

MODELING AND SIMULATION OF NAPHTHA CATALYTIC REFORMER

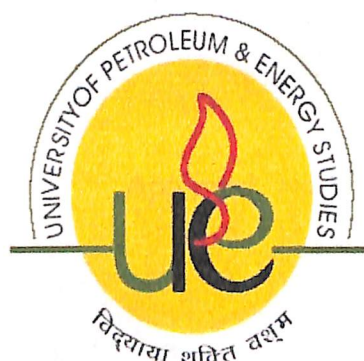
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M. Tech (Process Design)

REPORT ON MAJOR PROJECT (PROJ801)



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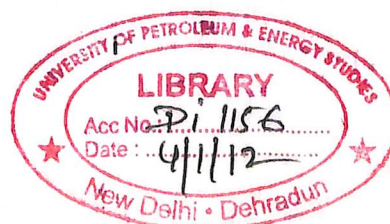
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MODELING AND SIMULATION OF NAPHTHA CATALYTIC REFORMER

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

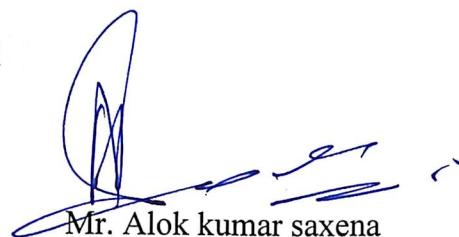
Master of Technology

(Process Design Engineering)

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CERTIFICATE

This is to certify that the work contained in this thesis titled “MODELING AND SIMULATION OF NAPHTHA CATALYTIC REFORMER” has been carried out by INDRADEEP THAMMISSETTI under my supervision and has not been submitted elsewhere for a degree.



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ABSTRACT

In this work, the mathematical modeling of a semi-regenerative catalytic reformer is developed. A naphtha catalytic reforming unit with three reactors in series is analyzed. Kinetic and thermodynamic equations are selected to describe the naphtha catalytic reforming reactions based on idealizing the complex naphtha mixture by representing the paraffin, naphthene, and aromatic groups by single lumped components (Smith's model).

In the first part of the work, naphtha catalytic reforming unit is simulated with the reforming unit data of Haldia refinery and effect of operating parameters of the reformer unit such as reactor inlet temperatures on reformate composition are studied. In the second part of work, the simulation process is validated with reactor data of Barauni Refinery.

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I sincerely thank to Dr. ALOK KUMAR SAXENA, my project guide, for his time to time suggestions and technical support which have helped me to accomplish this work and improve my technical abilities.

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NOMENCLATURE

r- rate of reaction, Kmol/hr

kf-reaction rate constant, kmol/(hr.kgcat.Mpa) for reactions 1 &2;
for reaction 3&4 Kmol/(hr. kgcat)

keq-equilibrium rate constant, (Mpa)³ for reaction 1;
(Mpa)⁻¹ for reaction 2

ΔH -enthalpy of reaction KJ/Kmol H₂

p_i- partial pressure of component i, Mpa

P-Pressure, Mpa

L-length of the catalyst bed, m

R-Radius of the catalyst bed, m

N-Number of moles, Kmol

T-Temperature, °C

C_p-heat capacity, KJ/Kmol °C

ρ_b - Bulk density, kg/m³

Subscripts

1-Reaction 1

2-Reaction 2

3-Reaction 3

4-Reaction 4

N-Naphthenes

A-Aromatics

P-Paraffins

T-Total

x

CHAPTER 1

1.1 INTRODUCTION

The catalytic reforming process is one of the operations in petroleum refineries to produce gasoline with high octane number. This process uses naphtha as feedstock to produce aromatic compound rich reformat with high octane number through reactions such as aromatization, cyclization and hydrocracking. At the same time, it produces hydrogen (H₂) and liquefied petroleum gas (LPG) as its by-products. In this process, products with different octane number are produced unlike the production of certain octane number in others such as catalytic cracking, alkylation and isomerization.

Octane rating has been used for many years to measure the antiknock performance of gasoline. The higher the octane number, the less the tendency for an engine to produce a knocking sound in an automobile engine. Until 1974, almost all gasoline contained tetraethyl lead additive as an octane booster. However, with the advent of catalytic converters on most 1975 model U.S. cars, unleaded gasoline appeared, followed by lead phase down in leaded gasoline. The 1990 amendment to the clean air act completely prohibits the use of lead in gasoline. Coupled with these stricter environmental regulations, there has been a consistent increase in the demand for higher fuel efficiency standards of engines. This requires the use of engines with higher compression ratio and therefore even greater octane number of the motor fuel. These considerations have continually forced the refiner toward producing higher octane number gasoline. The gasoline boiling range compounds obtained from the crude fractionation column in the refinery are collectively known as naphtha in the refinery.

Although oxygenated hydrocarbons, e.g., alcohols, have their uses, refiners depend upon catalytic reforming for providing the high-octane gasoline. The process may also be alternatively operated to produce high yields of aromatics like, benzene, toluene, and xylenes for petrochemical feed stocks. However, the focus of this research work are those reformers whose objective is to upgrade low-octane naphtha to high-octane compounds for use as motor fuel. The reformer unit is located downstream of the crude distillation unit and the feed naphtha to the reformer is produced as one of the lighter fractions of the crude column.

1.2 LITERATURE SURVEY

With the objective to prepare model of a catalytic naphtha reformer, phenomenological in nature and detailed enough to represent the actual process characteristics, following literature was referred.

A number of articles have appeared in the literature studying the chemistry of reforming reactions. A detailed study classifying different types reactions in naphtha reforming was published by Mohan Taskar (1996)[9].

The main reactions taking place in the reformer are the dehydrogenation of naphthenes, isomerization of paraffins and naphthenes, dehydrocyclization of paraffins, and hydrocracking of paraffins. Proper kinetic modeling of reforming reactions was the key to effectively represent the process over a wide operating range was published by D.Bommannan et al. (1989)[1] and Padmavathi (1997)[3]

The operating variables of the process, like reactor inlet temperature affect the important product properties and kinetics of the reactions taking place was published by Liang Ke-min (2005) [5] .

In view of the fact that we lacked means of developing the kinetic model of our own, the kinetic model had to be based on the work done previously and published in the literature. Because of its importance, it was thought to be well worth the effort to extensively investigate the information on different types of kinetic models of naphtha reforming available in literature. The problem is further complicated by the fact that there are literally hundreds of pure chemical components taking part in the reaction system. In order to reduce the complexity of the problem, various chemical species are lumped together and represented as a pseudo component. Almost all the kinetic models derived so far, differ from each other with respect to the kind of lumping strategy used. Some of the earliest attempts lumped the whole feed naphtha into a single species. The first significant attempt to recognize different components within naphtha was performed by Smith (1959)[7]. He characterized naphtha by three of its basic constituents; paraffins, naphthenes, and aromatics. However, within each class, no distinction is made on the basis of the number of carbon atoms. In a more extensive attempt to model reforming reactions of whole naphtha, Krane et al. (1960) divided naphtha into twenty components. They accounted for the presence of various carbon numbers from C_6 to C_{10} as well as the difference between paraffins, naphthenes, and

aromatics within each carbon number group. A total of fifty-three reaction steps each represented by a pseudo-first order rate equation with respect to hydrocarbon concentration were derived from experimental studies on whole naphtha. Henningsen and Bundgaard-Nielson (1970) expanded on this model by expressing the rate constants in the form of Arrhenius type of equation. This accounted for influence of reactor operating temperatures on the rates of reactions. That model is also noteworthy before concluding the survey of kinetic modeling of reforming reactions; we would like to mention a few other informative papers published recently on the modeling of catalytic naphtha reforming. These are Padmavati (1997)[3]; Mirko and Aleksandra (2008)[7]; Bommannan et al. (1989)[1]. Bench marking of the model with the given data involved adjusting coefficients in the model.

CHAPTER 2

2.1 CATALYTIC REFORMING OF NAPHTHA

Naphtha reforming is extensively used in petroleum refineries and petrochemical industry. The use of catalytic naphtha reforming as a process to produce high-octane gasoline continues to be important as it has been over the 55 yr of its commercial use. The catalytic reformer occupies a key position in a refinery providing high value-added reformate for the gasoline pool, hydrogen for hydroprocessing operations, and frequently, for producing benzene, toluene, and xylene aromatics for petrochemical uses. The main objective of catalytic reforming is to transform paraffins and naphthenes in naphtha to aromatics-rich products. Aromatics have very high octane numbers (>100) and can be tolerated in gasoline up to almost 50 vol%. However, because of stringent environmental regulations, the refining industry has taken significant steps to reduce the level of aromatic compounds in gasoline by adapting its formulation. Many countries have reduced the total aromatics content in gasoline from 42-35vol%.

Naphtha feed to the reformer contains a mixture of C_6 - C_{11} paraffins, naphthenes, and aromatic hydrocarbons in the temperature range of 85-200°C. Most reformers process is using straight-run naphtha's with qualities that vary significantly depending on the crude oil origin. Typical straight-run naphtha contains 65 wt% paraffins, 20 wt% naphthenes, and 15 wt% aromatics. In motor gasoline applications, naphtha contains the full range of C_6 - C_{11} components to maximize gasoline production. In petrochemical applications, naphtha feed may be adjusted to contain a more select range of hydrocarbons to maximize the production of aromatics.

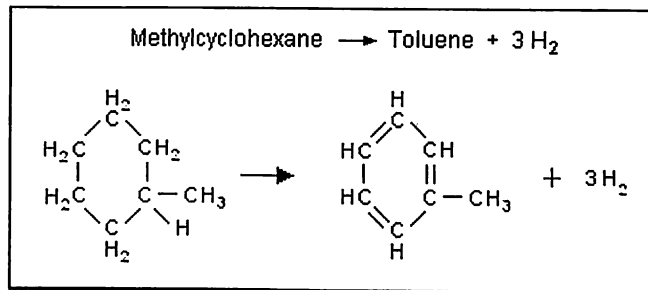
A variety of commercial processes are available which differ in the catalyst make, its regeneration procedure or catalyst bed and interstage heater configurations. The process consists of three reactors in series. Most of these reformers are multi-bed reactors operated at relatively high pressure (- 1.408 mpa), temperature (498-525 °C) and high hydrogen to hydrocarbon molar ratio (5 to 10). Bifunctional catalysts such as Pt/ Al_2O_3 , Pt-Re/ Al_2O_3 or Pt-Sn/ Al_2O_3 are commonly used which have a metal component (Pt) for hydrogenation- dehydrogenation reactions and an acidic component (Al_2O_3) for isomerization, cracking, polymerization etc. Naphtha being a complex mixture of hydrocarbons, undergoes a variety of reactions such as dehydrogenation and dehydroisomerization of naphthenes to aromatics, dehydrogenation of paraffins to olefins, dehydro-cyclization of paraffins and olefins to aromatics, isomerization or hydroisomerization

to isoparaffins, isomerization of alkylcyclopentanes and substituted aromatics and hydrocracking of paraffins and naphthenes to lower hydrocarbons.

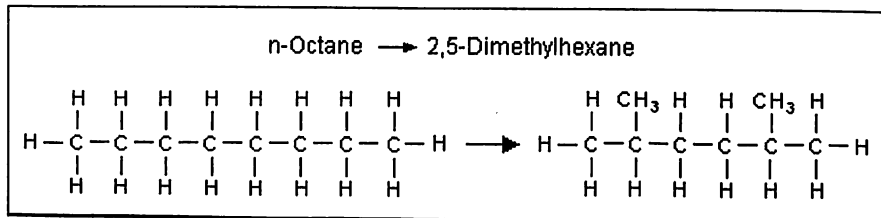
2.2 REACTION CHEMISTRY

The four major catalytic reforming reactions are:

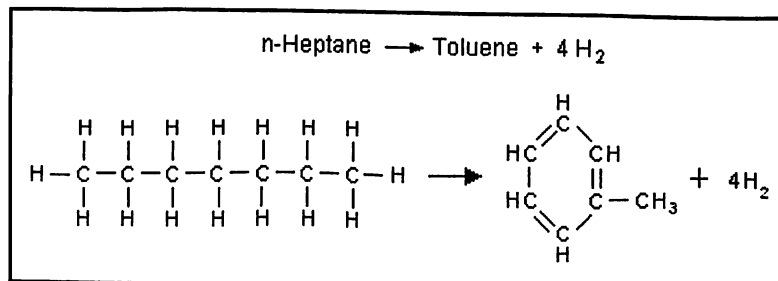
1: Dehydrogenation of naphthenes to convert them into aromatics as exemplified in the conversion methylcyclohexane (a naphthene) to toluene (an aromatic), as shown below:



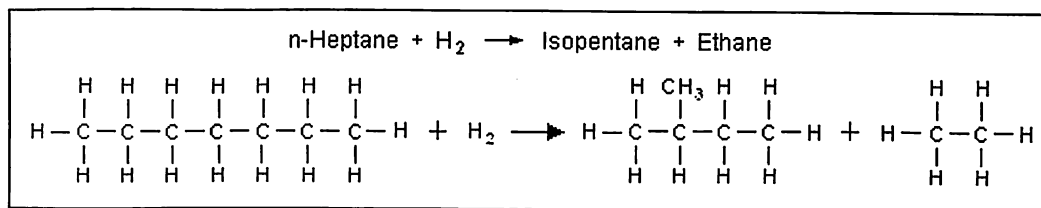
2: Isomerization of normal paraffins to isoparaffins as exemplified in conversion of normal octane to 2, 5-Dimethylhexane (an isoparaffin), as shown below:



3: Dehydrogenation and aromatization of paraffins to aromatics (commonly called dehydrocyclization) as exemplified in conversion of normal heptane to toluene, as shown below:



4: Hydrocracking of paraffins into smaller molecules as exemplified by cracking of normal heptane into isopentane and ethane, as shown below:



Hydrocracking of paraffins is the only one of the above four major reforming reactions that consume hydrogen. Isomerization of normal paraffins does not consume or produce hydrogen. However, both the dehydrogenation of naphthenes and the dehydrocyclization of paraffins produce hydrogen. In many petroleum refineries, the net hydrogen produced in catalytic reforming supplies a significant part of the hydrogen used elsewhere in the refinery (for example, in hydrodesulphurization processes). The hydrogen is also necessary in order to hydrogenolyze any polymers that form on the catalyst.

2.3 PROCESS FLOW SHEET

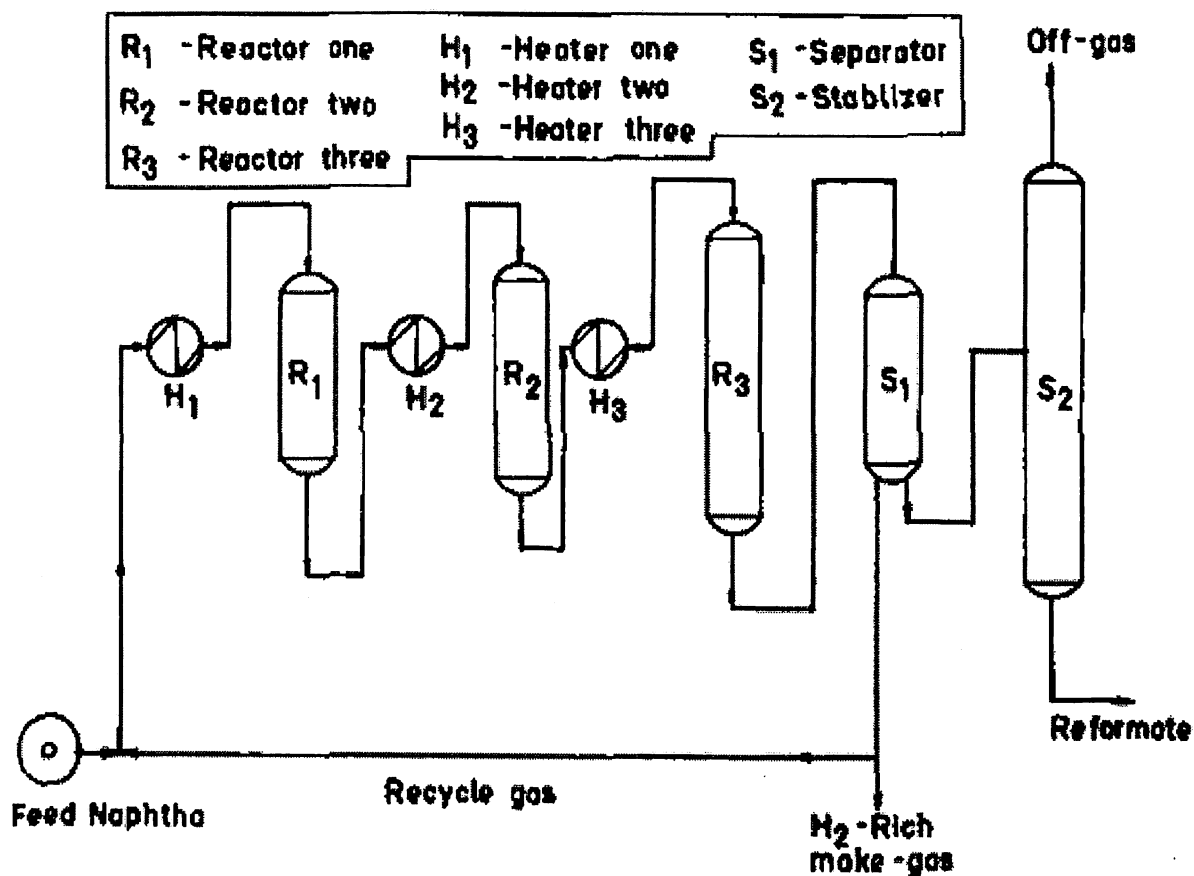


Figure1: Process Flow sheet

The most commonly used type of catalytic reforming unit has three reactors, each with a fixed bed of catalyst, and all of the catalyst is regenerated in situ during routine catalyst regeneration shutdowns which occur approximately once each 6 to 24 months. Such a unit is referred to as a semi-regenerative catalytic reformer (SRR).

The liquid feed (at the bottom left in the diagram) is pumped up to the reaction pressure (5 to 45 atm) and is joined by a stream of hydrogen-rich recycle gas. The resulting liquid-gas mixture is preheated by flowing through a heat exchanger. The preheated feed mixture is then totally vaporized and heated to the reaction temperature (495 to 520 °C) before the vaporized reactants enter the first reactor. As the vaporized reactants flow through the fixed bed of catalyst in the reactor, the major reaction is the dehydrogenation of naphthenes to aromatics (as described earlier

herein) which is highly endothermic and results in a large temperature decrease between the inlet and outlet of the reactor. To maintain the required reaction temperature and the rate of reaction, the vaporized stream is reheated in the second fired heater before it flows through the second reactor. The temperature again decreases across the second reactor and the vaporized stream must again be reheated in the third fired heater before it flows through the third reactor. As the vaporized stream proceeds through the three reactors, the reaction rates decrease and the reactors therefore become larger. At the same time, the amount of reheat required between the reactors becomes smaller.

The hot reaction products from the third reactor are partially cooled by flowing through the heat exchanger where the feed to the first reactor is preheated and then flow through a water-cooled heat exchanger before flowing through the pressure controller (PC) into the gas separator.

Most of the hydrogen-rich gas from the gas separator vessel returns to the suction of the recycle hydrogen gas compressor and the net production of hydrogen-rich gas from the reforming reactions is exported for use in the other refinery processes that consume hydrogen (such as hydrodesulphurization units and/or a hydrocracker unit).

The liquid from the gas separator vessel is routed into a fractionating column commonly called a stabilizer. The overhead off gas product from the stabilizer contains the byproduct methane, ethane, propane and butane gases produced by the hydrocracking reactions as explained in the above discussion of the reaction chemistry of a catalytic reformer, and it may also contain some small amount of hydrogen. That off gas is routed to the refinery's central gas processing plant for removal and recovery of propane and butane. The residual gas after such processing becomes part of the refinery's fuel gas system. The bottoms product from the stabilizer is the high-octane liquid reformat that will become a component of the refinery's product gasoline.

CHAPTER 3

3.1 MODELING OF CATALYTIC REFORMING OF NAPHTHA

Catalytic reforming process is often modelled based on the following factors:

- 1-The number of reactive species
- 2-The type of used kinetic model

Because of many components as reactants or intermediate products in the reactive mixture and new reactions as a consequence, it will extremely make a sophisticated situation for modeling the process. To mitigate the complication, reactants in the mixture are classified in certain and limited groups, called Pseudo Components. The number of selected pseudo components in the feed is a characteristic factor, the key in presented models.

Arrhenius and Langmuir–Hinshelwood kinetics are used for catalytic reforming models. It should be noted that for all of the presented models, the reactions are considered as Pseudo homogeneous.

Smith proposed the first kinetic model for catalytic reforming process in 1959 he assumed that naphtha includes of three fundamental groups: paraffins, naphthenes, and aromatics. Moreover, he introduced hydrogen, ethane, propane, and butane into the system in addition to these groups. Based on these assumptions, he could give a simple and accurate kinetic or catalytic reforming process. Reactions according to Smith model are as the following:

- 1- Naphthenes to aromatics
- 2- Naphthenes to paraffins
- 3- Hydrocracking of paraffins
- 4- Hydrocracking of naphthenes

In present work, Smith model was used for simulation of a process with 3 reactors in series. To evaluate the accuracy of the model, we are running plant data of reforming unit and comparing it with another industrial data.

3.1.1 MATHEMATICAL MODEL

In our present work a steady state flow sheet for a naphtha reforming unit is used for modeling and simulation. A simple kinetic model (Smith's model) has been used to simulate catalytic naphtha reformers. According to this model we consider naphtha in to three constituents, namely, paraffins, naphthenes and aromatics, with average properties assigned to each class. Then four major reactions (such as aromatization, cyclization and hydrocracking) have been considered with kinetic parameters of the reactions.

The present work is to develop a generalized model for catalytic reformers and running this model with plant data for verification. To find how sensitive a process is with respect to the operating parameters such as inlet temperature of the reactor. Such a model can be run off-line to emulate the plant and determine optimized operating conditions. Smith's model can be tuned with its specific parameters for catalyst activity. The model predicted temperature drop of each reactor and aromatic content of stream leaving third reactor can be statistically correlated to the corresponding parameters from the plant. Though there are detailed models for reforming, a simple model (Smith's model) has been intentionally selected as in a later stage all models need to be tuned to the plant based on past operation data from the plant.

3.1.2 ASSUMPTIONS

The following assumptions are proposed on the basis of the features of catalytic reforming reactions, reactor and its operation conditions:

1. There is no temperature and concentration gradient in the radial direction
2. Reactions are in homogenous phase

Reactions within the model are classified in four groups. They are as the following:

- i) Dehydrogenation of naphthenes to aromatics.
- ii) Dehydrocyclization of paraffins to naphthenes.
- iii) Hydrocracking of naphthenes to lower hydrocarbons (C_1 , to C_5).

iv) Hydrocracking of paraffins to lower hydrocarbons (C1 to C₅).

REACTION 1

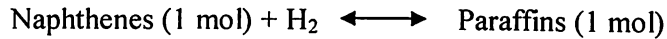


The rate of disappearance of naphthenes is given by

$$r_1 = k_{f1} \left(p_N - \frac{p_H^3 p_A}{K_{eq1}} \right)$$

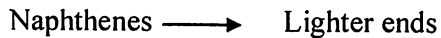
REACTION 2

The rate of disappearance of naphthenes is



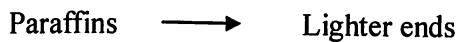
$$r_2 = k_{f2} \left(p_N p_H - \frac{p_P}{K_{eq2}} \right)$$

REACTION 3



$$r_3 = k_{f3} \frac{p_N}{P_T}$$

REACTION 4



Assuming paraffins hydrocracking to be similar to naphthene hydrocracking with reaction rate constant to be the same

$$r_4 = k_{f3} \frac{p_P}{P_T}$$

Where

$$k_{f1} = 9.87 e^{\left(23.21 - \frac{34750}{1.8T}\right)}$$

$$k_{f2} = 9.87 e^{\left(23.21 - \frac{59600}{1.8T}\right)}$$

$$k_{f3} = e^{\left(42.97 - \frac{62300}{1.8T}\right)}$$

3.1.3 THERMODYNAMICS

The most important reaction in the catalytic reforming is the transformation of cycloalkane into aromatics. It is a rapid reaction which approaches equilibrium in very short time. For reactions of cycloalkane transformation into aromatics and alkane, their reaction equilibrium constants are as follows

$$K_{eq1} = 1.04 \times 10^{-3} e^{\left(46.15 - \frac{46045}{1.8T}\right)}$$

$$K_{eq2} = 9.87 e^{\left(\frac{8000}{1.8T} - 7.12\right)}$$

$$C_p = 4.1868(a + bT + cT^2 + dT^3)$$

K_{eq1} , K_{eq2} are equilibrium rate constants

For the above four model reactions, considering the reaction enthalpy and the number of moles of hydrogen consumed or released during the reaction, the reaction enthalpies based on the number of moles of hydrogen (ΔH_1 reaction enthalpy of model(1), kJ/(kmol H); ΔH_2 reaction enthalpy of model reaction (2), kJ/(kmol H); ΔH_3 reaction enthalpy of model reaction (3), kJ/(kmol H); ΔH_4 are as reaction enthalpy of model reaction (4), kJ/(kmol H) follows:

$$\Delta H_1 = 71038.06 \text{ kJ/(kmol H)}$$

$$\Delta H_2 = 36953.33 \text{ kJ/(kmol H)}$$

$$\Delta H_3 = -56597.54 \text{ kJ/(kmol H)}$$

$$\Delta H_4 = -51939.31 \text{ kJ/(kmol H)}$$

The reactants and products of a catalytic reforming unit are gases. The relation between its heat capacity (C_p , kJ/kmol°C).

$$C_p = 4.1868(a + bT + cT^2 + dT^3)$$

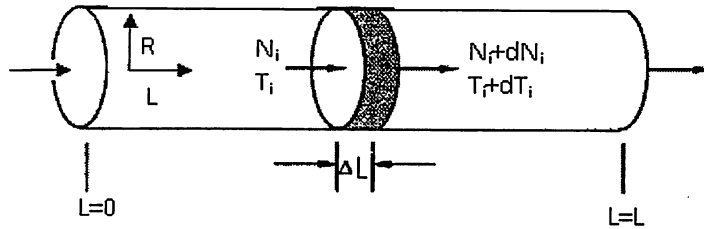
Where, T is in °C, then a, b, c and d can be obtained from physical properties manual and is listed in Table1.

Table1: Coefficients of heat capacity equation of gases

ID	a	$b \times 10^3$	$c \times 10^6$	$d \times 10^9$
H ₂	6.483	2.215	-3.298	1.826
C ₁	4.598	12.45	2.680	-2.703
C ₂	1.292	45.84	-16.57	2.081
C ₃	-1.009	73.15	-37.89	7.678
C ₄	2.266	79.13	-26.47	-0.674
C ₅	-0.866	116.4	-61.63	13.67
P	-1.456	184.2	-100.24	21.15
E	-14.789	187.3	-106.0	22.37
A	-5.817	122.4	-66.05	11.73

3.1.4 MODELING EQUATIONS

The outer radius of the catalyst bed is R . For a catalyst bed of length L , with mass and enthalpy balances for the element combining kinetic and thermodynamic equations, the concentration and temperature distributions along the reactor length can be derived as:



$$\frac{dN_A}{dL} = \pi R^2 \rho_b r_1$$

$$\frac{dN_N}{dL} = \pi R^2 \rho_b (-r_1 - r_2 - r_3)$$

$$\frac{dN_P}{dL} = \pi R^2 \rho_b (r_2 - r_4)$$

$$\frac{dN_H}{dL} = \pi R^2 \rho_b \left(3r_1 - r_2 - \left(\frac{n_c - 3}{3} \right) \times r_4 - \frac{n_c}{3} \times r_3 \right)$$

$$\frac{dT}{dL} = \frac{\pi R^2 \rho_b}{N_T \sum C_{pi} M_w} \left((\Delta H_1) r_1 + r_2 (\Delta H_2) + \left(\frac{n_c}{3} \right) \times r_3 (\Delta H_3) + \left(\frac{n_c - 3}{3} \right) \times r_4 (\Delta H_4) \right)$$

CHAPTER 4

4.1 SIMULATION

The process with three reactors in series, with conditions at the reactor inlet as boundary conditions, the concentration and temperature distributions can be calculated by solving above equations with fourth order Runge-Kutta method. The input data for simulation of reformer is from Haldia refinery[2].

4.1.1 INPUT

- The inlet temperatures of all reactor I, II and III were 510 °C.
- The operating pressure was 25kg/cm²
- Flow rate of feed 574 MT/day
- Hydrogen to feed ratio=5
- Bulk Density of feed = 600kg/m³
- Reforming feedstock content of catalytic reforming reactors

P - 151.981 kmol/h

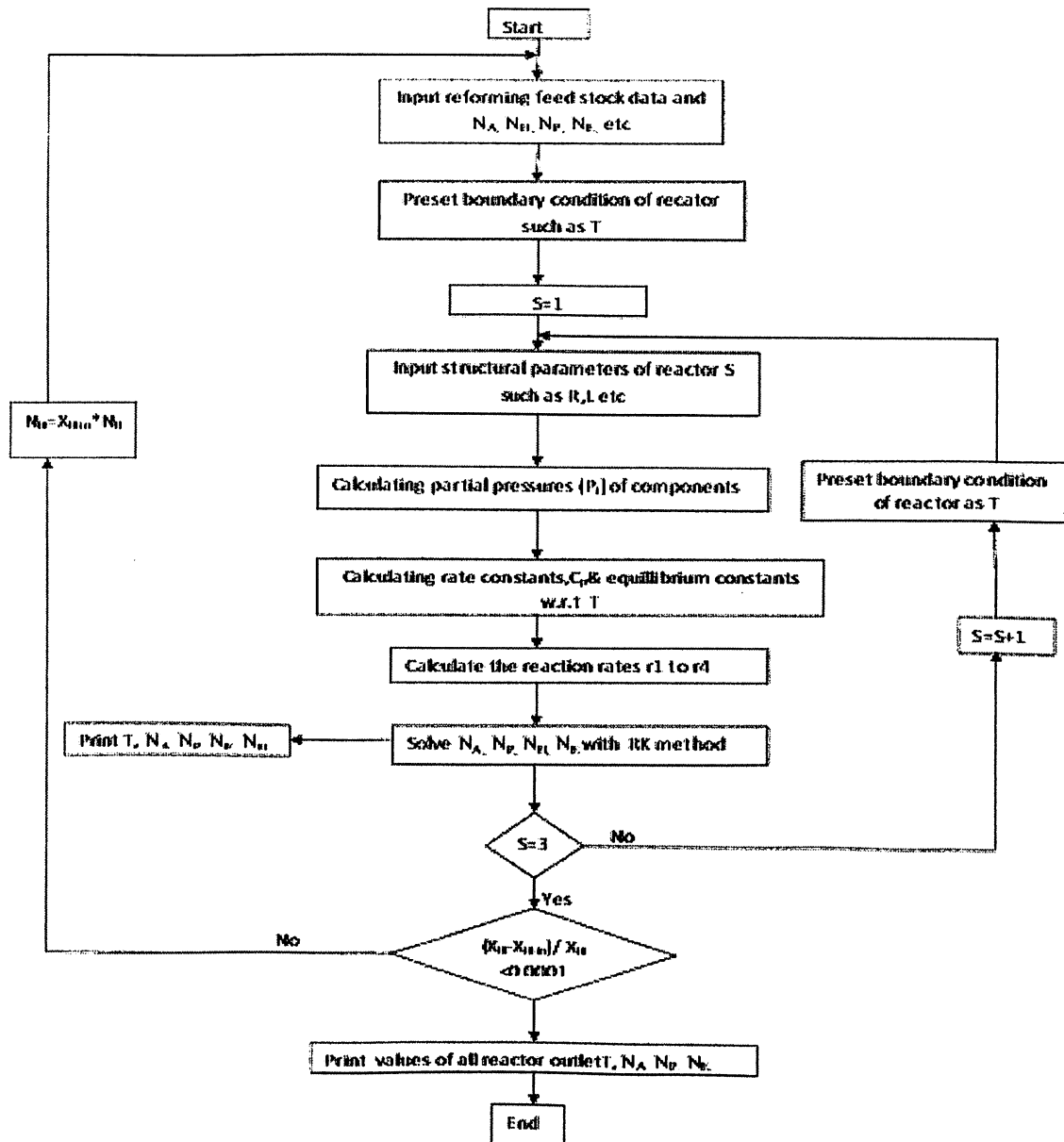
N - 53.33 kmol/h

A - 17.8539 kmol/h

- Hydrogen flow rate - 1115.87 kmol/h
- Light end flow rate - 406.46 kmol/h
- Reactor I Radius R=1.175m, Length L =0.6m
- Reactor II Radius R=0.751m, Length L =1m
- Reactor III Radius R=0.6614m, Length L =0.9m

Simulation was carried out using data listed above. Model equations (ODEs) are solved using MATLAB (RK 4th order method). The temperature, arene, cycloalkane, alkane and hydrogen varying with length of the beds are presented. Simulation is carried for 3 reactors in series until the steady state process is reached. The algorithm of process is shown below.

Figure2: Schematic flow diagram for computation



4.1.2 RESULTS AND DISCUSSION

The concentration of components and the temperature are predicted along the length of reactor as predicted from the simulation are plotted in figures below. The outputs of three reactors are listed in Table 2.

Table2: Output of the three Reactors

Reactor	Inlet temperature(°C)	Outlet temperature(°C)	Alkane (mol%)	Cycloalkane (mol%)	Aromatics (mol%)
I	510	455	67.94	10.76	21.29
II	510	481.7	67.09	3	29.19
III	510	514	64.58	0.67	34.75

It is obvious, from the data listed in Table .3 , that in reactor I the main reaction happened is cycloalkane aromatization, is an endothermic reaction and the bed layer temperature drop of this reactor is large. In reactor II and III, alkane dehydrogenization, cyclization, and hydrocracking reactions are dominant there. At the same time, the cycloalkane produced there through cyclization continues to aromatize, but the amount is not large. Furthermore, a large amount of heat was released by cyclization and hydrocracking reactions. Therefore, the bed temperature drop in these two reactors, the last one especially is smaller. The cycloalkanes are more important for increasing aromatic production yield.

The temperature distribution curve in the catalyst bed, that is, the temperature variation within the length of the catalyst bed is shown in Figure 3 showing that at the inlet temperature of the reactor I the bed temperature changes rapidly. Therefore, more aromatic compounds were generated and more heat was absorbed. For reactor II and III in spite of the trend being similar to that of reactors I, the temperature varied more gently because the reactions were exothermic.

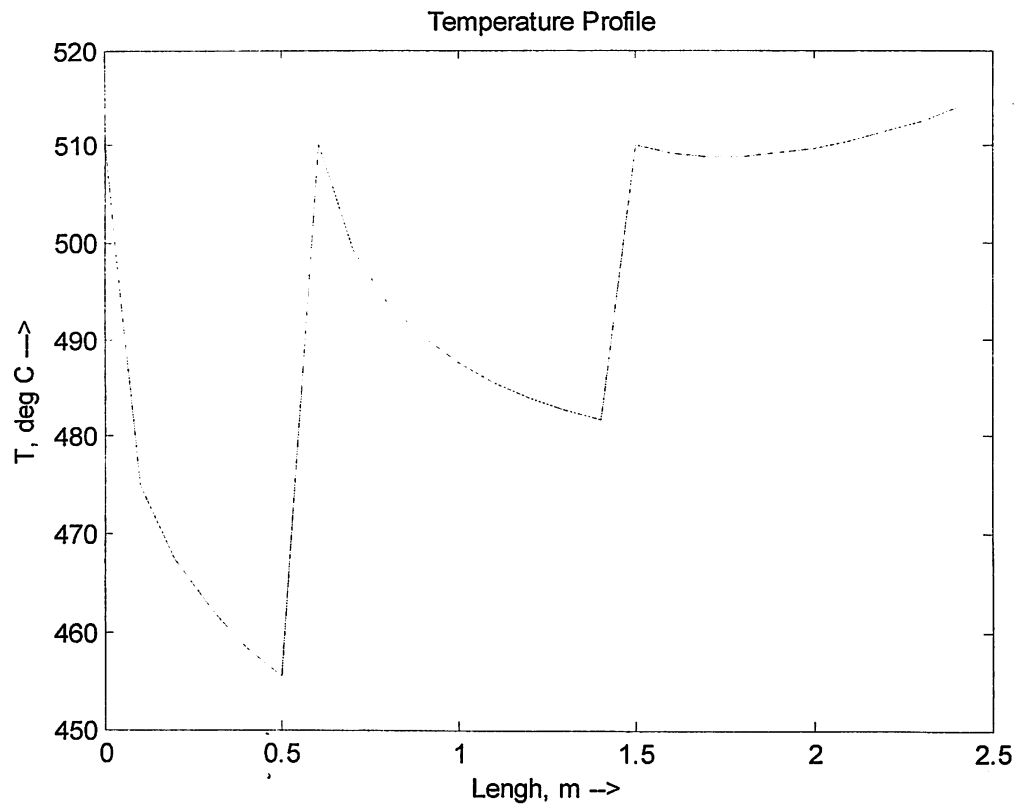


Figure3:Temperature profile along the length of reactor

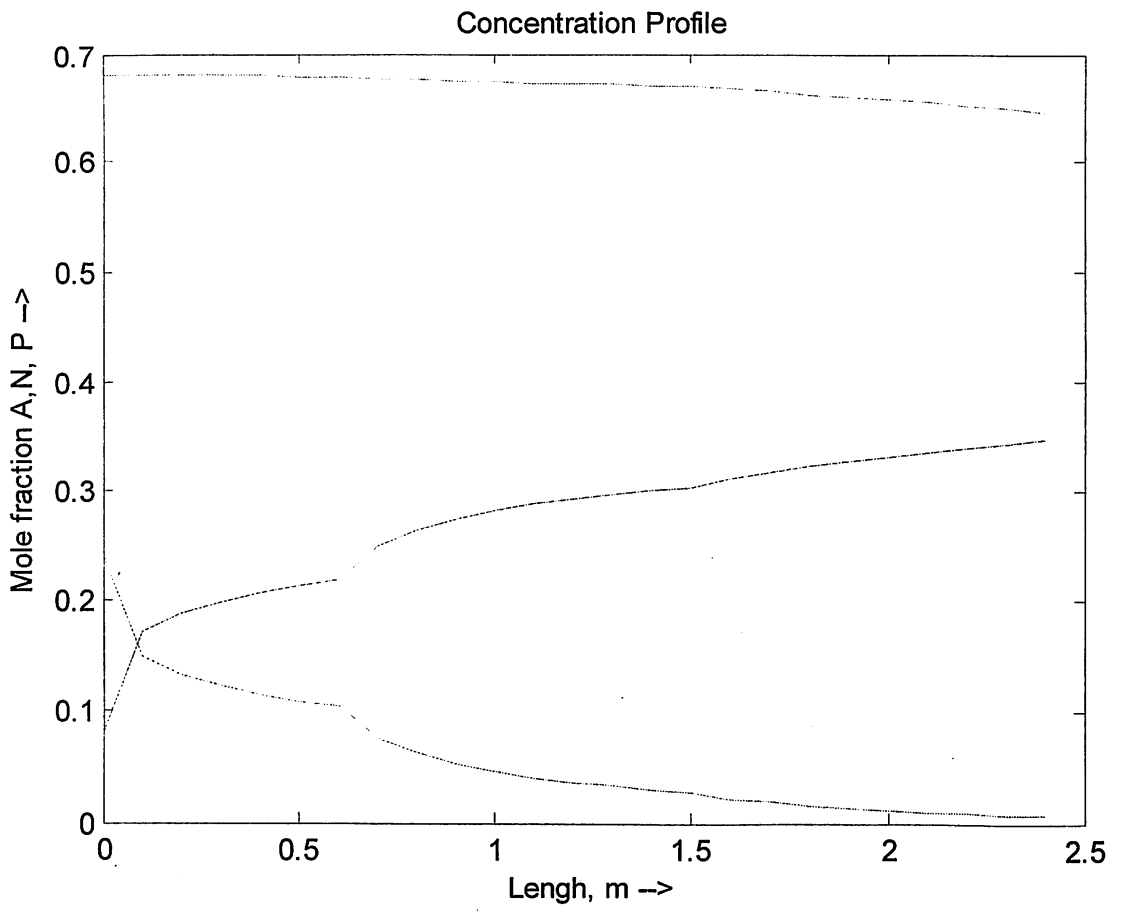


Figure4:A,N,P concentration profile along the length of reactor

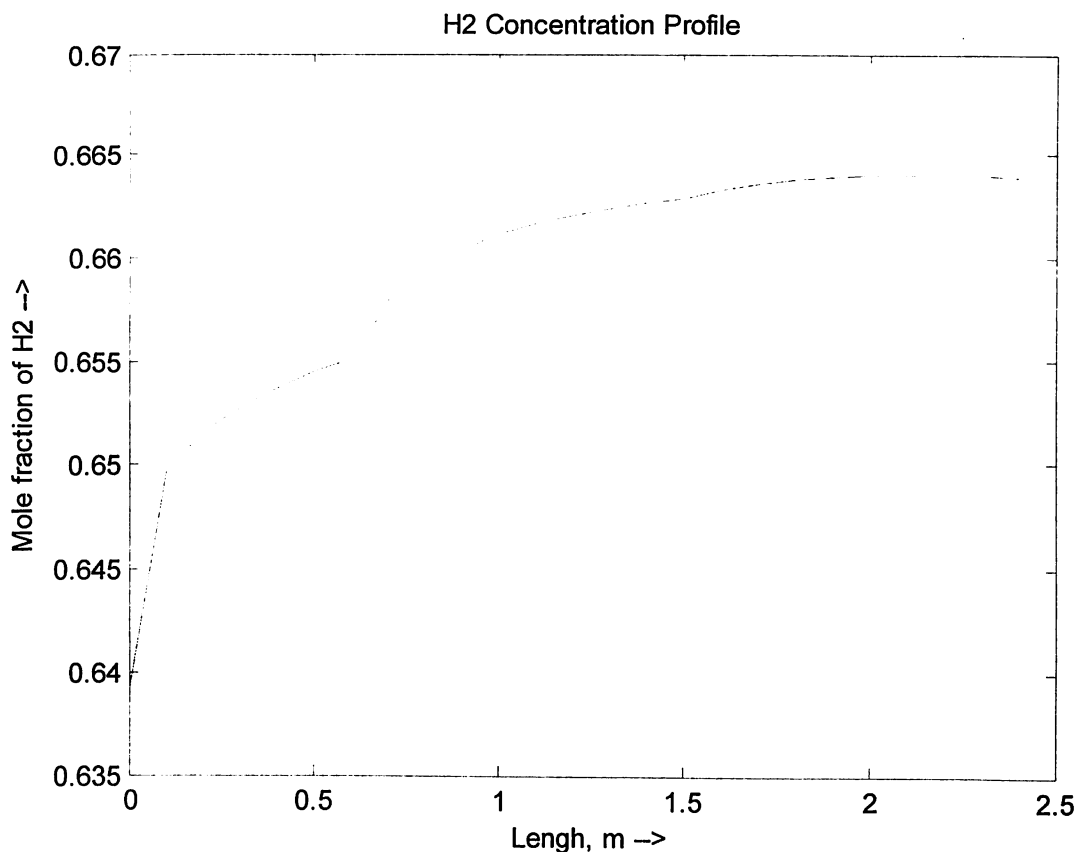


Figure5: H₂ Concentration profile along the length of reactor

4.2 SENSITIVE ANALYSIS

A simulation model can be used to optimize the plant performance by considering the optimal set of operating conditions such as temperature, pressure, flow rate, etc. However, before optimizing, it is desirable to find how sensitive a process is with respect to the decision variables. In this section, effects of variation in process parameters (inlet temperatures, recycle flow rate and pressure) for the aromatics content in the reformat are presented.

4.2.1 TEMPERATURE

The effect of variation in inlet temperature in reactor on the resulting aromatics content the product has been plotted in Figure. 10. For this study the inlet temperatures have been changed. The curves are nearly linear and monotonically increasing. The first, second and third reactors are increasingly more sensitive to temperature changes in that order. The aromatic content increases

with increasing temperature. This is because according to thermodynamics with increasing temperature for endothermic reaction the equilibrium conversion increases therefore aromatic composition increases

Table3: Variation of P,N,A concentrations at the outlet of the reactor with inlet temperature of the reactor

Temperature($^{\circ}$ C)	Paraffins(mol%)	Naphthenes(mol%)	Aromatics(mol%)
470	72	7.5	25
480	71	5	28
490	70	2.7	31.6
500	69	1.5	34.5
520	68	1.7	35.7
525	65	1.35	39

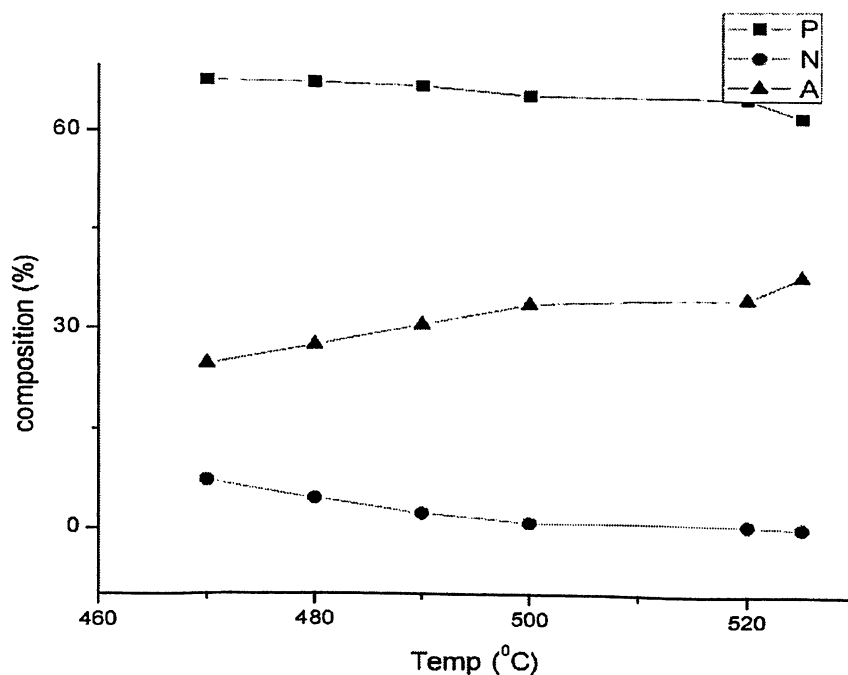


Figure6: Variation of P,N,A concentrations at the outlet of reactor with inlet temperature of the reactor

CHAPTER 5

5 VALIDATION OF MODEL

Simulation was carried out using data listed below that is from Barauni refinery using the same model that is used for simulating naphtha catalytic reformer of Haldia refinery. Simulation is carried for 3 reactors in series until the steady state process is reached. The algorithm of simulation process is same that is used for simulating Haldia refinery

5.1 INPUT

- The inlet temperatures of all reactor I, II and III were 494⁰C.
- The operating pressure was 25kg/cm²
- Flow rate of feed 33.1 MT/day
- Hydrogen to feed ratio=5.22
- Bulk density of feed 600kg/m³
- Weight % of reforming feedstock content of catalytic reforming reactor

P - 41.52

N - 42.8

A - 15.4

- H₂ purity of recycle gas - 91.34(%vol)
- Reactor I Radius R=1m, Length L =0.7m
- Reactor II Radius R=1m, Length L =1.1m
- Reactor III Radius R=0.8m, Length L =1.7m

Simulation was carried out using data listed above using the same simulation code that is used for simulating naphtha catalytic reformer of Haldia refinery. The temperature, arene, cycloalkane,

alkane concentrations (wt%) and hydrogen concentrations(mol%) varying with length of the beds are presented. Simulation is carried for 3 reactors in series until the steady state process is reached. The algorithm of process is same that is used for simulating Haldia refinery.

5.1.1 RESULTS AND DISCUSSION

The temperature, arene, cycloalkane, alkane concentrations (wt%) and hydrogen concentrations(mol%) varying along the length of the beds are as following.

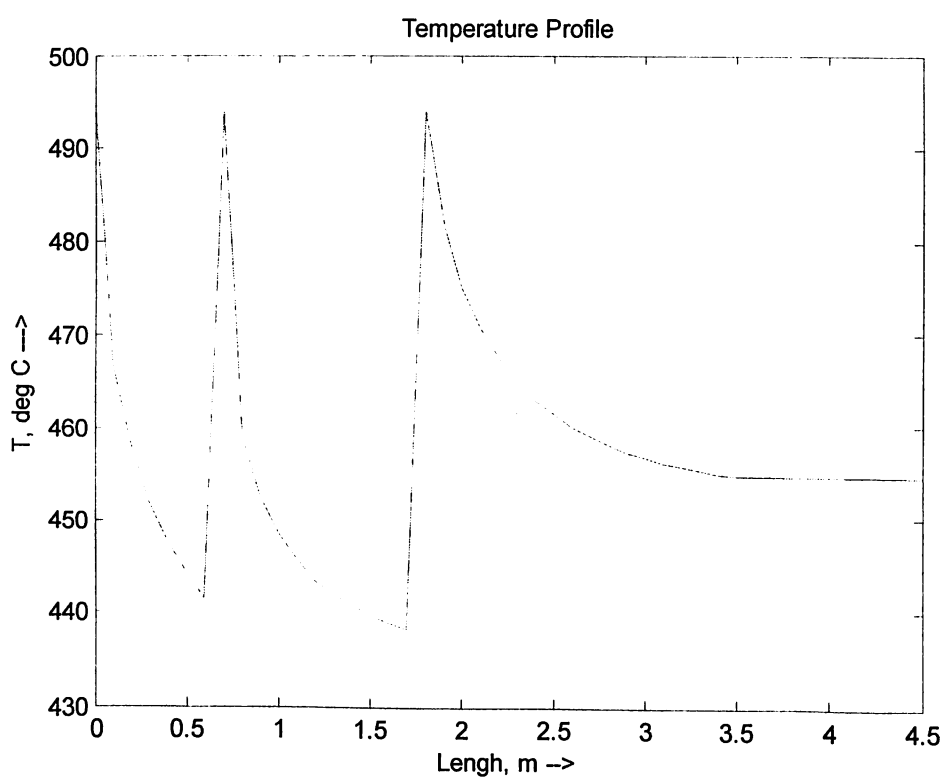


Figure7:Temperature profile along the length of the reactor

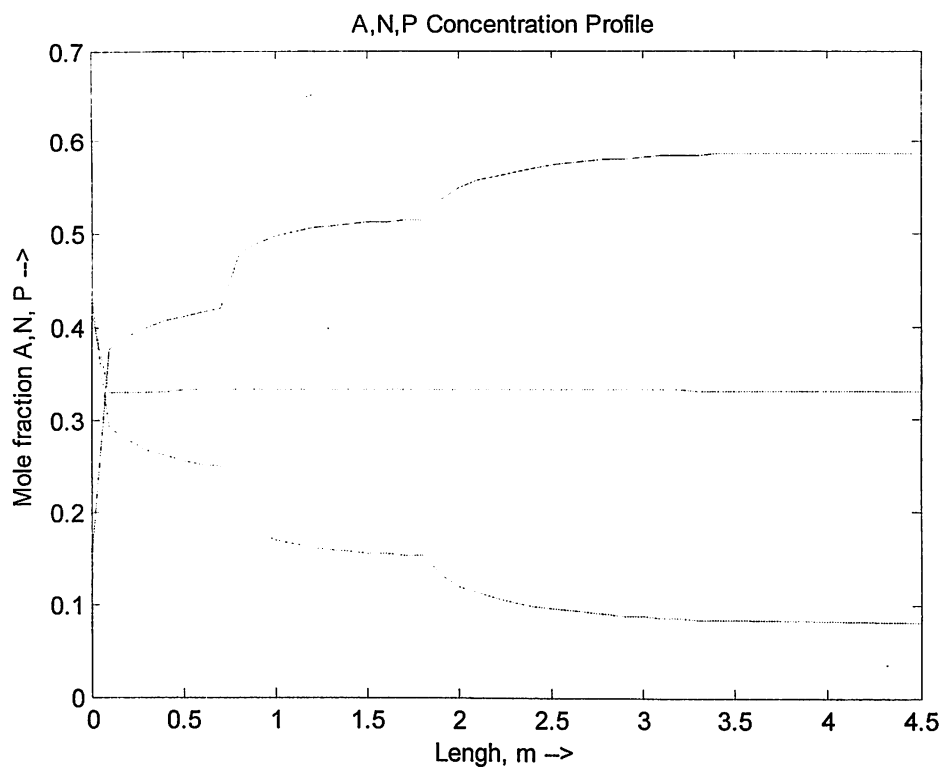


Figure8: A,N,P concentration profile along the length of the reactor

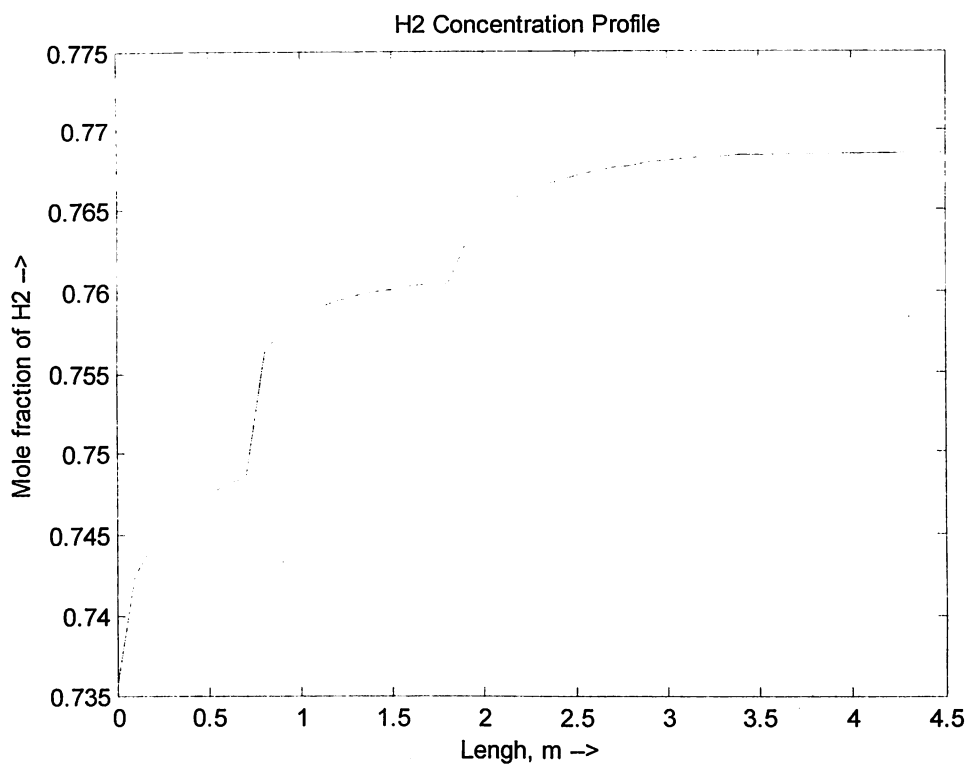


Figure9: H₂ concentration profile along the length of the reactor

The temperature, arene, cycloalkane, alkane concentrations (wt%) that are calculated are very much close to the plant data. Hence the developed simulating model of the catalytic naphtha reformer adequately representing the actual plant behaviour. The comparison of calculated values with the plant values is presented in the table 3.

Table3: Comparison of calculated values with plant values

Outlet temperature of Reactor1		Outlet temperature of Reactor2		Outlet temperature of Reactor3		Aromatic concentration (wt%)		Paraffin concentration (wt%)		Naphthene concentration (wt%)	
Plant	Calc	Plant	Calc	Plant	Calc	Plant	Calc	Plant	Calc	Plant	Calc
440	441.5	425	438	450	454	63.16	58.73	37.95	33.13	5.2	8.14

Above comparison suggest the model rightly simulate the unusual behaviour of larger temperature drop for second reactor as compared to that for first reactor This is with out any tuning of parameters. Further tuning of parameters in the model can be done for specific applications.

CHAPTER 6

6. CONCLUSION

This chapter is essentially a final commentary on how far successful we were in meeting these targets, and also on the techniques and the knowledge we gained during the course of this work. Amongst the major steps the first step, i.e., modeling of catalytic reformer. A mathematical model of the catalytic naphtha reformer was developed with the intention of adequately representing the actual plant behavior. As expected, simulating the complex chemistry of reforming reactions occurring in the fixed-bed reactors was the most crucial part. It was felt that detailed kinetic modeling of the reactions was essential in order to improve the prediction accuracy of the model.

- A model has been developed for simulating catalytic reformer.
- The model has been simulated with industrial data(Haldia refinery).
- The model predicts the reformer performance in terms of reactor inlet temperatures and concentration profiles of each reactor, individual yields of reformate, hydrogen and light ends.
- The temperature affects the aromatics production significantly
- The model has been validated with industrial data(Barauni refinery)

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