PROCESS SIMULATION AND OPTIMIZATION OF CYCLOHEXANE MANUFACTURING PLANT USING UniSim AND HINT.

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ABSTRACT: The Energy crisis and Low production rate are the important parameters in industrial operations. In this point, the simulation and optimisation of plant is highly desirable. This study shows the simulation of cyclohexane manufacturing plant. Cyclohexane is mainly used as an intermediate chemical compound for the production of adipic acid. It prepared by the hydrogenation reaction of benzene at elevated temperature and pressure. Honeywell's UniSim software R470 was used for the simulation and optimization processes and the fluid package employed was PRSV. Heat exchanger network design for pinch method has been carried out using HINT educational software. Pinch technology is used for Energy and Cost optimisation. This study reveals with all the stages of the design, which include cost targeting, area targeting, utility selection and heat exchanger network designing (HEN). The results of the base and optimized cases were compared and analysed. It has been shown that the developed UniSim model of this work can be used to represent, simulate and optimize a cyclohexane stabilization system successfully. This simulation helps engineers to create steady-state plant design, performance monitoring and troubleshooting.

Key words: Cyclohexane, Hydrogenation, Simulation, UNISIM, HINT.

1. INTRODUCTION

Process simulation is a model based representation of different processes like chemical, physical, biological, and other technical and unit operations in software [Rhodes C.L, 1996]. Using the knowledge of chemical and physical properties of pure components and mixtures, of reactions, and of mathematical models, allow the calculation of a processes in computers. In process simulation software, the unit operations are connected by product or

product streams as process flow diagrams. The ultimate intension of process simulation is optimization required process. [UniSim training Guide, 2009]. Process simulation always use different models which introduce approximations and assumptions but allow the description of a property over a wide range of temperatures and pressures which might not be covered by real data. Models also allow interpolation and extrapolation- within certain limits- and enable the search for conditions outside the range of known properties [M. Edwin1et al., 2017].

All industries need huge amount of energy for the safe running of operations. The amount of energy required depends on operations carrying out in the industries, size of the plant etc. the main concern about the energy is the cost [Jacobson et al. 2010]. The cost of energy increasing dramatically. The rapid increasing trend is expected to continue. The large amount of energy requirement and the cost is become major concern to chemical engineers. The optimisation of energy consumption and energy sources need attention and skilled engineers [Linnhoff, B et al., 1978]. Pinch analysis is the best-known technique used for finding the maximum efficiency condition of particular plant. In this work the steady state simulation of the plant is done in UniSim design software and the pinch analysis is carried out using hint software [Zamora et al., 1997].

The main objective of a chemical and refining industry is to produce products with precise quality values and at minimal costs. It is necessary to use modelling, simulation, and optimization tools to satisfy these goals [UniSim training Guide, 2009]. A chemical simulator is defined as an instrument that solves a complex chemical problem [Marsh K et al., 1994]. we can solve the problems like Thermodynamic models of the calculation of liquid-vapour equilibrium, Components database, which contains the needed values for the calculation of physical Properties starting from the thermodynamic models, Mathematical model components of the main operating units, Flow sheet section that calculates mass balances, energy balances, liquid-vapours [Sokolowski, J.A et al., 2009]

Steady state analysis determines the operating behaviour of the system at a specific point or under steady state conditions [Gagniuc et al., 2017]. The results that are obtained from this type of analysis are instantaneous values of the system a few hours, or even a few minutes, later in time [Linnhoff, B et al., 1978]. Initially process simulation was used to simulate steady state processes and then which is extended to dynamic simulation. Steady-state models perform a

mass and energy balance of a stationary process (a process in an equilibrium state) it does not depend on time.

In this study, The Simulation of cyclohexane production unit is carried out by using UniSim design software R470. Honeywell's UniSim design software is a tool for design, optimize and operating of a chemical process [C. Patrascioiu et al., 2018]. Importance of this study is, Cyclohexane (C_6H_{12}) is an important intermediate compound for the production of adipic acid and caprolactam is the prior raw material of Nylon preparation [Campbell et al., 2011]. The commercial demand for nylon as fibre in increasing day by day. Aromatic recovery reduces the aromatic content in fuel oil which can cause toxic effect while burning [A. A. Gaile et al., 2004]. This study focusing on the Model and Simulation of Cyclohexane production plant, Optimize the process conditions, Energy and Cost.

2. MATERIALS AND METHODS

2.1. MATERIALS:

2.1.1. HONEYWELL UNISIM DESIGN SOFTWARE R 470

Simulation of cyclohexane production unit is carried out by using UniSim design software R470, provides a tool for design, optimize and operating of a chemical process [Michael Pearson et al.]. The main objective of a chemical and refining industry is to produce products with precise quality values and at minimal costs. It is necessary to use modelling, simulation, and optimization tools to satisfy these goals.

2.1.2. HINT EDUCATIONAL SOFTWARE

Heat integration is a non-commercial software used for Heat Exchanger Network design for required problem. It is more complex at the same time more powerful software for the designing purpose. It also gives the insight of area and cost targeting [Igor Bulatov, 2013]. It is a well-known software for HEN designing. The Energy optimisation done by the method of heat exchanger network synthesis (HENS).

2.2. METHODOLOGY:

2.2.1. MANUFACTURIN OF CYCLOHEXANE:

Before going to simulate a plant, a proper plant study needed. This paper based on the cyclohexane manufacturing process from Benzene. The process is hydrogenation of Benzene at elevated temperature and pressure gives Cyclohexane [Hubner et al., 2017]. The hydrogenation

of benzene to cyclohexane has an importance in the chemical and petroleum industry, due to its application in the synthesis of many useful chemical intermediates [Hongli Liu et al., 2015]. For this first a detailed plant study needed. First of all we have to understand the process of separation of Benzene from Naphtha. The plant is called aromatics (Benzene, Toluene etc) recovery unit.

PLANT STUDY: AROMATIC RECOVERY UNIT

The Aromatic Recovery Unit can be divided into different section for easy description. ARU (Aromatic Recovery Unit) feed section, Extraction section, Extract stripping section, Solvent recovery section, Clay treatment section (CTS), Benzene section, Toluene section. In this ARU to CTS section is generally known as Extraction section and Benzene and Toluene is known as Fractionation section. The process sequence, arrangement of process equipment with major control schemes for extraction and aromatics fractionation section are shown in P & I diagrams. Fig.1 shows the schematic diagram for aromatic recovery unit. In the diagram ZV01, ZV03, ZV04, ZV07 and ZV08 represents extraction column, extract stripper, solvent recovery column, benzene fractionation column and toluene fractionation column respectively.

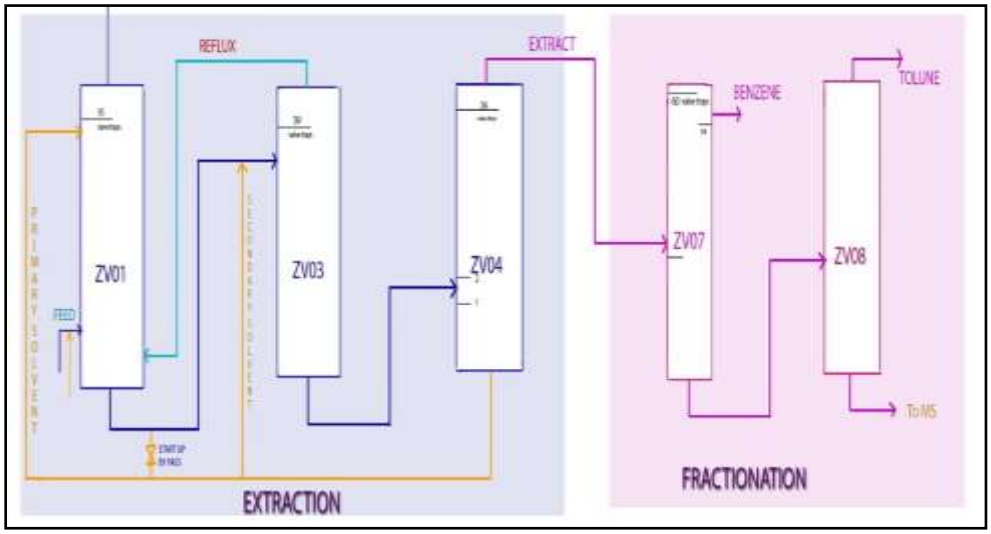

Fig.1. The process sequence of extraction and aromatics fractionation section

EXTRACTION SECTION

Aromatics are extracted from stabilized C3 + reformate by liquid-liquid exchange with sulfolane solvent in the extraction column at a suitable temperature to obtain optimum solubility and selectively for aromatics. The extract phase, composed of aromatic-rich solvent is withdrawn

from the bottom of the extraction column and introduced into the extract stripper, which strips the extract of dissolved non-aromatics (extractive distillation). The stripper overhead vapours composing of aromatics is condensed and taken out. The stripped extract from extract stripper is introduced into the solvent recovery column where aromatics are distilled overhead from the higher boiling solvent in vacuum to prevent degradation of solvent. The high purity aromatics is sent to the charge day tank and used as the fractionation section feed. The aromatics free solvent from the bottom of solvent recovery column is sent back to the extraction column.

FRACTIONATION SECTION

Pure extract from the charge day tank is pumped to the clay towers or clay treater where it contacts activated clay, whereby the unsaturated (olefins) get absorbed enabling benzene and toluene to meet colour specification. The extract after absorption is fed to the benzene column where benzene and toluene-rich stream gets fractionated. Benzene column operates under total reflux and product benzene is taken off as a side stream. Saturates, if any, in the overhead are returned to the extraction section/slop/gasoline as drag. Toluene-rich stream from the bottom of benzene column is again fractionated in the toluene column, where we get toluene as the overhead product. Toluene column, bottom containing mainly xylene are routed to the gasoline pool/mixed aromatic solvent tank.

MANUFACTURING PROCESS:

Cyclohexane manufactured by the hydrogenation reaction of benzene at elevated temperature and pressure. The hydrogenation reaction is an exothermic reaction. Vapour phase Equilibrium reaction that take place on the surface of the catalyst (0.3 wt% Pt on Al2O3) at a pressure of about 31 Kg/cm2 absolute and at a temperature from 350-400 deg. The heat of reaction is removed by circulating thermal oil around the reactor tubes.

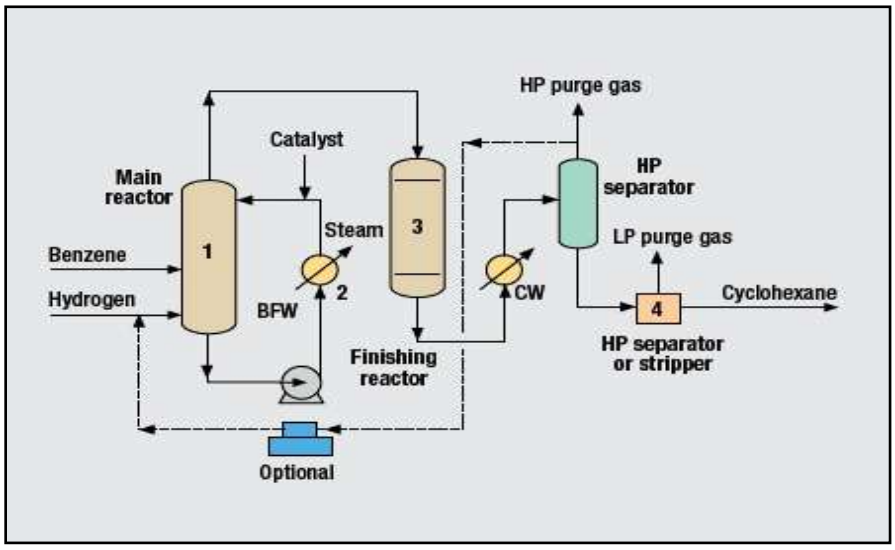

Fig.2.Plant overview of cyclohexane Manufacturing.

Benzene is supplied to a benzene evaporator in which benzene is injected into the evaporator via distributed plate supplied with nozzle. The benzene flow determines the load of benzene hydrogenation section and for 100% load benzene flow is 7.5 m3/hr. Pure hydrogen is passed through the benzene evaporator in order to lower the evaporation temperature of benzene. The heat required for benzene evaporation in order to lower the evaporation temperature of benzene.

The heat required for benzene evaporation is supplied by circulation of thermal oil coming out from the hydrogenation reactor around the tubes. The mixture of vapours of benzene and hydrogen coming out of the evaporator id then compressed to 30kgf/cm2 through a multi stage compression process is then finally fed to the hydrogenation reactor. Hydrogenation reactor is fixed bed tubular reactor. The hydrogenation of benzene into cyclohexane is an exothermic vapour phase equilibrium reaction of about 350-450^0 C. The hydrogenation catalyst consists of 0.3wt% Pt on Al_2O_3 tablets, the Pt being deposited as thin layer on the outside of these tablets. The hydrogenation reactor consists of 4m long tubes filled with catalyst. From the benzene evaporator, the mixture of benzene. Hydrogen and nitrogen was introduced at the top of the hydrogenation reactor. The hydrogenation reaction occurs in the tubes of the reactor as the reaction gas passes through the tubes. The efficiency of the hydrogenation reaction is very high about 99.9% and no by-products formed under proper reaction condition. Thermal oil circulated around the tubes of reactor sufficiently cooled down the reaction mixture to allow complete benzene conversion. The heat gained by thermal oil is utilized for evaporating the benzene feed stock in the benzene evaporator and also producing low pressure steam in the waste heat boiler.

Sulphur present in the benzene feed stock is a catalyst poison. In order to remove sulphur from the reaction gas mixture and from the reactor, it is passed through another after reactor of which the upper part contain a ZnO bed. The sulphur removal, the converted benzene will be hydrogenated to cyclohexane in the lower part reactor, which is supplied with affixed bed Pt on Al2O3 catalyst. After the completion of benzene hydrogenation, the cyclohexane is liquefied by condensation. Following this step, separation of cyclohexane and the reaction gas takes place. The liquid cyclohexane is transferred to the heptane distillation in order to remove n-heptane and other high boiling components. After the reaction, liquid cyclohexane is liquefied in a condenser and get separated in a separator from the gas mixture. Cyclohexane is collected in a buffer vessel after that. The cyclohexane transport is due to the difference in operating pressure of the separator (about 30Kg/cm2 abs) and the separating vessel (about 10Kg/cm2 abs). Before cyclohexane is fed into cyclohexane storage tank, the concentration of n-heptane and other higher boiling hydro carbon has to be reduced into a level acceptable for the preparation of caprolactam. n- Heptane and other high boing hydrocarbons are separated from the cyclohexane by fractional distillation in heptane column as the bottom product and pure cyclohexane which obtained as the top product is discharged to cyclohexane storage tank. Fig.2 represents the plant overview of cyclohexane manufacturing plant. The reaction is carried out in plug flow reactor. Two reactors are placed in series. In diagram 1 and 3 are the PFR in series. Cooler (no.3 in diagram) is place to remove the generated heat.

2.2.2. SELECTION OF THERMODYNAMIC MODEL

The first and the major step before beginning the simulation is the selection of thermodynamic model. UniSim design software provides different types of thermodynamic packages. Each package performs wide variety of physical property calculations, a particular temperature range, compounds etc. The property package used for cyclohexane production is PRSV. The PRSV model is a two- fold modification of Peng- Robinson equation of state [Al-Matar et al., 2015]. It has the potential to predict the behaviour of hydrocarbon system more accurately for system of dissimilar compounds [http://www.razifar.com/ description package].

2.2.3. BACKGROUND INFORMATION

Naphtha is selected as the starting material for the process. This contain various types of hydrocarbon. Components in the naphtha should be added before beginning the simulation. The composition of components may vary according to the source of crude [CDC- Pocket Guide to

Chemical Hazards]. The component list of naphtha and their composition is shown in the figure 3.

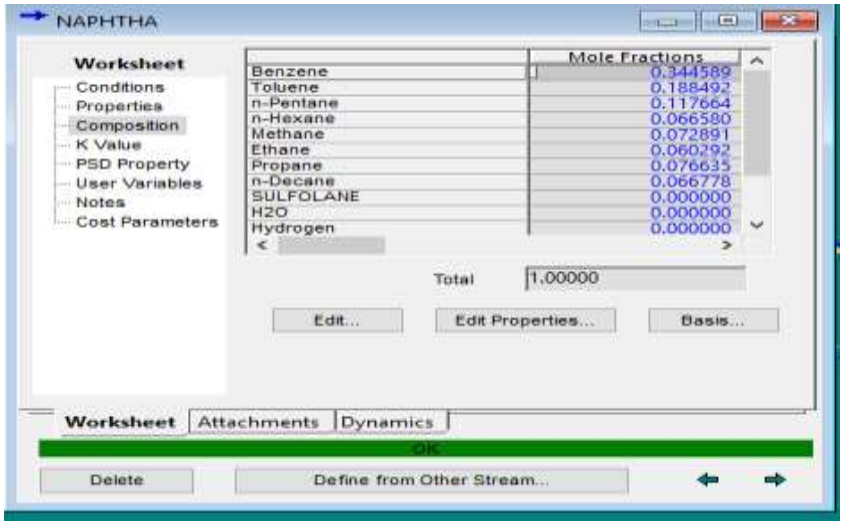

Fig.3-Composition of naphtha

2.2.4. PROCESS MODELLING AND STEADY STATE SIMULATION

Honeywell UniSim design software provide different predefines templates for columns and equipment. Which are available from object palette. Equipment specifications are important while simulating a plant. We can use arbitrary values or otherwise software provide default values. The specification for columns are given in table 1. The composition of various compounds from the columns after processing is given in table 2. 65% conversion is achieved in PFR by hydrogenation reaction of benzene. After purification the cyclohexane is separated from the un-reacted hydrogen and benzene. Cyclohexane composition obtained from the final operation is 0.99.

Table-1

EQUIPMENT	DIAMETER (m)	LENGTH / HEIGHT (m)	OPERATING PRESSURE [kPa]	TYPE OF VESSEL	NO. OF TRAYS
Extraction column	1.5	6.1	120	Tray	95
Extract stripper	1.372	6.1	190	Tray	39
SRC	1.372	6.1	323	Tray	34
Absorption column	1.372	6.1	485	Packed	-
Benzene column	1.372	6.1	470	Tray	60
Toluene column	1.372	6.1	442	Tray	35
PFR	0.0270	2.2	2200	-	-
Cyclohexane Column	1.372	6.1	600	Tray	45

Table 1. Main equipment specifications

Table 2. Main feed conditions & material and energy balance result from the simulation

Table-2

STREAMS		EXTRACT-OR FEED	ABSORPTION COLUMN	BENZENE COLUMN	PFR	CYCLOHEXANE COLUMN
Vapour fraction		0	0.6033	0	1	0
Flow rate [kmol/hr]		76.5	14.1	13.1	38.4	7.5
Temperature [°C]		70	115	118.5	776	100
Pressure [kPa]		101	199.5	489.8	3000	2950
Mole fraction	C_6H_6	.391519	.496921	.777305	0	0
	C_7H_8	.321862	.351951	.000539	.00023	.000721
	C_8H_{10}	.052457	.0666633	.104230	.04633	0
	CH_4	.000381	.0000484	.000757	.00033	0
	C_2H_6	.001472	.001870	.002925	.00130	0
	C_3H_8	.001472	.006580	.010292	.00457	0
	$C_{10}H_{22}$	.005180	.007753	0	0	0
	$C_6H_6O_2S$	0	0	0	0	0
	H_2O	0	0	0	0	0
	H_2	0	0	0	.55549	0
	s-rhombic	.004061	0	0	0	0
	C_6H_{12}	.004061	.001333	0	0	0
	C_6H_{14}	.009507	0	0	.34653	.99

Fig. 4 and 5 shows the steady state simulation of aromatic recovery unit and cyclohexane production plant respectively. Later plant is an extension of aromatic recovery plant.

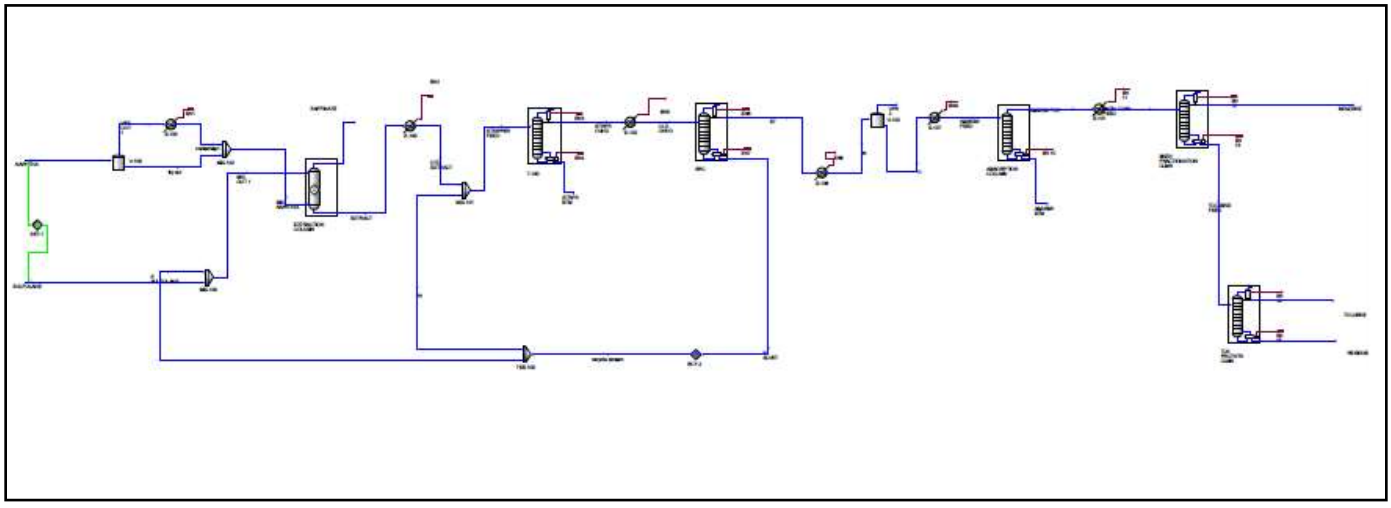

Fig. 4 Process flow diagram for aromatic recovery unit.

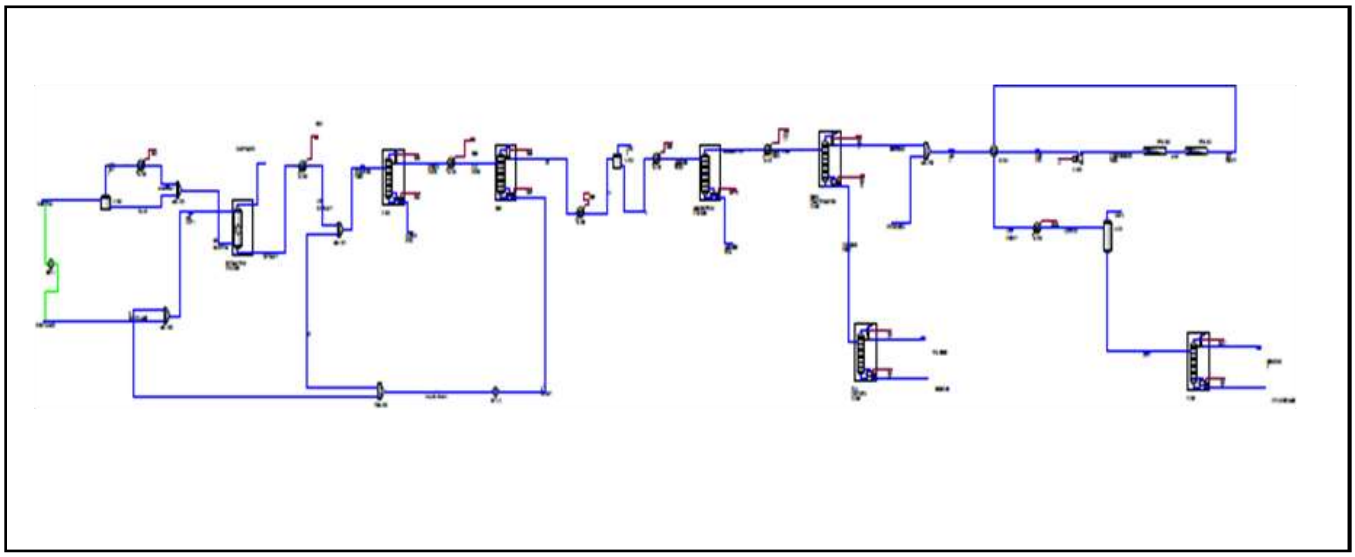

Fig.5. Process flow diagram for cyclohexane production plant.

2.2.5. ENERGY OPTIMISATION

This methodology has been successfully used in industries to minimize the usage of energy in chemical processes. There are mainly two methods of Energy optimisation. The first method is heat exchanger network synthesis (HENS) [Linnhoff, B et al., 1994]. With the help of HEN can formulate the optimisation problem. The major advantage of this problem is the ability to find out the best and suitable solution for the problem. However, there is some drawbacks for this method. In this method, which provide only a few information about the factors that affects the energy consumption in the operation and for the plant modification.

The second method is more acceptable, which is mainly based on thermodynamic principles, known as Pinch method. The pinch technology focusing to minimise the external heat transfer to or from the site [Desmond E. Winterbone FR et al., 2015]. Which is a simplified method to find the energy and cost targets. It gives a minimum value for energy consumption and for cost for the required process. Also, a suitable plant modification as per graphical representation from available data. It gives possibilities for heat exchanger network design by satisfying the all energy requirement [E. K. Macdonald et al., 1988]. For these reasons pinch method become more popular and would wide acceptably tool for HEN design. Pinch methodology required simple calculations. It can be done by hand. But it is a time consuming and tedious process. To reduce the human effort and time, a software which have the ability to do repetitive tasks is used. The software used is HINT. Heat integration is a non-commercial software used for heat exchanger network design for required problem [Angel Martin et al., 2008].

2.2.6. PROBLEM DESCRIPTION

To achieve minimum energy and cost target in cyclohexane production plant pinch method is used by the assistance of HINT software [M. Hassan Panjeshahi et al., 2004]. There are several steps to calculate the energy and designing a heat exchanger network. The first step is extraction of data. The software requires temperature, enthalpy, and heat transfer coefficient etc. data from the plant. The data can be taken from converged process flow diagram. Here which is from UniSim design model. The extraction of data required more attention.

The table shows the thermal properties of the stream. Which include both hot and cold fluids with the design parameter minimum temperature difference of 10^0 C. The ΔT_{min} is the minimum vertical distance between hot and cold curves that is the minimum approach temperature for thermal exchanges. There are 4 cold fluids and 3 hot fluids shown in the table 3.

Table 3. Stream data for pinch analysis

Stream	Description	Type	Heat Type	T1 (K)	T2 (K)	H (kW)	m.Cp (kW/K)
1	C1	Cold	Sensible	330.84	373	4054.44	96.1679
2	C2	Cold	Sensible	381.7	523	1370.08	9.67001
3	C3	Cold	Sensible	319.2	523	776.76	3.8112
4	C4	Cold	Sensible	303	368	689.5	10.74
5	H1	Hot	Sensible	399	348	- 588.0	11.7539
6	H2	Hot	Sensible	512	373	-580.24	4.83469
7	H3	Hot	Sensible	367.37	303	-780.04	12.3890

In these case, the streams are considered as linear streams, that is the streams have constant m.Cp values over a given temperature interval. The software can also be able to receive non-linear streams with varying m.Cp values.

2.2.7. AREA AND COST TARGETING

The cascade/ stream diagram from the hint represents the energy and cost targets calculations. Schematic representation of the stream population on a vertical temperature scale. The fig.6.a. represents the calculations for energy target with problem table algorithm for the given data. The minimum heating duty required is 5087.91 kW and cooling duty required is 145.74kW.

The HINT also generates composite curves, which is closely related to energy targeting. The composite curves are indication of possible energy recovery in the process. The fig.6. b. shows both cold and hot composite curves. The overlapped area between the hot and cold curves indicates the possible amount of energy extraction.

With the parameters presented in Table3. Minimum temperature difference of 10℃, the minimum area of 3229.74 m2 and a Minimum cost of $ 587832 / year.

The main step in the HEN design is the estimation of cost and area using HINT software. These calculations and the network design help to modify the flow sheet design by proposing alternatives. This may result in the improvement in energy efficiency of the system. From the energy target, the cost and area target calculations can be calculated in hint. The calculations are complementary to energy target calculations. The energy and also the area contribute to the total cost of the process. Energy cost and the cost of utilities are the two major parameters which affects the operating cost.

As per the entered data in the hint, which also gives different diagrams like energy v/s DT min., cost v/s DT min., area v/s DT min. Which is useful for optimising DTmin.

The relationship between energy or area or cost (TAC) of the HEN with respect to DTmin, as shown in Fig 6.c,6.d,6e. The variation in DTmin will slightly affect the dependent variable (Energy, Area and Cost) to a considerable extent, observes a continuity in the value of Energy, Area or TAC at a certain value of DTmin in the graphs of energy or area or TAC with respect to DTmin.

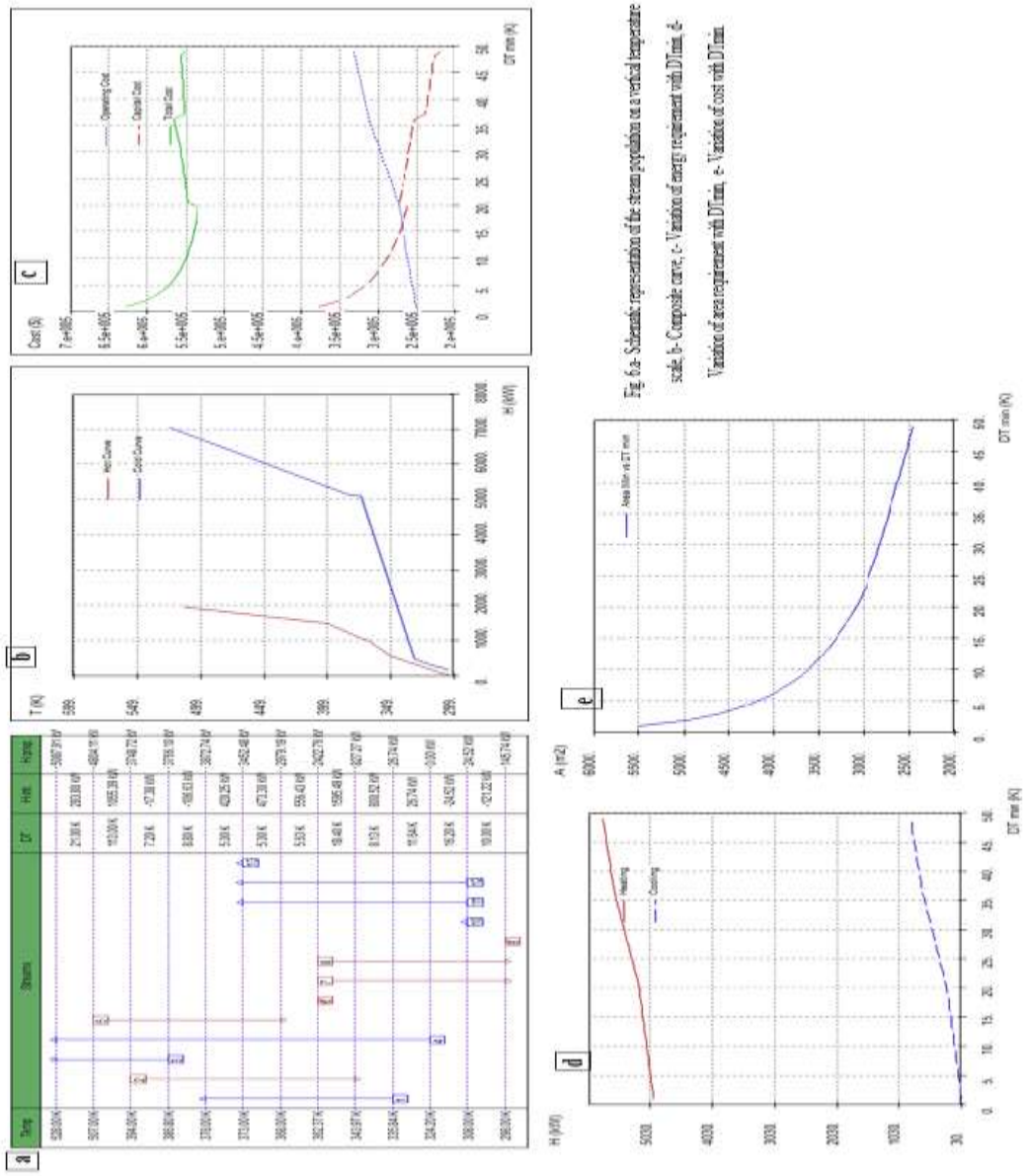

Fig. 6.a- Schematic representation of the stream population on a vertical temperature scale, b- Composite curve, c- Variation of energy requirement with DTmin, d- Variation of area requirement with DTmin, e- Variation of cost with DTmin

2.2.8. SELECTION OF UTILITY

Utilities for energy requirement can supply after completing Thermal property data. The very efficient tool for the utility selection is grand composite curve (GCC). GCC represents the hot and cold utility required for the process at each temperature. The utility selection optimized the use of available temperature difference.

Table 4. The energy targets for utility level.

No.	Description	Utility	Heat	Sup T(K)	Tar T(K)	H max (kW)
1	Hot utility	Heating	Latent	600	600.	-5087
2	Cold utility	Cooling	Latent	250	250.	145.74

The temperature at which utility is needed is identified by using GCC curve. Based on this information can add the utility depends upon the energy requirement. After the addition of utility, which are combined to obtain utility GCC. That satisfy the energy requirement of the process.

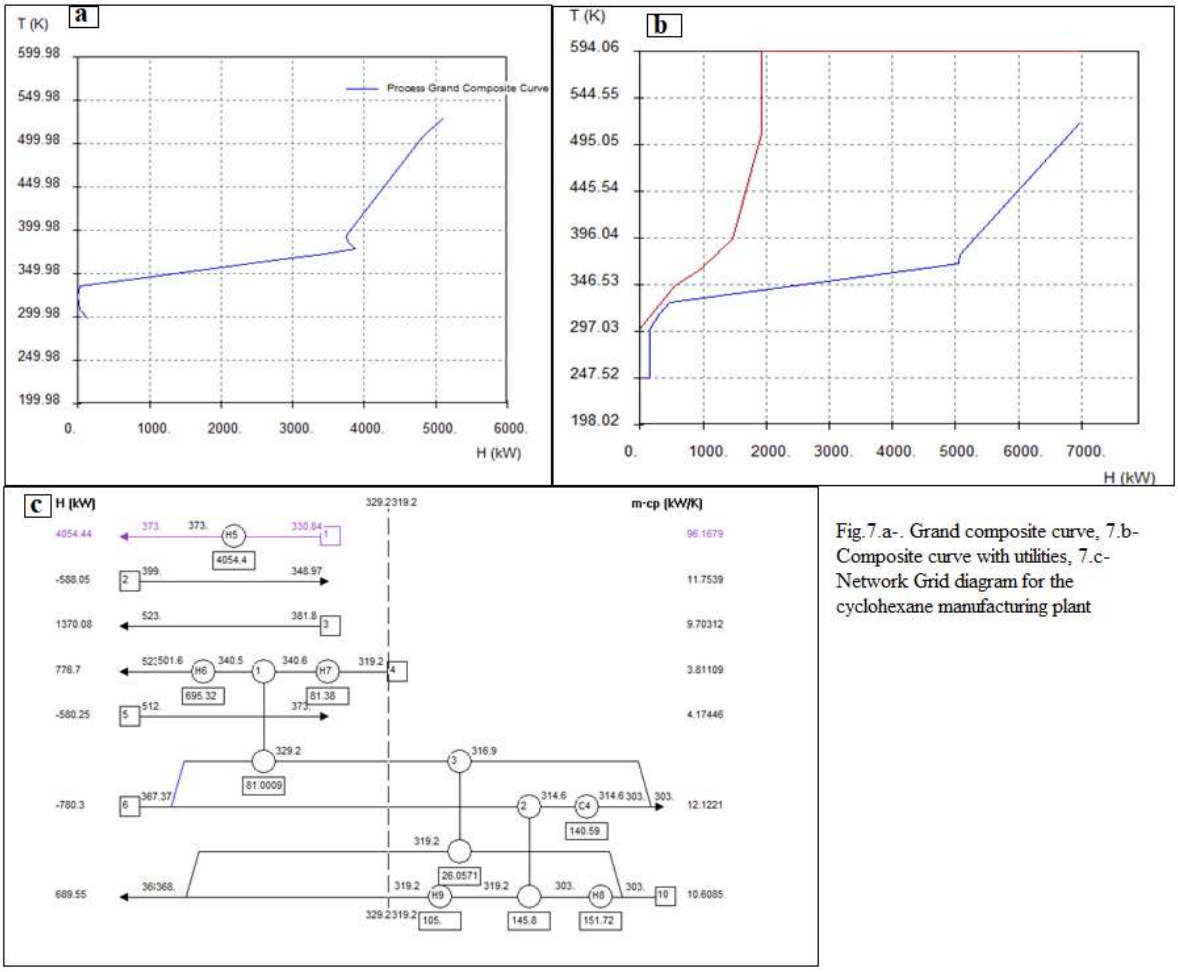

Fig.7.a-. Grand composite curve, 7.b-Composite curve with utilities, 7.c-Network Grid diagram for the cyclohexane manufacturing plant

Fig. 7.a. shows the grand composite curve. It can be seen that the separation between process and utilities GCCs is much smaller. Very steep GCCs indicates for the use of sensible-heat transmitting utilities, others with flat GCCs indicates adequate use of latent heat utilities and others with different sections which make convenient the selection of multiple heating and/or cooling utilities. Fig. 7. b-.gives the composite curve with utilities.

2.2.9. HEAT EXCHANGER NETWORK DESIGN (HEN)

The pinch heat exchanger design is done by obeying some feasibility criteria. Which have the minimum temp difference in one end. To satisfy the criteria, sometime it is necessary to split the process streams. Here two process streams are split to fulfil the criteria. After finding the feasible match from the split cold and hot stream, the pinch heat exchangers are specified. Along with the heat exchangers heaters and coolers are also added to satisfy the required minimum cooling and heating duty. Pinch method is not a mechanical design methodology. Which follow certain rules to obtain optimum HEN design.

Fig. 7.c. shows network grid diagram for this synthesis loop based on the available information from the plant. After heat exchanger network designing the heating and cooling duty should not be more than the required duty. At this condition the network obtained from hint have minimum energy consumption and maximum energy efficiency. As per design done in the software the process flow diagram can modify. After completing the design, the cost estimation can be done by assigning values for heat transfer coefficients and relation of cost to each heat exchanger placed in the design instead of the stream.

3. RESULT AND DISCUSSION

3.1. STEADY STATE ANALYSIS

In the steady state analysis of plant model, analyse each equipment placed in the plant model and the reaction or the unit operation carried out in the plant. Optimization of process conditions and process parameters are find out in different case studies. Case studies for each equipments are mentiones as below;

FOR EXTRACTION COLUMN

CASE STUDY 1

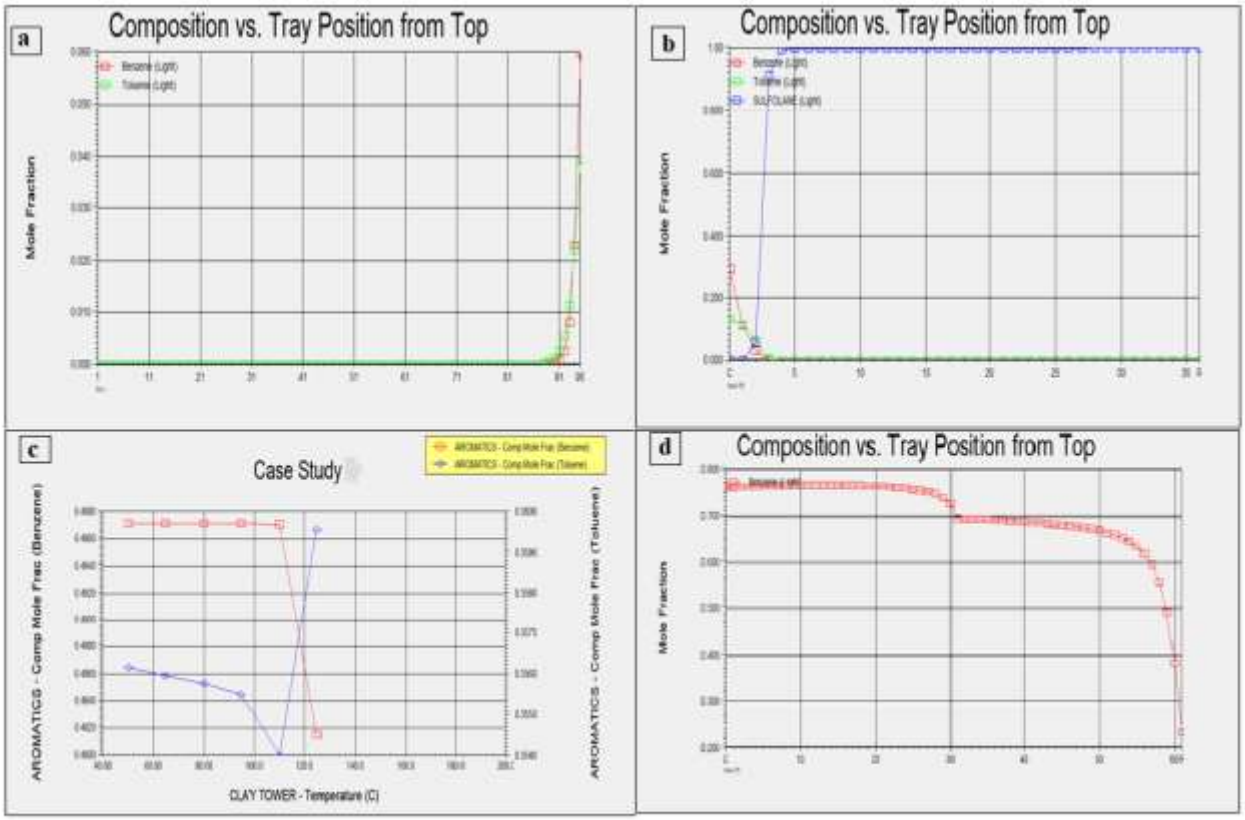

Fig 8.a-Relation between composition and Tray position from top for extraction column., b- Relation between composition and tray position from top for solvent recovery column, c- Relation between composition of benzene and toluene and temperature, d-Relation between composition and tray position from top for benzene fractionation column.

The fig.8.a- shows the case study for liquid- liquid extraction column. The plot of composition v/s tray position is drawn. The extraction process is a counter current operation in which the feed is entered from the bottom of the column and the solvent is given from the top of the column. The solvent used is sulfolane. There is about 95 number of trays in the extraction column. In this operation we separate aromatics and non-aromatics from the feed solution. The extract phase coming out from the bottom of the column contain aromatic compounds and the raffinate phase is coming out from the top of the column contain large amount of non-aromatics. Graph shows two components. One is benzene and the other is toluene. It is clear that the major amount of extraction is taking place is from the 90^{th} tray. Separation of aromatics mainly benzene and toluene take place near the last tray.

FOR SOLVENT RECOVERY COLUMN

CASE STUDY 2

Case study 2 gives the relation between composition and tray position for the solvent recovery column. The product stream coming out from the extract stripper contains large amount of

sulfolane solvent. In SRC column the sulfolane is separated from the stream and then which is given back to the extraction column and also to the extract stripper. The separation of sulfolane from aromatics is a simpler process because sulfolane is a heavier component than aromatics. So lean sulfolane is separated from the bottom of the distillation column. Aromatic stream is separated from the top of the column. There are 35 no. of trays present in the solid recovery column. Fig. 8.b- gives the plot for relationship.

FOR ABSORPTION COLUMN

CASE STUDY 3 -COMPOSITION VS. TEMPERATURE

The case study 3 shows that the relation between composition of benzene and toluene with temperature of the operation. From the fig.8.c.it is understood that at absorption operation prefer lowest temperature. Beyond a particular temperature the composition goes down rapidly. A small increase in temperature causes a large decrease in the composition. In the case of toluene, as the temperature increases the composition decreases up to a temperature level. Beyond that temperature level the composition increases rapidly.

FOR BENZENE FRACTIONATION COLUMN

CASE STUDY 4

The fig.8.d gives the relation between composition and tray position for top for benzene fractionation column. There approximately 60 no. of trays. About 75 % of composition for benzene is obtained from this fractionation section. The benzene is separated from the top of the column.

FOR SEPARATOR

CASE STUDY 5-COMPONENT MOLE FRACTION VS. TEMPERATURE

The case study 5 shows in fig 9.a- the temperature- component mole fraction relationship of input stream and the outlet flow respectively. In separator we separate the cyclohexane and the unreacted hydrogen from the feed stream. The graph shows that initially as the temperature increases the composition of cyclohexane in the outlet increases, after a certain temperature the composition falls down. Therefore, temperature of 160-180 ^{0} C is maintained for maximum level of separation.

FOR CYCLOHEXANE FRACTIONATION COLUMN

CASE STUDY 6

The fig.9.b-. Gives the relation between composition and tray position from top for cyclohexane fractionation column. There approximately 45 no. of trays. About 98 % of composition for cyclohexane is obtained from this fractionation section. The product stream is obtained as the bottom of the fractionation column.

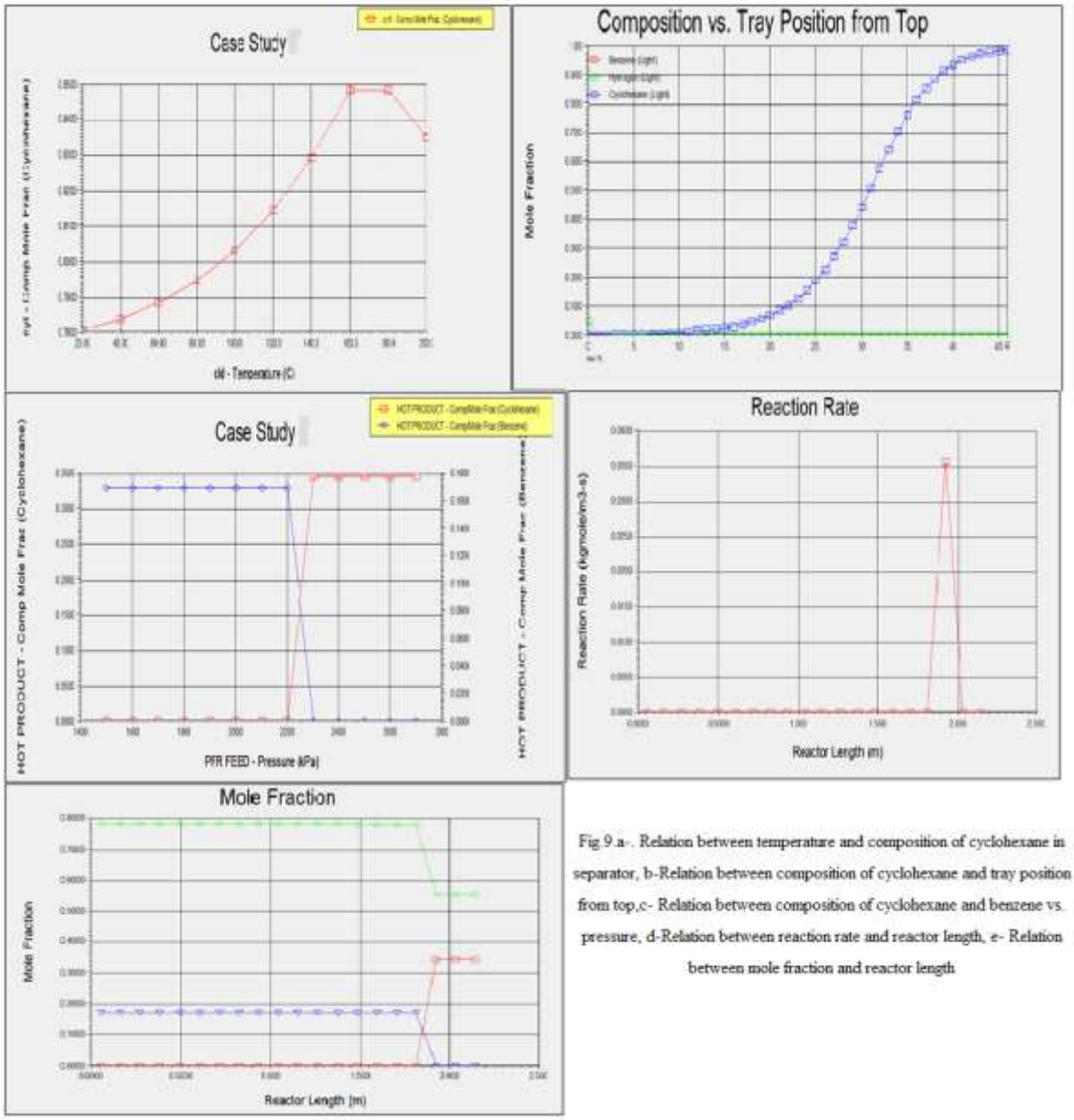

Fig 9.a-. Relation between temperature and composition of cyclohexane in separator, b-Relation between composition of cyclohexane and tray position from top,c- Relation between composition of cyclohexane and benzene vs. pressure, d-Relation between reaction rate and reactor length, e- Relation between mole fraction and reactor length

FOR PLUG FLOW REACTOR

CASE STUDY 7- COMPOSITION VS. PRESSURE

Case study based on pressure of the PFR vs. component mole fraction of cyclohexane and benzene is shown in fig.9.c. From this it can be seen that high pressure favours more yield of reaction for cyclohexane. Hence a pressure of 2200 kPa is found to be suitable.

REACTION RATE VS. REACTOR LENGTH

CASE STUDY 8

Case study to find the optimum length of PFR is observed. In PFR benzene and hydrogen is reacted at elevated temperature and pressure to form cyclohexane. From this it can be seen that a tube length of 1.9 m favours good reaction extent. shown in Fig.9. d.

MOLE FRACTION VS. REACTOR LENGTH

CASE STUDY 9

The case study 9 shows the relation between mole fraction and reactor length. The Fig. 9.e. gives at tube length of 1.9 m the mole fraction of cyclohexane is more.

3.2. PINCH ANALYSIS

Through pinch analysis in conjunction with conventional optimisation technique can reduce the 20% cost reduction in proposed design and 30% energy saving. The main objective of pinch method is to modify the heat exchanger network. The modified network design should have maximum improvement in energy efficiency, minimum energy consumption and also minimum cost.

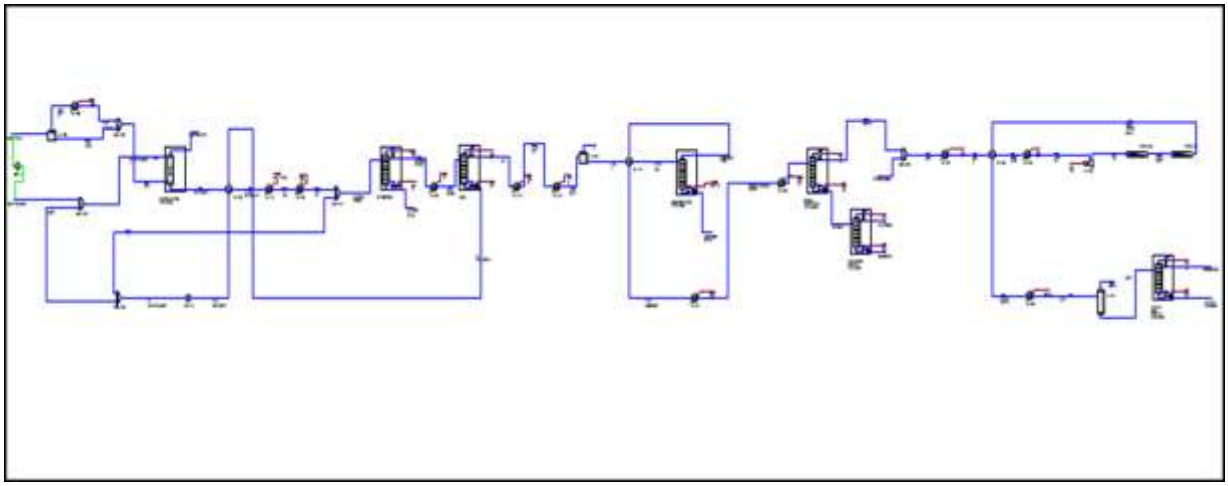

Fig.10. Modified process flow diagram for cyclohexane production plant after pinch analysis.

The calculation for area and cost is done after HEN design by the aid of remaining problem analysis. Which is unnecessary for small system. It can also be done using hint. The modification of process flow sheet in UniSim design software is carried out. Modification of process flow diagram is done by including 9 no. of heat exchangers. The area required for this is only 1461.06 m^2, and its total cost is about 6.009*10^5 $/ year.

The table 5. shows the result of remaining problem analysis. However, the direct modification can be done only when operating with heat exchanger path and utility loops. The fig.10.shows the modified plant diagram of cyclohexane plant after pinch analysis.

Table 5. Remaining problem analysis

	Minimum	Installed
No. of heat exchangers	13	9
Area target (m^2)	2064.44	1461.06
Capital cost target ($/ Yr)	2.032*10^6	6.009*10^5
Heating (kW)	5087.91	5087.82
Cooling (kW)	145.742	145.52

4. CONCLUSION

The process simulation and optimization of cyclohexane manufacturing plant has successfully performed and developed. This paper presented the design and simulation of a plant for the production of cyclohexane by hydrogenation of benzene. The entire plant is divided into two section- aromatic recovery unit and the hydrogenation unit. Both the steady state model and the dynamic model of the plant were completed. The Performance of the steady-state model has been studied by comparing the material and energy balances with actual data from a pilot plant. The various operating parameters along with product specification data for a real-life plant with UniSim simulation results, show only 2.2% variation.

Pinch analysis method is the best method for HEN designing. It can implement both for existing and for new plants. The design of heat exchanger network for the cyclohexane plant is done by using hint educational software. The area targeting, cost targeting and utility design also. Done in

HINT. As per pinch analysis the plant design is modified in UniSim design software to achieve maximum energy efficiency.

Therefore, it has been shown that the UniSim model of this research work can be used to represent, simulate and optimize a plant operation system successfully.

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