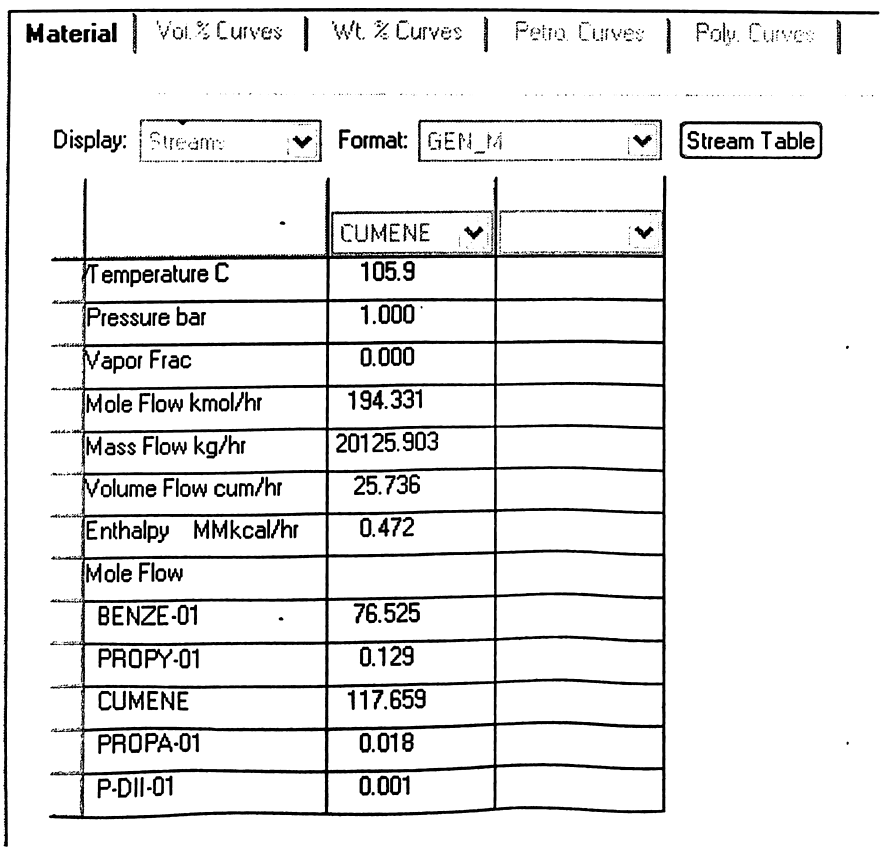

Polar,
non-electrolyte
P?
P < 10 bar
P > 10 bar
LL?
LL?
LL?
Y
N
Y
N
Y
N
NRTL, UNIQUAC,
and their variances
WILSON, NRTL, UNIQUAC,
and their variances
UNIF-LL
UNIFAC, UNIF-LBY,
UNIF-DMD
SR-POLAR, PRWS,
RKSWS, PRMHV2,
RKSMHV2
PSRK, RKSMHV2
Pressure
Liquid-Liquid
Interaction parameters available

RK-SOAVE Method:



Result for the RK-SOAVE Method:



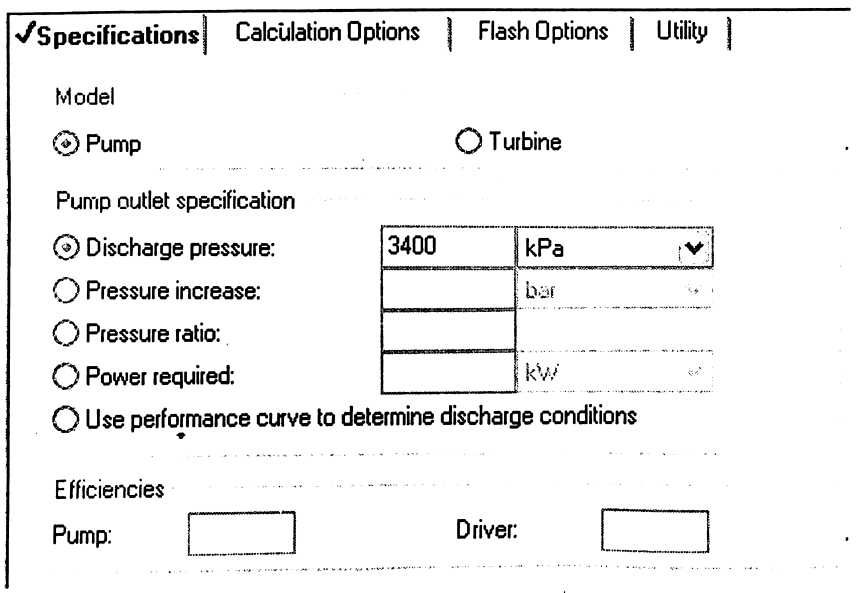
	CUMENE	
Temperature C	105.9	
Pressure bar	1.000	
Vapor Frac	0.000	
Mole Flow kmol/hr	194.331	
Mass Flow kg/hr	20125.903	
Volume Flow cum/hr	25.736	
Enthalpy MMkcal/hr	0.472	
Mole Flow		
BENZE-01	76.525	
PROPY-01	0.129	
CUMENE	117.659	
PROPA-01	0.018	
P-DII-01	0.001	

Final Result:

The reason to arrive in this conclusion is the component benzene, propylene and cumene are non-polar and real. Also with the help of user guide of Aspen, I have arrived to the the conclusion that by comparing results with selected thermo package, **RK-SOAVE showed better results and is also justified very clearly above.**

BASE CASE SIMULATION RESULTS:

Pump1 Input:



Pump 1 result:

Material

Display: Streams | Format: | Stream Table

	BEN-RECY	BEN[illegible]	[illegible]	
Temperature C	20.0	25.0	24.6	
Pressure bar	1.000	1.013	34.000	
Vapor Frac	0.000	0.000	0.000	
Mole Flow kmol/hr	227.921	210.000	437.921	
Mass Flow kg/hr	17200.025	16403.864	33603.889	
Volume Flow cum/hr	20.062	18.810	38.972	
Enthalpy MMkcal/hr	2.421	2.475	4.946	
Mole Flow				
BENZE-01	211.053	210.000	421.053	
PROPY-01	15.189		15.189	
CUMENE	0.009		0.009	
PROPA-01	1.670		1.670	
P-DII-01	TRACE		TRACE	

Pump2 Input:

✓**Specifications** | Calculation Options | Flash Options | Utility

Model

(•) Pump ( ) Turbine

Pump outlet specification

(•) Discharge pressure: 3400 kPa

( ) Pressure increase:

( ) Pressure ratio:

( ) Power required:

( ) Use performance curve to determine discharge conditions

Efficiencies

Pump: Driver:

Pump2 Results:

Material | Vol.% Curves | Petro. Curves

Display: Streams Format: Stream Table

Temperature C	25.0	23.3
Pressure bar	1166.000	34.000
Vapor Frac	0.000	0.000
Mole Flow kmol/hr	220.540	220.540
Mass Flow kg/hr	9301.712	9301.712
Volume Flow cum/hr	18.334	18.229
Enthalpy MMkcal/hr	0.164	-0.087
Mole Flow		
BENZE-01		
PROPY-01	210.000	210.000
CUMENE		
PROPA-01	10.540	10.540
P-DII-01		

Mixer Input:

Flash Options

Mixer specifications

Pressure: 0 bar

Valid phases: Vapor-Liquid

Temperature estimate

C

Convergence parameters

Maximum iterations: 30

Error tolerance: 0.0001

Mixer Result:

Material | Heat | Work | Vol.% Curves | Wt. % Curves | Petro. Curves | Poly. Curves

Display: Streams Format: GEN_M Stream Table

	P2OUT	P1OUT	M-OUT	
Temperature C	23.3	24.6	25.2	
Pressure bar	34.000	34.000	34.000	
Vapor Frac	0.000	0.000	0.000	
Mole Flow kmol/hr	220.540	437.921	658.461	
Mass Flow kg/hr	9301.712	33603.889	42905.601	
Volume Flow cum/hr	18.229	38.972	55.828	
Enthalpy MMkcal/hr	-0.087	4.946	4.859	
Mole Flow				
BENZE-01		421.053	421.053	
PROPY-01	210.000	15.189	225.189	
CUMENE		0.009	0.009	
PROPA-01	10.540	1.670	12.210	
P-DII-01		TRACE	TRACE	

ults

Heater Input:

✓Specifications | Flash Options | Utility

Flash specifications

Temperature	400	C
Pressure	3200	kPa

Valid phases

Vapor-Liquid

Heater Result:

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petro. Curves

Display: Streams Format: GEN_M Stream Table

	M-OUT	HEOUT	
Temperature C	25.2	400.0	
Pressure bar	34.000	32.000	
Vapor Frac	0.000	1.000	
Mole Flow kmol/hr	658.461	658.461	
Mass Flow kg/hr	42905.601	42905.601	
Volume Flow cum/hr	55.828	1068.522	
Enthalpy MMkcal/hr	4.859	15.811	
Mole Flow			
BENZE-01	421.053	421.053	
PROPY-01	225.189	225.189	
CUMENE	0.009	0.009	
PROPA-01	12.210	12.210	
P-DII-01	TRACE	TRACE	

Plug Flow Reactor Input:

Specifications:

✓Specifications | ✓Configuration | Streams | ✓Reactions | Pressure | Holdup | ✓Catalyst

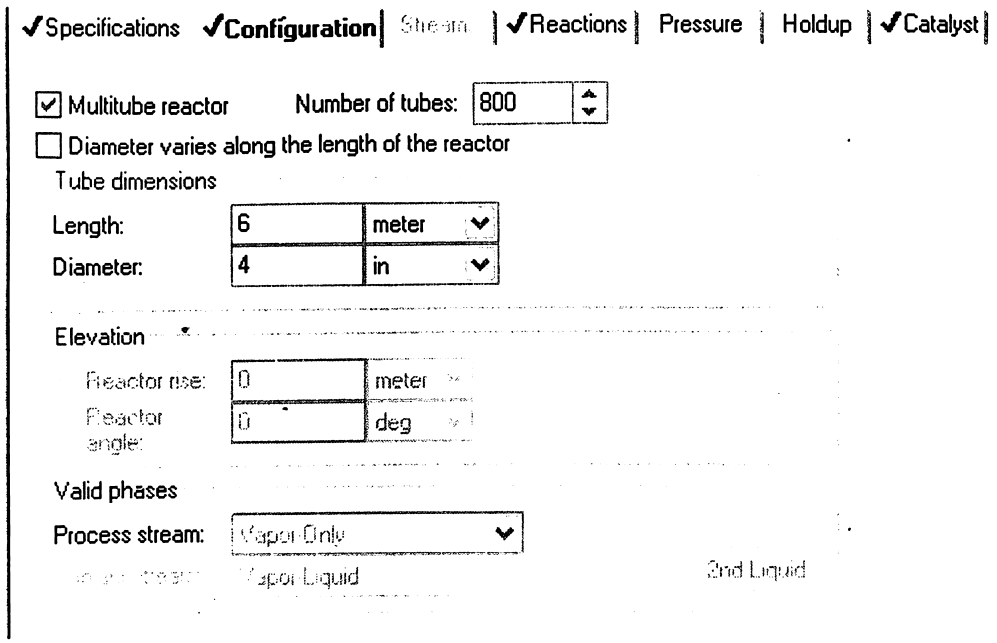
Reactor type: Reactor with specified temperature

Operating condition

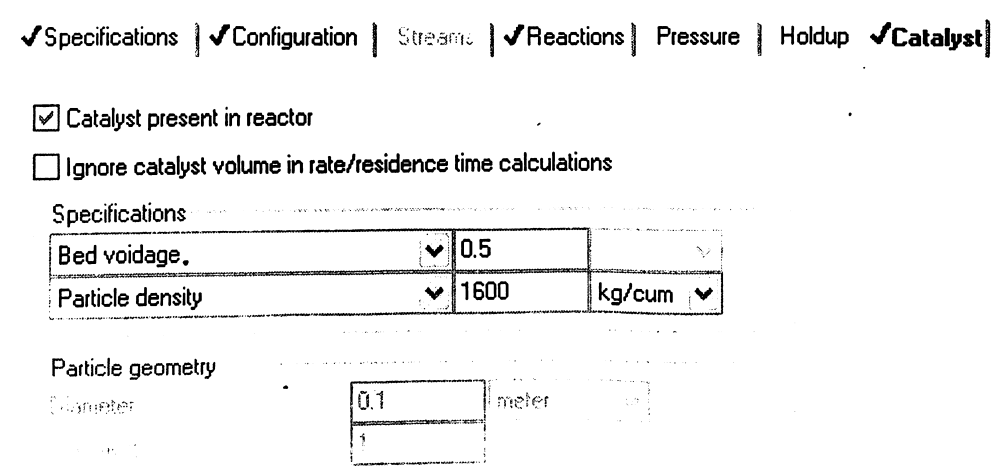
- (•) Constant at inlet temperature
- ( ) Constant at specified reactor temperature C
- ( ) Temperature profile

	Location	Temperature C
*		

Configuration:



Catalyst:



Plug Flow Reactor Results:

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petro Curves

Display: Streams Format: GEN_M Stream Table

	HEOUT	PFROUT	
Temperature C	400.0	400.0	
Pressure bar	32.000	32.000	
Vapor Frac	1.000	1.000	
Mole Flow kmol/hr	658.461	534.601	
Mass Flow kg/hr	42905.601	42905.601	
Volume Flow cum/hr	1068.522	824.474	
Enthalpy MMkcal/hr	15.811	12.882	
Mole Flow			
BENZE-01	421.053	298.104	
PROPY-01	225.189	101.329	
CUMENE	0.009	122.047	
PROPA-01	12.210	12.210	
P-DII-01	TRACE	0.911	

Cooler Input:

✓Specifications | Flash Options | Utility

Flash specifications

Temperature	120	C
Pressure	1	atm

Valid phases

Vapor-Liquid

Cooler Result:

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petro. Curves

Display: Streams Format: GEN_M Stream Table

	PFROUT	COOLOUT	
Temperature C	400.0	120.0	
Pressure bar	32.000	1.013	
Vapor Frac	1.000	1.000	
Mole Flow kmol/hr	534.601	534.601	
Mass Flow kg/hr	42905.601	42905.601	
Volume Flow cum/hr	824.474	16872.253	
Enthalpy MMkcal/hr	12.882	7.488	
Mole Flow			
BENZE-01	298.104	298.104	
PROPY-01	101.329	101.329	
CUMENE	122.047	122.047	
PROPA-01	12.210	12.210	
P-DII-01	0.911	0.911	

Flash Column Input:

✓Specifications | Flash Options | Entrainment | Utility

Flash specifications

Temperature	20	C
Pressure	1	bar

Valid phases

Vapor-Liquid

Flash Column Result:

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petro Curves | Poly Curves

Display: Streams Format: GEN_M Stream Table

	RAD1-TOP	FLUEGAS	BEN-RECY	
Temperature C	-25.6	20.0	20.0	
Pressure bar	1.000	1.000	1.000	
Vapor Frac	0.000	1.000	0.000	
Mole Flow kmol/hr	334.723	106.802	227.921	
Mass Flow kg/hr	22085.505	4885.481	17200.025	
Volume Flow cum/hr	26.695	2559.327	20.062	
Enthalpy MMkcal/hr	1.914	0.344	2.421	
Mole Flow				
BENZE-01	221.321	10.268	211.053	
PROPY-01	101.200	86.012	15.189	
CUMENE	0.009	< 0.001	0.009	
PROPA-01	12.192	10.522	1.670	
P-DII-01	TRACE	TRACE	TRACE	

Rad Frac1 Input:

✓Configuration | ✓Streams | ✓Pressure | ✓Condenser | ✓Reboiler | 3-Phase

Setup options

Calculation type: Equilibrium

Number of stages: 10

Condenser: Total

Reboiler: Kettle

Valid phases: Vapor-Liquid

Convergence: Standard

Operating specifications

Reflux ratio	Mole	0.8
Distillate to feed ratio	Mole	0.62611664

Free water reflux ratio:

Feed basis

Rad Frac1Result:

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petro. Curves | Poly Curves

Display: Streams Format: GEN_M Stream Table

	COOLOUT	RAD1-TOP	RAD1-BOT	
Temperature C	120.0	-25.6	106.7	
Pressure bar	1.013	1.000	1.000	
Vapor Frac	1.000	0.000	0.000	
Mole Flow kmol/hr	534.601	334.723	199.878	
Mass Flow kg/hr	42905.601	22085.505	20820.093	
Volume Flow cum/hr	16872.253	26.695	26.647	
Enthalpy MMkcal/hr	7.488	1.914	0.437	
Mole Flow				
BENZE-01	298.104	221.321	76.783	
PROPY-01	101.329	101.200	0.129	
CUMENE	122.047	0.009	122.038	
PROPA-01	12.210	12.192	0.018	
P-DII-01	0.911	TRACE	0.911	

Rad Frac2 Input:

✓Configuration | ✓Streams | ✓Pressure | ✓Condenser | ✓Reboiler | 3-Phase

Setup options

Calculation type: Equilibrium

Number of stages: 11

Condenser: Total

Reboiler: Kettle

Valid phases: Vapor-Liquid

Convergence: Standard

Operating specifications

Reflux ratio	Mole	0.8
Distillate to feed ratio	Mole	0.97224722
Boilup ratio		

Feed basis

Rad Frac2 Result:

Material | Heat | Vol% Curves | Wt% Curves | Petro Characterization | Pay Curves

Display: Streams Format: GEN_M Stream Table

	RAD1-BUT	CUMENE	DIP	
Temperature C	106.7	105.9	148.7	
Pressure bar	1.000	1.000	1.000	
Vapor Frac	0.000	0.000	0.000	
Mole Flow kmol/hr	199.878	194.331	5.547	
Mass Flow kg/hr	20820.093	20125.903	694.190	
Volume Flow cum/hr	26.647	25.736	0.930	
Enthalpy MMkcal/hr	0.437	0.472	-0.028	
Mole Flow				
BENZE-01	76.783	76.525	0.258	
PROPY-01	0.129	0.129	< 0.001	
CUMENE	122.038	117.659	4.379	
PROPA-01	0.018	0.018	TRACE	
P-DII-01	0.911	0.001	0.910	

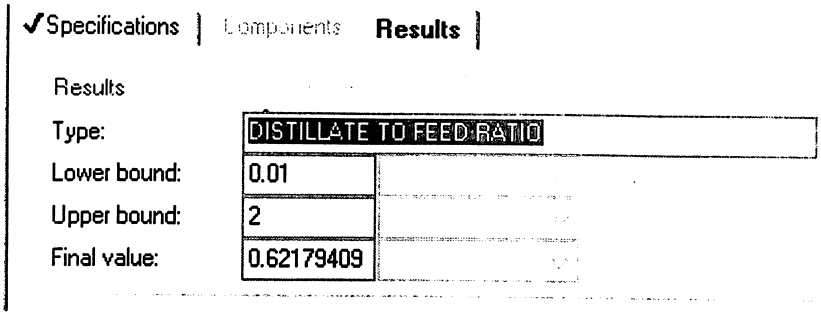
CUMENE

DESIGN SPECIFICATIONS:

In using this option, we have to define two variables, one is DEFINE variable and the other is VARY variable. We have to check how the DEFINED variable varies if the VARY variable is changed.

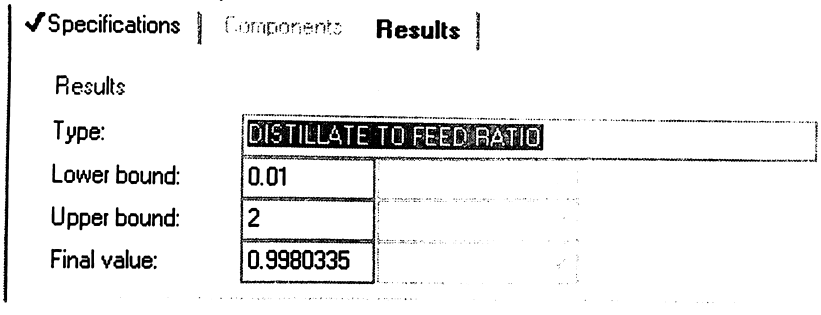
Rad Frac1:

Here mole recovery of Cumene in the top stream and DIP in the bottom stream is DEFINED variables. Distillate to Feed ratio is VARY variables in the rad frac column1.



Rad Frac2:

Here mole recovery of Cumene in the top stream and DIP in the bottom stream is DEFINED variables. Distillate to Feed ratio is VARY variables in the rad frac column2.



SENSITIVITY ANALYSIS:

1. Sensitivity analysis was performed for the **Rad Frac1**

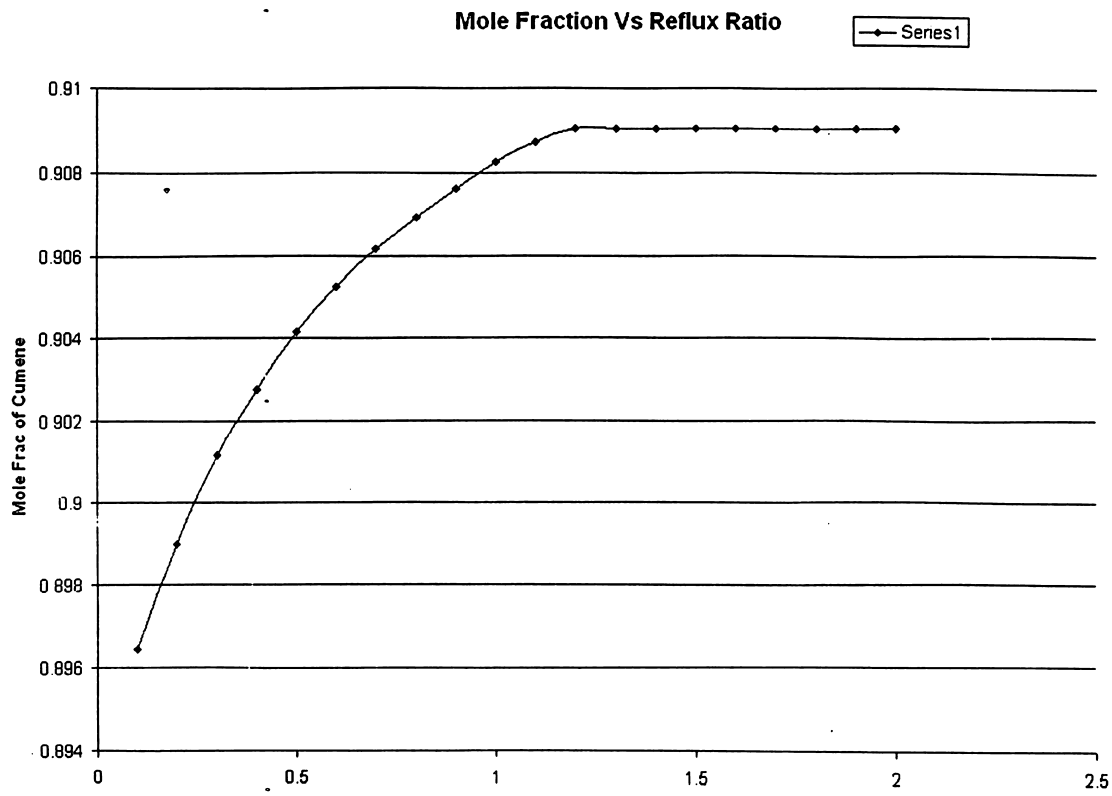
A sensitivity study between reflux ratio and mole recovery of cumene in bottoms of distillation column, gives the optimum reflux ratio required for maximum flow of cumene in bottoms.

In this sensitivity study we can know how a variable changes when the other parameters are changed. With this we can know at what point would be the maximum flow.

The results obtained by Sensitivity Analysis are plotted below.

Summary | Define Variable |

Row / Case	Status	VARY 1 RADFRAC1 COL-SPEC MOLE-RR	REFLU	SPEC
1	OK	0.1	0.1	0.89645195
2	OK	0.2	0.2	0.89899376
3	OK	0.3	0.3	0.90116824
4	OK	0.4	0.4	0.90274
5	OK	0.5	0.5	0.90412918
6	OK	0.6	0.6	0.90524098
7	OK	0.7	0.7	0.9061798
8	OK	0.8	0.8	0.90693025
9	OK	0.9	0.9	0.90760767
10	OK	1	1	0.90825395
11	OK	1.1	1.1	0.90871817
12	OK	1.2	1.2	0.90902757
13	OK	1.3	1.3	0.90904668
14	OK	1.4	1.4	0.90904841
15	OK	1.5	1.5	0.90904919
16	OK	1.6	1.6	0.90904966
17	OK	1.7	1.7	0.90905
18	OK	1.8	1.8	0.90905027
19	OK	1.9	1.9	0.90905049
20	OK	2	2	0.90905067



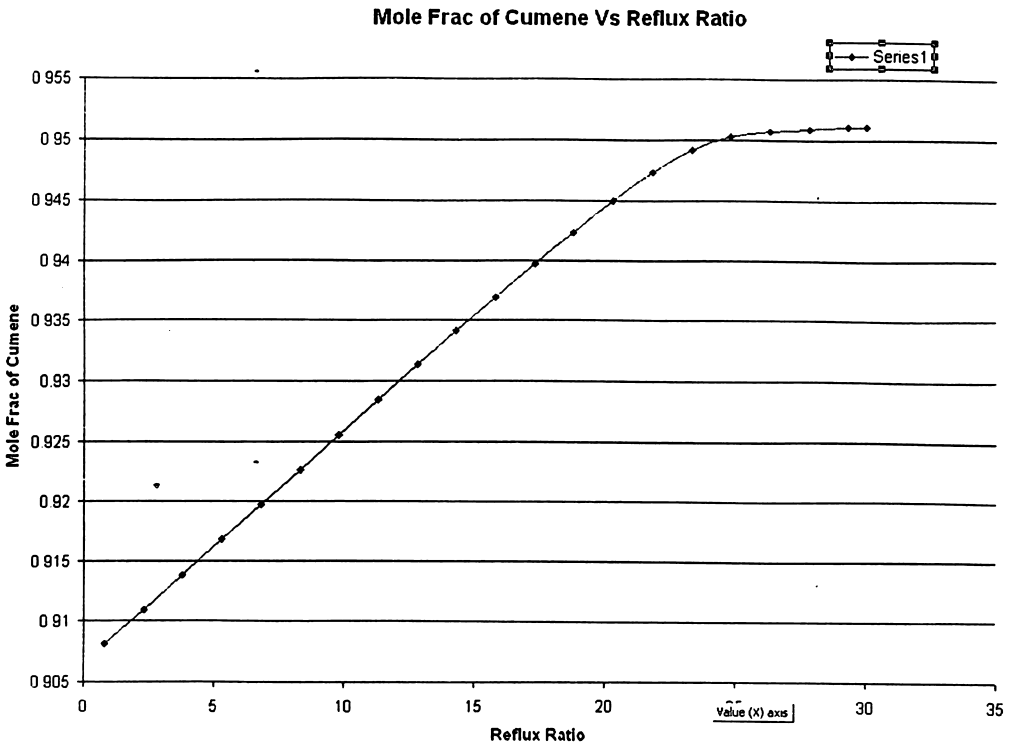
From the above graph the optimum reflux ratio for the rad frac 1 is found to be 1.25.

2. Sensitivity analysis was performed for the **Rad Frac2**

A sensitivity study between reflux ratio and mole recovery of cumene in top of distillation column, gives the optimum reflux ratio required for maximum flow of cumene in tops.

Summary | Define Variable |

Row / Case	Status	VARY 1 RADFRAC2 COL-SPEC MOLE-RR	REFLUX	SPEC
1	OK	0.8	0.8	0.90807059
2	OK	2.3	2.3	0.91090613
3	OK	3.8	3.8	0.91383671
4	OK	5.3	5.3	0.916774
5	OK	6.8	6.8	0.91971142
6	OK	8.3	8.3	0.9226359
7	OK	9.8	9.8	0.92554475
8	OK	11.3	11.3	0.92843541
9	OK	12.8	12.8	0.9313052
10	OK	14.3	14.3	0.93414909
11	OK	15.8	15.8	0.93696101
12	OK	17.3	17.3	0.93972944
13	OK	18.8	18.8	0.94243173
14	OK	20.3	20.3	0.94501866
15	OK	21.8	21.8	0.94736843
16	OK	23.3	23.3	0.94920496
17	OK	24.8	24.8	0.9502579
18	OK	26.3	26.3	0.95073325
19	OK	27.8	27.8	0.95095733
20	OK	29.3	29.3	0.9510787
21	OK	30	30	0.95111666



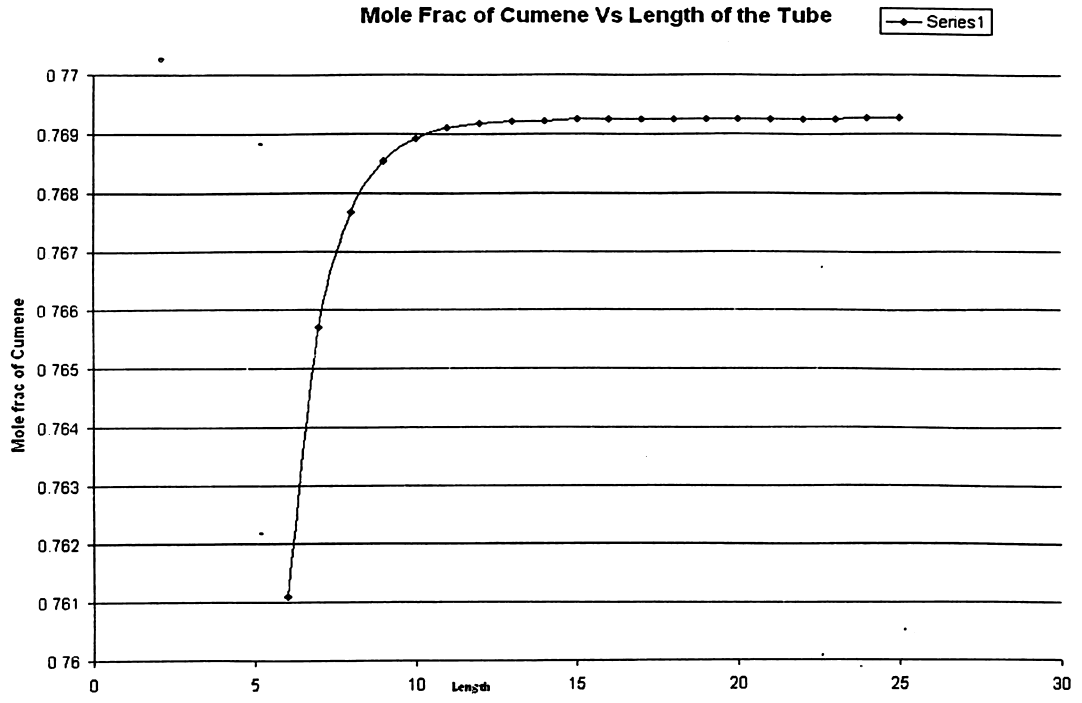
From the above graph the optimum reflux ratio for the rad frac 2 is found to be 26.

3. Sensitivity analysis was performed for the **Plug Flow Reactor.**

A sensitivity study between length of the tube and mole recovery of cumene in the PFR out stream, gives the optimum Length of the tube required for maximum flow of cumene from the PFR out.

Summary | Define Variable |

	Row / Case	Status	VARY 1 PFR PARAM LENGTH METER	LENGTH METER	SPEC
▶	1	OK	6	6	0.76108747
	2	OK	7	7	0.76570766
	3	OK	8	8	0.76768131
	4	OK	9	9	0.76855157
	5	OK	10	10	0.76892976
	6	OK	11	11	0.76910536
	7	OK	12	12	0.76918094
	8	OK	13	13	0.76921226
	9	OK	14	14	0.76922139
	10	OK	15	15	0.76925097
	11	OK	16	16	0.76926331
	12	OK	17	17	0.76926331
	13	OK	18	18	0.76926123
	14	OK	19	19	0.76925945
	15	OK	20	20	0.76925869
	16	OK	21	21	0.7692588
	17	OK	22	22	0.76926101
	18	OK	23	23	0.76926487
	19	OK	24	24	0.76927728
	20	OK	25	25	0.76927943



From the above Graph the optimum length of the tube is found to be 15m.

Base case results before sensitivity

Material | Heat | Load | Work | Vol % Curves | Wt % Curves | Petro Curves | Poly Curves

Display: Preferred Format: GEN_M Stream Table

	HEOU	PFROU	[illegible]	[illegible]	[illegible]	[illegible]	DIP
Temperature C	400.0	400.0	120.0	-25.6	106.7	105.9	148.7
Pressure bar	32.000	32.000	1.013	1.000	1.000	1.000	1.000
Vapor Frac	1.000	1.000	1.000	0.000	0.000	0.000	0.000
Mole Flow kmol/hr	658.461	534.601	534.601	334.723	199.878	194.331	5.547
Mass Flow kg/hr	42905.601	42905.601	42905.601	22085.505	20820.093	20125.903	694.190
Volume Flow cum/hr	1068.522	824.474	16872.253	26.695	26.647	25.736	0.930
Enthalpy MMkcal/hr	15.811	12.882	7.488	1.914	0.437	0.472	-0.028
Mole Flow kmol/hr							
BENZE-01	421.053	298.104	298.104	221.321	76.783	76.525	0.258
PROPY-01	225.189	101.329	101.329	101.200	0.129	0.129	< 0.001
CUMENE	0.009	122.047	122.047	0.009	122.038	117.659	4.379
PROPA-01	12.210	12.210	12.210	12.192	0.018	0.018	TRACE
P-DII-01	TRACE	0.911	0.911	TRACE	0.911	0.001	0.910

Base case results after sensitivity

Material | Heat | Balance | Vapor | Vol% Curves | Wt% Curves | Petro Curves | Plug Curves

Display: Streams | Format: GEN_M | Stream Table

	HEOUT	FFROUT	COOLOUT	R-DISTOP	RADFEED	CUMENE	DIP	
Temperature C	400.0	400.0	120.0	-1.7	141.2	140.7	164.9	
Pressure bar	32.000	32.000	1.013	1.000	1.000	1.000	1.000	
Vapor Frac	1.000	1.000	0.923	0.000	0.000	0.000	0.000	
Mole Flow kmol/hr	749.931	554.507	554.507	347.185	207.321	201.567	5.754	
Mass Flow kg/hr	49845.587	49845.587	49845.587	25427.385	24418.147	23640.730	777.418	
Volume Flow cum/hr	1211.221	816.668	16079.299	29.578	32.446	31.395	1.058	
Enthalpy MMkcal/hr	18.333	13.686	7.108	2.731	-0.461	-0.409	-0.049	
Mole Flow kmol/hr								
BENZE-01	506.427	313.046	313.046	299.106	13.940	13.937	0.003	
PROPY-01	223.901	28.477	28.477	28.477	TRACE	TRACE	TRACE	
CUMENE	0.006	191.344	191.344	0.006	191.338	187.630	3.708	
PROPA-01	19.597	19.597	19.597	19.595	TRACE	TRACE	TRACE	
P-DII-01	TRACE	2.043	2.043	TRACE	2.043	< 0.001	2.043	

After comparing the results before sensitivity and after sensitivity the mole fraction of cumene is increased from **96.04%** to **98%**.

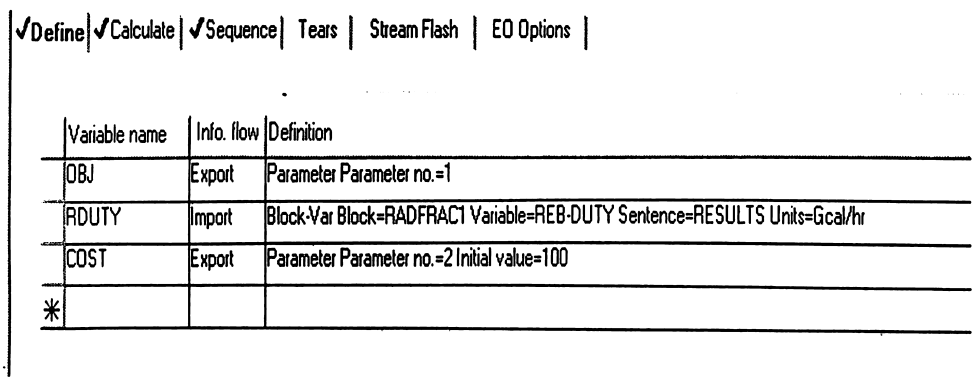
OPTIMIZATION

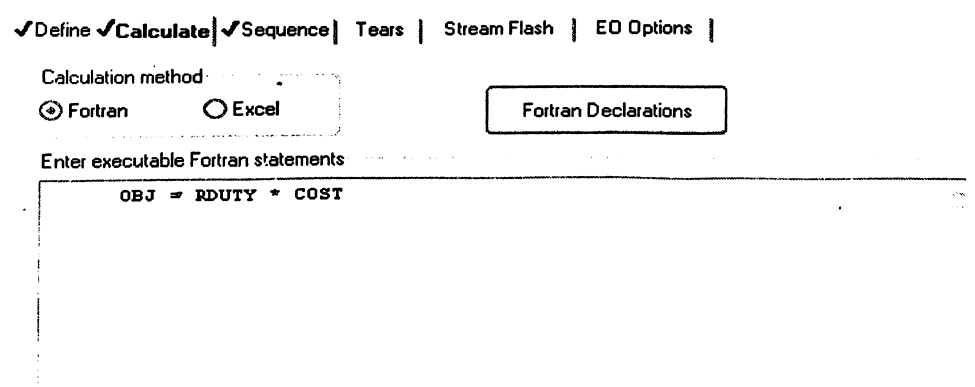
Optimization is done to decrease the re-boiler duty of the rad farc1 in order to decrease the operating cost.

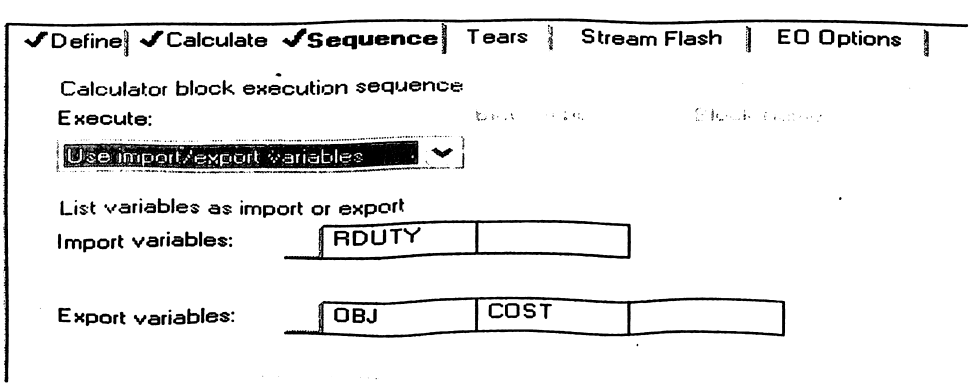
The Objective function is defined as product of re-boiler duty and cost.

So, as the re-boiler duty is minimized the objective function is also minimized and the cost is also reduced.

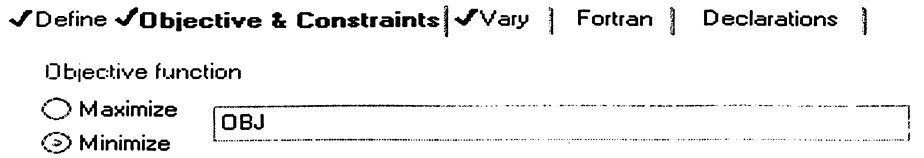
Calculator Operation:

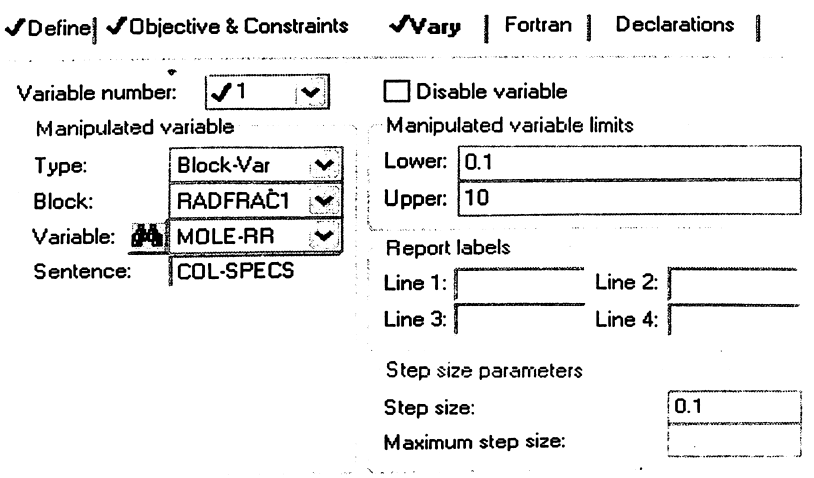




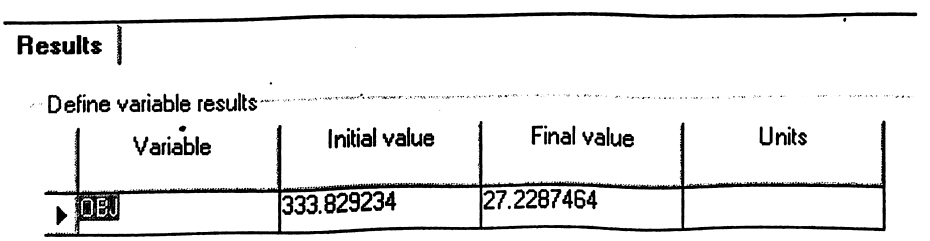


Optimization Input:





Optimization Result:



COST ESTIMATION:

The advantage of using the calculator option is that we can do all the mathematical operations of any number of variables from our flow sheet. By using this I have found out the total profit of the plant

The cost for the different reactants and products taken into consideration are:

Benzene: 11.75Rs/kg.

Propylene: 1.4Rs/kg.

Cumene: 27.73Rs/kg.

Heat duty = 42.3 Gcal/hr.

Cost of the power= 94KW.

Here all variables which are used in the calculator are defined.

✓Define | ✓Calculate | ✓Sequence | Tears | Stream Flash | EO Options |

	Variable name	Info. flow	Definition
	BENZ	Import	Mass-Flow Stream=BENZ Substream=MIXED Component=BENZENE Units=kg/hr
	PROPY	Import	Mass-Flow Stream=PROPY Substream=MIXED Component=PROPYLEN Units=kg/hr
	P1	Import	Block-Var Block=PUMP1 Variable=BRAKE-POWER Sentence=RESULTS Units=kW
	P2	Import	Block-Var Block=PUMP2 Variable=BRAKE-POWER Sentence=RESULTS Units=kW
	HDUTY	Import	Block-Var Block=HEATER Variable=QCALC Sentence=PARAM Units=Gcal/hr
	CDUTY	Import	Block-Var Block=COOLER Variable=QCALC Sentence=PARAM Units=Gcal/hr
	R1COND	Import	Block-Var Block=RADFRAC1 Variable=COND-DUTY Sentence=RESULTS Units=Gcal/hr
	R1REBO	Import	Block-Var Block=RADFRAC1 Variable=REB-DUTY Sentence=RESULTS Units=Gcal/hr
	R2COND	Import	Block-Var Block=RADFRAC2 Variable=COND-DUTY Sentence=RESULTS Units=Gcal/hr
	R2REBO	Import	Block-Var Block=RADFRAC2 Variable=REB-DUTY Sentence=RESULTS Units=Gcal/hr
	FLASH	Import	Block-Var Block=FLASH Variable=NET-DUTY Sentence=PARAM Units=Gcal/hr
	CUMENE	Export	Mass-Flow Stream=CUMENE Substream=MIXED Component=CUMENE Units=kg/hr
	PROF	Export	Parameter Parameter no.=1 Physical type=Unit-Price Units=$/kg
	SP	Export	Parameter Parameter no.=2 Physical type=Unit-Price Units=$/kg
	CP	Export	Parameter Parameter no.=3 Physical type=Unit-Price Units=$/kg
	FEEDCO	Export	Parameter Parameter no.=4 Physical type=Unit-Price Units=$/kg
	TDUTY	Export	Parameter Parameter no.=5 Physical type=Unit-Price Units=$/kg
	PUMPCO	Export	Parameter Parameter no.=6 Physical type=Unit-Price Units=$/kg
*			

✓Define | ✓Calculate | ✓Sequence | Tears | Stream Flash | EO Options |

Calculator block execution sequence

Execute: Block type: Block name:

Use import/export variables

List variables as import or export

Import variables:	BENZ	PROPY	P1	P2	HDUTY	CDUTY	R1COND	R1REBO	R2COND	R2REBO	FLASH	

Export variables:	CUMENE	SP	PROF	CP	FEEDCO	TDUTY	PUMPCO	

Profit Results:

Summary **Define Variable**

Define variable results

Variable	Value read	Value written	Units
BENZ	16403.8644		KG/HR
PROPY	8836.9344		KG/HR
P1	73.7156093		KW
P2	-292.36005		KW
HDUTY	13.4458217		GCAL/HR
CDUTY	-8.3563649		GCAL/HR
R1COND	-4.3257685		GCAL/HR
R1REBO	0.27228746		GCAL/HR
R2COND	-52.592992		GCAL/HR
R2REBO	52.6110993		GCAL/HR
FLASH	0.46134798		GCAL/HR
CUMENE	20708.2801	20708.2801	KG/HR
PROF	3326.77683	3326.77683	$/KG
SP	12217.8846	12217.8853	$/KG
CP	7826.17945	7826.11743	$/KG
FEEDCO	7812.47855	7812.47855	$/KG
TDUTY	13.7009057	13.6388799	$/KG
PUMPCO	0	0	$/KG

The profit is calculated taking into account the amount of cumene produced, amount of benzene, propylene, expenditure due to energy and the cost of power.

The expressions are given as input to the calculator and profit is estimated.

Profit obtained is 156322.67 Rs/hr.

CONCLUSION:

The simulation of a plant manufacturing Cumene has been successfully carried out. The main introduction of the product is explained such as its properties and uses. Base case results are shown and the base case flow sheet involves units such as reactor, columns, flash column, mixer which are successfully simulated. Also cases for design spec, sensitivity are presented and the optimum values are determined from the sensitivity. A suitable thermodynamic package is considered for the simulation of the plant and justified it by comparing the results with other methods. Optimization is done in order to minimize the objective function. Costs are calculated using calculator and the profit is determined. This project truly helps us to understand and implement the concepts of Aspen Plus.

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