

**STEADY STATE SIMULATION OF TUBULAR FLOW
REACTOR USING HYSYS PROCESS SIMULATOR**

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NOVEMBER, 2007.

DECLARATION

I, HENRY ENUDI declare that this work was done by me and has never been presented any where for the Award of a degree. I also hereby relinquish the copyright to the federal university of technology, Minna.

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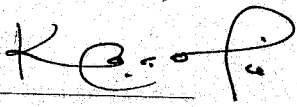
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(External Supervisor)

CERTIFICATION

This is to certify that this project titled "Steady State Simulation of a Tubular Flow Reactor (TFR) using Hysys Process Simulator." under the supervision of Professor K.R. Onifade and submitted to the Chemical Engineering Department, Federal University Of Technology, Minna in partial fulfillment of the requirement for the award of bachelor of Engineering(B.Eng) degree in Chemical Engineering.



29/11/07

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My appreciation goes to my almighty **God** in his love and mercy who has made everything possible for me. Also my loving and caring parents Late Mr. F. N Enudi and Mrs. R Enudi, my brothers and sisters who supported me financially and academically I say thank you.

There is a golden rule that states that when you are climbing to the top do not forget those that helped you as you will certainly need them again when they are no longer rosy up there.

Going by the above claim, I deeply acknowledge and appreciate my project supervisor's effort Prof K. R Onifade who assisted me at every stage with useful comments, corrections and advice.

My appreciation also goes to my noble colleagues and to my friends I say thank you for my stay worthwhile.

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CHAPTER ONE

1.0 INTRODUCTION

The use of simulation has expanded rapidly during the past decades because of the availability of high speed computer and computer workstation. In the chemical process industry, large, realistic nonlinear problems are now routinely being solved through computer simulation. Also, the recent trends toward personal computing and specialized industrial software allude for the expanded use of computers in engineering practice. This means that virtually all engineering computations will shortly be computerized and engineers needs to understand the principles behind available software and how to effectively use software to solve pertinent process engineering problems (Seider *et-al*, 1999).

The increasing use of computer simulation techniques has broadened the usefulness of the scientific approach to engineering. Developing competency in process simulation requires that the engineer develop the following skills:

- A sound understanding of engineering fundamentals: the engineer must be familiar with the physical system and its mechanism in order to be able to intelligently simulate a real process and evaluate the simulation the process cannot be viewed as a black box
- Modeling skills: the engineer has to be able to develop a set of mathematical relations, which adequately describes the significant process behaviour.
- Computational skills: rapid and inexpensive solutions to simulation problems must be obtained. The engineer must be capable of choosing and using the pro computational tool. For realistic problems, the tool of interest is usually a digital computer. The engineer must be able to evaluate and use correctly available commercial software packages.

Since simulation relies upon a scientific rather than empirical approach to engineering, it has served to stimulate developments in inter disciplinary areas such as

bioengineering and environmental engineering. Engineers have found that they have been able to make significant contribution to society through the successful simulations of biological and environmental systems. Chemical process simulations have investigated both the steady-state and dynamic behavior of processes (Douglas, 1988).

The Thermal Hydro-Dealkylation (THDA) is a unit in Kaduna refinery and Petrochemicals Company designed to convert alkylbenzene present in light reformate to benzene by reacting it with hydrogen. The unit consists of pre-fractionation section, reaction section, make-up hydrogen treating section, product stripping section, benzene column, chiller unit, hydrogen purification unit, and heavy aromatic stripping unit. Data generated from this unit are analyzed using the analog control system. The outputs from this control system are displayed in forms of graphs, blinks of lights, level rise or decrease. The constant start-up and shut-down of the thermal hydro dealkylation unit, and the need to obtain trends and behavior of the plant has prompted the need to evaluate the performance of the unit using a process simulator. For an effective performance evaluation of the THDA unit, it goes beyond the study and interpretation of data obtained from the unit operations. The major advantage of this computerized method of evaluation over the ordinary method is that it shows the trend and behavior of the plant that cannot be visualized or obtained experimentally. Such behavior as flow trends, heat flows, concentration profile and pressure drop across reactor length, which may not be obtained from the control panel and other parameters which might be difficult to obtain. The major benefit of the THDA unit includes the production benzene used for manufacture Linear Alkyl Benzene (LAB) and the production of feedstock used in production of other petrochemicals.

1.1 Aim and Objectives:

The aim and objective of this project is to carry out steady state simulation of a tubular flow reactor (TFR) using Hysys Process Simulator.

1.2 Scope of the Project

The scope of this project are the following:

1. To design a tubular flow reactor using steady state stimulation.
2. To determine the effect of temperature, pressure and molar flow across the reactor length.
3. To determine the effect of enthalpy, entropy, reactor duty and mass flow across reactor length.

CHAPTER TWO

2.0 LITERATURE SURVEY

2.1 Thermal Hydrodealkylation (THDA)

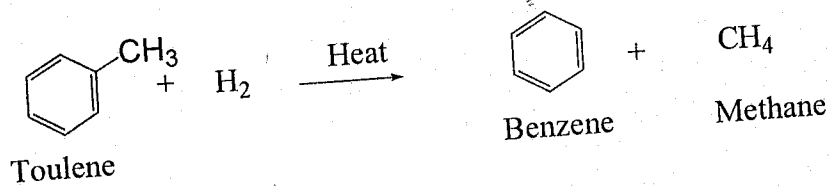
This is a non-catalytic process for the thermal dealkylation of toluene and other alkylbenzene to benzene (Betts *et al*, 1957).

Hydrocarbon feed such as toluene from petroleum reformat and a hydrogen-rich gas are heated in a furnace to an elevated temperature and pumped into a specially design reactor. The reaction effluent goes through a waste heat boiler and is then heat-exchanged with fresh toluene feed. It is cooled further and the gas is separated. The liquid is pumped to a fractionating tower where benzene, recycle toluene, and a very small amount of biphenyl and higher hydrocarbons are separated. The yield of benzene from toluene is greater than 95% of the theoretical. Less than 1% of biphenyl and higher hydrocarbons is formed (Betts *et al*, 1957).

2.2 THEORETICAL EXPLANATION OF THERMAL HYDRO-DEALKYLATION (THDA) UNIT.

Thermal hydrodealkylation in a strict sense refers to the reaction between an alkyl aromatic compound and hydrogen in the presence of heat to produce the parent aromatic hydrocarbon and corresponding alkane. In its simple form, benzene is made from toluene.

This simple reaction can be represented as:-



This type of reaction takes place at high temperatures (i.e. 650-750°C) and it consumes a lot of hydrogen. Fresh charge stock (mixture of naphtha containing high percent of aromatic compound or toluene) is combined with recycled unconverted aromatic mixture and recycled hydrogen which contains some methane and other light

hydrocarbons. This mixture is heated and passed through one or more reactors in series where the desired hydro-alkylation occurs with the release of a substantial quantity of heat. This heat is recovered by the reactor effluent/combined feed exchanger (Chiyoda, 1979).

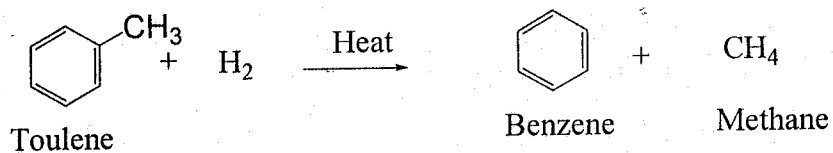
2.2.1. Chemistry

The principal reaction of the thermal hydro dealkylation (THDA) process is the elimination of the alkyl groups from the aromatic nucleus of the alkyl aromatic hydrocarbon if the reaction is conducted at the proper condition and the conversion enhanced by the recycle of unconverted alkyl aromatics. The ultimate products are benzene and light hydrocarbons, principally methane. Alkyl benzene in the theory is a charge stock for the production of benzene through hydroalkylation. From the standpoint of minimum hydrogen consumption and highest benzene yield, the best charge for the above mentioned reaction is pure toluene.

However, for the plant the most % of charge is combined hydrocarbon in the range C₅-C₉. Saturated hydrocarbon hydrocrack more readily than alkyl aromatics dealkylate. So there is a practical limit to their concentration in the charge stock with respect to hydrogen consumption and to loss normally liquid material. Virgin single-ring aromatics produced from petroleum are associated with large quantities of unsaturated hydrocarbons that aromatics extraction step is always required. Prior to any thermal hydrodealkylation sulphur compounds are partially decomposed to H₂S. The feedstock must be relatively free of sulphur. Little amount of sulphur can be allowed. Alkylation of C₇, C₈, and C₉ aromatic compound is about the same as that for the conversion of benzene in the normal cause of operation. It is expected that the reactor inlet temperatures will range from 670°C and the reactor outlet temperatures, before the quench, from 740°C. The rate of demethylation reaction appears to be unaffected by the presence of moderate amount of contaminating materials such as chlorine, sulphur and water.

2.2.2 Demethylation Reaction

The principal reaction between an alkyl benzene and hydrogen in which the alkyl side chain is removed from the aromatic ring



The overall reaction is shown above although the actual reaction is believed to involve several free radical steps. This reaction is strongly exothermic to the extent that about 150kcal/kg of charge is converted at normal efficiency. It is essentially uninhibited by any equilibrium considerations. Its rate increases slowly with an increase in temperature since it takes about 30°C to double the reaction rate.

At low conversion, the product will contain some materials, which has being partially hydrodealkylated. The reactor product will contain benzene, toluene, and ethylbenzene than other components because longer side chains are more readily decomposed.

2.2.3 Process Variables

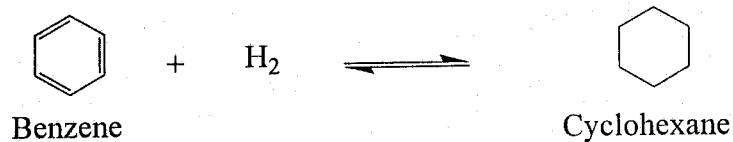
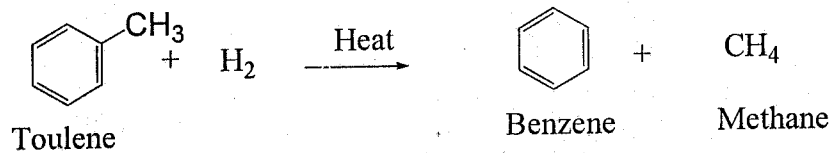
In the preceding section, the reactions that govern the thermal hydrodealkylation were examined. In this section, a review of the variables that govern these chemical reactions will be taken.

The process variables are the following

- *Reaction temperature*
- *Pressure*
- *Recycle gas ratio*
- *Hydrogen purity*
- *Sulphur injection*

2.2.3.1 Reaction Temperature

Let's now examine the reaction of toluene to benzene, the reaction is written for toluene conversion, but it is a representative of any of the hydrodealkylation reactions.



For a light reformer feed stock, reactor inlet temperature will range from 670°C – 760°C. At these temperature levels, the less favourable hydrogenation equilibrium provides somewhat a limit to the extent to which these side reactions occur. The use of excessively high temperature could lead to loss due to direct rupture of the aromatic ring.

Consequently apart from the plant design aspect, there is an upper limit to the allowable reaction temperature. As already mentioned, this highly exothermic reaction occurs very rapidly, especially with compound as heavy as C₁₀. Lighter paraffins such as ethane or propane hydrocracked at much slower rate and may be expected from the kinetic data to survive a hydro dealkylation reaction despite the favourable equilibrium towards further hydrocracking to methane.

2.2.3.2 Pressure

Pressure is a fixed process condition. Its value is fixed by design taking into account the feed composition and conversion level. The pressure is generally in the range of (2.50*10⁶ - 2.90*10⁶) N/m². Increase in the reactor pressure increases the residence

time in the reactor. This results in a greater loss of rings to light paraffin gases since this particular reaction involves a step which is favoured by higher pressure. A decrease in pressure on the other hand, reduces the residence time and hence conversion and also encourages carbon formation.

2.2.3.3 Recycle Gas Ratio

The recycle gas ratio is defined as the number of moles of total gas divided by the number of moles of total liquid charged. The recycle gas has two functions; the first one is that it provides hydrogen to the reaction zone. The second is that it acts as a heat sink in the reactor. An increase in recycle gas ratio reduces the residence time somewhat. The greater volume per unit time of gas tends to take away the heat of reaction faster than before. This results in a slight decrease in conversion; other conditions being constant. A reduction in recycle gas ratio on the other hand increases the residence time and thereby increases conversion. The usual design recycle gas ratio is fixed at 10 to 12. However, there is no objection to an increased gas ratio provided a satisfactory conversion is achieved. Such operation is considered beneficial because it keeps the reactor internals clean.

2.2.3.4 Hydrogen Purity

Hydrogen purity and hydrogen partial pressure are both quality and quantity of hydrogen which are very important. The process must satisfy the stoichiometric demand of the hydrodealkylation reaction. Though hydrogen must be available for hydrodealkylating saturated hydrocarbons contained in the charged stock, some hydrogen is also consumed during the cracking of aromatic ring to light paraffinic fragments. The basic side reactions are divided as the evidence of the first and second reaction is not experimental. It actually takes place except in unusually high temperature. Reaction 3, however, is believed to be of considerable importance. The decomposition of methane is thoroughly endothermic and will occur at normal operating pressure. Methane is stable

provided the hydrogen purity of the system is not too low. We require a high temperature and hydrogen purity in excess of about 55% to normally avoid massive carbon formation. For design purposes, it is to allow some variation in the reactor, minimum hydrogen purity has been fixed at 58%. If excess hydrogen is available, it is advantageous to operate at the highest possible purity to encourage reaction rate and also to maintain a greater gap between the equilibrium line and the actual operating condition.

2.2.3.5 Sulphur Injection sulfur

Sulphur contained in the aromatic feed will be largely alkyl thiophene. In the thermal hydrodealkylation process, this is dealkylated to thiophene, with minor conversion of the thiophene to hydrogen sulphide (H_2S). The minimum sulphur content of the aromatic feed is therefore dependent on thiophene specification of the product (benzene). If the sulphur content of the feed and make-up hydrogen is too low to maintain this level, provision has to be made in the reactor. The presence of the small amount of H_2S in the recycle gas is an important factor in the control of ring loss.

If the sulphur level in the system is reduced too low such that aromatic hydrogenation and ring loss occurs, the reaction will be highly exothermic and hydrogen concentration will be quickly reduced. This can be avoided by maintaining a proper level of sulphur. The maintenance of about 1-2 grains of H_2S per 100 cubic meter of feed (15-30 mole ppm) is believed to be essential to forestall demethylation reaction. This small amount of sulphur will not cause any product purity problems.

2.3 PROCESS FLOW DESCRIPTION OF THERMAL HYDRO-DE-ALKYLATION UNIT (THDA)

The THDA unit consists of pre-fractionation section, reaction section, and make-up hydrogen treating section, product stripping section, and benzene column. In addition

The reactor effluent is cooled in the three exchangers by exchanging heat with the feed. The amount of heat transferred in the intermediate combined feed exchanger is generally controlled by sending a portion of the hot combined feed exchanger effluent to a steam generator and the remaining portion through the intermediate combined feed exchanger. The cold combining feed exchanger effluent is further cooled in a condenser. The cooled reactor effluent is separated into two phases, gas and liquid phase in the product separator. From the product separator, liquid is generally sent under level control to a stripper tower where the light hydrocarbon such as methane and ethane are stripped off. The stripper feed is heated in the stripper feed exchanger using the stripper bottoms material as a heating medium. The bottom liquid under level control is sent by to the clay tower treaters; prior to this the feed stripper is preheated with the bottom outlet of the clay treating tower. The product is cooled in a Preheater feed exchanger before sending it to the fractionator benzene column where at the top lighter products like methane, ethane etc are stripped off (Chiyoda, 1979).

From the fifth (5th) tray the product (benzene) is cooled with trim cooler and with a benzene pump under control of FRC and DTRC is sent to storage or to detergent alkylation. The bottom of the benzene column under level control is partly sent to a surge drum mixed with fresh feed, and the other part is sent to a heavy aromatic stripper where it is separated into light aromatics and sent back to the benzene column as reflux and bottom through the reboiler. The bottom of the heavy aromatic stripper is sent to the fuel oil tank (Chiyoda, 1979).

The demethylation reaction being one of the most important of the thermal hydrodealkylation processes is carried out in THDA Reactor. The THDA Reactor is a continuous plug flow process non-catalytic Tubular Reactor. Tubular Reactors are essentially vertical cylindrical vessels (Perry, 1993)

2.4 REACTORS

The plug flow reactor (R01) is one of the major equipment of the thermal hydrodealkylation (THDA) unit of Kaduna Refining Company (KRPC).

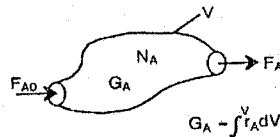
The purpose of the plug flow reactor is to react the light reformat (containing toluene, xylene, E-benzene e.t.c) with hydrogen. The reactor is equipment with high conversion of reactant per volume, low operating cost, continuous operation, and good heat transfer. It is in a series of I and II. The effluent of reactor I is the feed of reactor II. The reactor is made of full carbon due to the corrosive nature of hydrocarbon. Tube length is 2500mm, wall thickness is 5.0mm, number of tubes in reactor is 50, and void fraction.

2.4.1 Design equations for PFR reactor

Energy balance about the tubular plug flow reactor is expressed as follows:

IN - OUT + GENERATION = ACCUMULATION

$$F_{A0} - F_A + \int_0^V r_A dV = \frac{dN_A}{dt}$$



At steady state-

$$\frac{dN_A}{dt} = 0$$

Differentiating, that gives-

$$\frac{dF_A}{dV} = r_A$$

For single reactions in terms of conversion-

$$X = \frac{(F_{A0} - F_A)}{F_{A0}}$$

The differential form of the PFR mole balance is-

$$F_{A0} \frac{dX}{dV} = -r_A$$

The integral form is-

$$V = F_{A0} \int_0^X \frac{dX}{-r_A}$$

This is derived as:

$$\frac{dF_A}{dV} = r_A$$

$$F_A = F_{A0} - F_{A0}X$$

$$dF_A = 0 - F_{A0} dX$$

$$-F_{A0} \frac{dX}{dV} = r_A$$

$$\boxed{F_{A0} \frac{dX}{dV} = -r_A}$$

$$\frac{F_{A0} dX}{-r_A} = dV$$

$$t=0 \quad X=0$$

$$\boxed{V = F_{A0} \int_0^X \frac{dX}{-r_A}}$$

Derivation of rate equations for non- isothermal reactor conditions is an involved process requiring experimental data, trial and error procedures, and calculated guesses.

There are three main parameters are necessary to derive the rate equation:

- The order of the reaction, n
- The rate constant, k
- The activation energy, E

Calculations are not perfect, since some reactions takes place in the preheat section of the reactor, and the outlet section, where it is cooler. The reactor is non-isothermal, but by using the Hougen and Watson method, the data can be reduced to isothermal conditions.

The idea of this section is to find a method for deriving approximate value for the rate constant.

2.4.1.1 Design parameters

- **Reactor Volume**

A good place to start is the equation for the equivalent reactor volume that is the volume under non-isothermal conditions applicable to the reactor design and is approximated by isothermal profiles. The equation, the Hougen-Watson method (Fogler, 1986) is as follows. $V_R = \int \exp(E/R(1/T_1 - 1/T))dV$

Where, T is the reactor temperature and E is the activation energy. Calculation of V_R requires knowledge of temperature profile along the reactor tube, and the activation energy, E, to solve this equation; the rate is based solely on the continuity equation:

$$FdX = rdV_R$$

There are two methods used to determine the activation energy. The Arrhenius' formula and the shortcut method.

The Arrhenius' method is a trial and error procedure calculated at several temperature levels. A value of E is guessed and with the values from a temperature profile, V_R is derived graphical integration. Then from this value rate constants can be derived. These values are expressed in Arrhenius form:

$$k = k_o e^{-E/RT}$$

If this consistent with that used in the calculation of V_R . The whole procedure has to be repeated with a better approximation of E.

- **Temperature profile**

Temperature profile along the reactor is the second calculation for determining the volume of the reactor. There are three assumptions in determining the temperature profile:

- Wall temperature is known
- Physical properties of the reaction mixture are known
- Flow composition is known

A temperature profile can be calculated using Sieder-Tate equation, (Froment, Pijcke, Goethals, 1960):

$$\phi = t_o - t_m / t_o - t_s VS.mc_p / k_R L$$

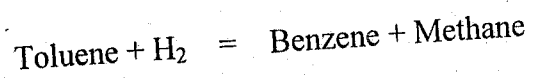
This equation can measure the temperature of the gas, t_m , at any point along the reactor: this is done by a graphical method, since the only unknowns are t_m and L

5. Selecting Components

- On the fluid property dialog box, **Components** tab was clicked on.
- **n-Nonane** was typed and **HYSYS** showed the formula **C₉H₂₀**
- The **Add Pure** button was pressed and n-Nonane was selected.
- The above selecting components procedure was repeated for the following components.
 - **n-Decane**
 - **Benzene**
 - **Toluene**
 - **m-Xylene**
 - **E-Benzene**
 - **n-PBenzene**
 - **Ethylbenzene**
 - **Hydrogen**
 - **n-BBenzene**
 - **Methane**

6. Defining the reaction

Move to **Reactions** tab the reaction was



7. Selecting the Reaction Components

From **RXN Components**.

The **Add component** was pressed.

Add This Group of Components was pressed.

The **Simulation Basis Manager** was returned to

8. Creating the Reaction

In the **Reaction**, **Add Rxn** was pressed

Kinetic type was selected.

Add Reaction was pressed.

The **Kinetic Reaction Rxn-1** page was displayed

In the **Component** column, the **Add** component was clicked on.

Select **Toluene** was selected from the dropped **Drop-Down** arrow.

This was repeated for **Hydrogen, Benzene** and **Methane**.

In the **Stoich Coeff.** Corresponding to **Toluene**.

-1 was typed for **Toluene**.

-1 was typed for **Hydrogen**

1 was typed for **Benzene**.

1 was typed for **Methane**

It is noted that the **Balance Error** is 0.0 indicating that the reaction was mass balanced.

The next step was to move to the **Basis** tab.

The **Basis** was selected to be in **Partial Pressure**.

Rxn phase = Vapour phase

For the **Base Component**, **Toluene** was chosen.

Then the **Parameters** tab was advanced to.

For forward reaction:

3.685 e⁻⁸ was entered for A

96.686 was entered for E.

The status indicator at the bottom of the **Kinetic**

Reaction property view changes from **Not Ready** to **Ready**, indicating that the

Reaction was completely defined.

The **Kinetic Reaction** property view was closed.

The **Reactions** view was closed.

9. Creating a Reaction Set

The **Add Set** button in the **Reaction Sets** group was clicked on.

DEDICATION

I wish to dedicate this project to God almighty.

In the **Active List** for the cell called <empty> from the **Drop-Down** arrow, Rxn-1 was selected.

The Rxn-1 was renamed to Demethylation reaction

The **Close** button was pressed.

10. Making the Reaction Set Available to the Fluid Package

Set-1 in the **Reaction Sets** on the **Reactions** tab was clicked on.

The **Add to FP** button was pressed; the **Add "Set-1"** view appeared.

The **Add Set to Fluid Package** button is pressed on.

11. At this point, the work was saved as a **New Case** and a name **Design Data** was given to it as a choice.

12. Installing the Feed Streams

13. Installing the Reactor.

The **Plug Flow Reactor** is double clicked on from the **Object Palette**. The **REACTOR** property View appeared and The **Connection** page was having focus.

The Reactor was renamed as **TDR**

The inlet and outlet streams were attached.

The inlet and outlet streams were attached.

Inlet dropdown was named as **Reformate Feed**.

A Second **Inlet** Stream was named **Hydrogen**

Outlet dropdown was named as **Product**.

Energy (Optional) stream was renamed as **TDR Duty**.

The reaction tab is clicked on and **TDR** is selected from the **Reaction set**.

The reaction Rating was clicked on and Reactor Tube dimensions were entered:

Diameter of 0.2 m

Length of 2.5 m

Number of tubes 1

Wall thickness 0.0050 m

The reaction Rating was clicked on and Reactor Tube Packing dimensions were entered:

Void Fraction of 1.000

From the Worksheet Tab the following were specified for Reactor Effluent:

- Temperature ($^{\circ}\text{C}$): inlet 632 and outlet 732
- Pressure (kPa): inlet 3177 and outlet 3030
- Molar Flow (m^3/hr): 100 and 1000 for hydrogen and reformat stream respectively.

On the composition tab the following were entered as the composition of the reformat stream:

- n-Nonane: 0.1261
- n-Decane: 0.0127
- Benzene: 0.0881
- Toluene: 0.2974
- m-Xylene: 0.1751
- E-Benzene: 0.0395
- n-PBenzene: 0.1939
- Hydrogen: 0.0000
- n-BBenzene: 0.0672
- Methane: 0.0000

The hydrogen stream was pure hydrogen.

The same was repeated for **Reactor (TDR)** for 2005 operating data but the inlet and outlet temperatures was 632°C and 712°C respectively. The inlet and outlet pressure was 3177 kPa and 2712 kPa respectively. The molar low for hydrogen and reformat stream was $92.24 \text{ m}^3/\text{hr}$ and $1114 \text{ m}^3/\text{hr}$ respectively.

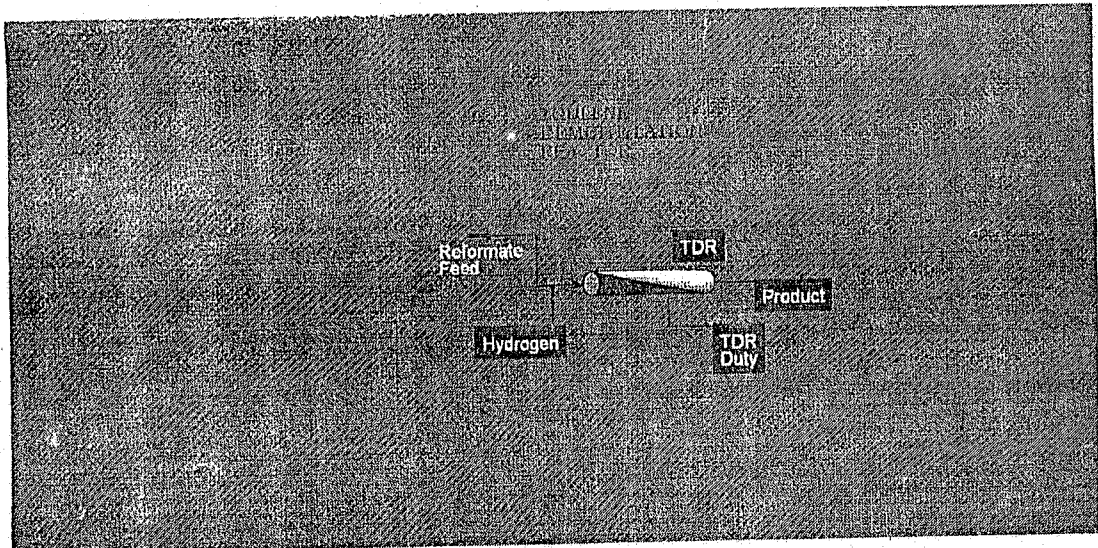


Figure 3.1 The Process Diagram for the Steady State Simulation of a Tubular Flow Reactor.

CHAPTER FOUR

4.0 RESULTS AND DISCUSSION OF RESULTS

4.1 Results

The results of the steady state simulation of tubular flow reactor using Hysys are shown below:

Table 4.1: Stream Properties of Reactor R-01 for 1993 and 2005 Respectively

Specification	Results
Total Volume	3.927 m ³
Length	2.500 m
Diameter	0.2000 m
Wall Thickness	5.000e-003 m
Void Fraction	1.0000
Void Volume	3.927 m ³
Number of Tubes	50

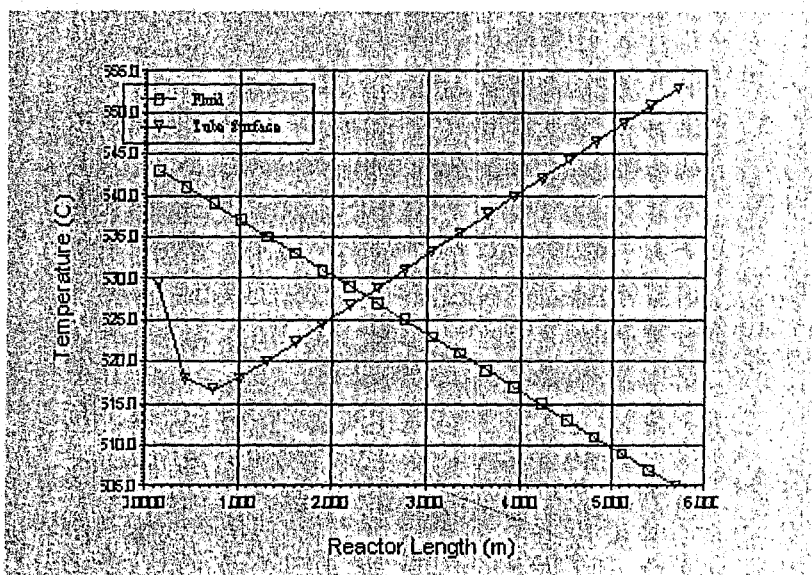


Figure 4.1 Plot of Temperature (°C) against Reactor Length (m) for Reactor (RO2) Design Parameters

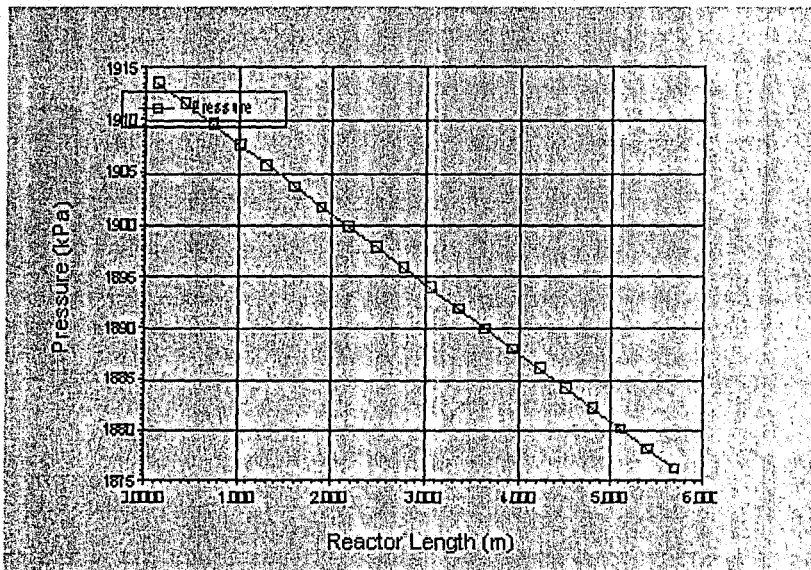


Figure 4.2 Plot of Pressure (kPa) against Reactor Length (m) for Reactor (RO2) Design Parameters

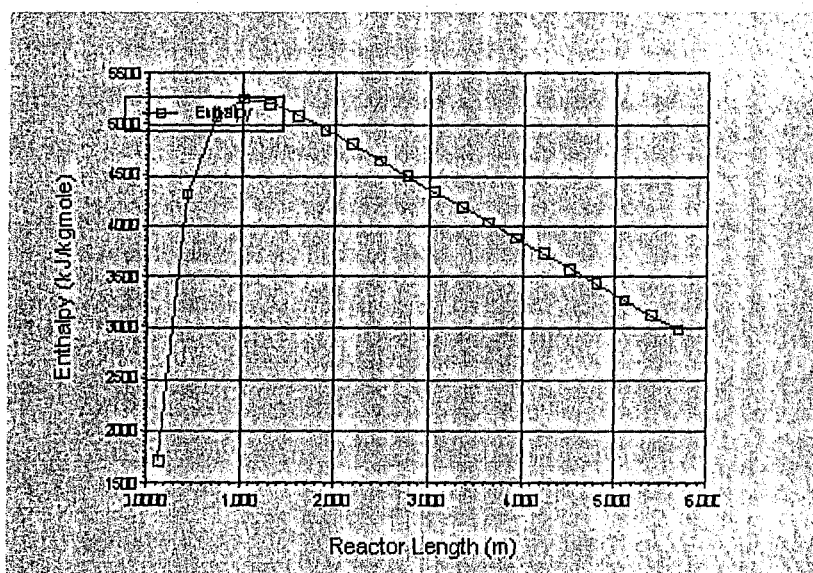


Figure 4.3 Plot of Enthalpy (kJ/kgmol) against Reactor Length (m) for Reactor (RO2) Operating Parameters

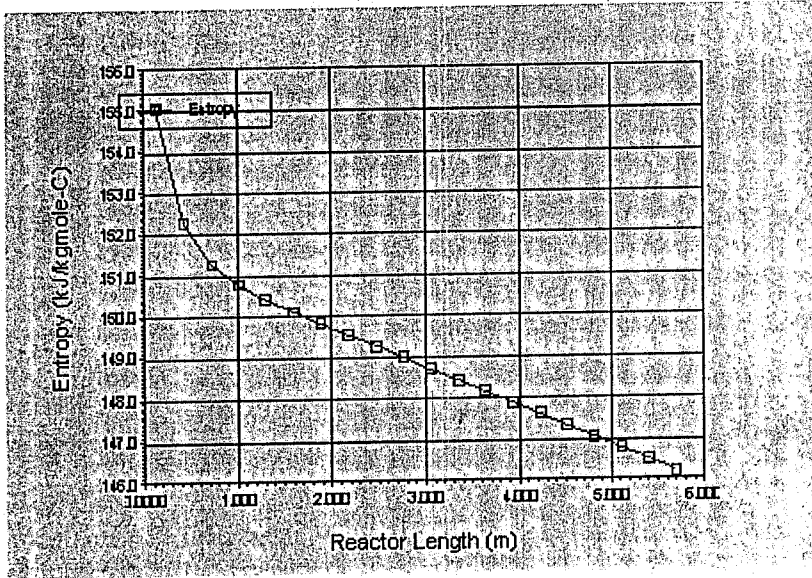


Figure 4.4 Plot of Entropy (kJ/kgmol °C) against Reactor Length (m) for Reactor (RO2) Design Parameters

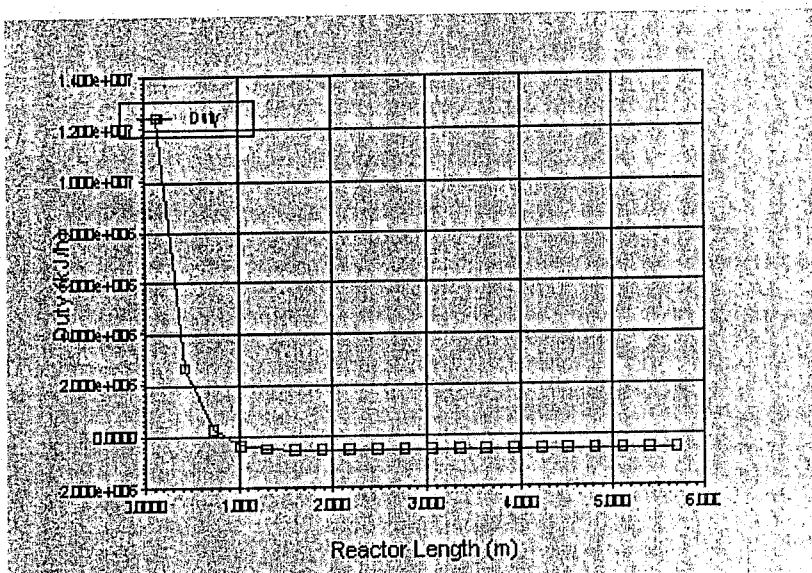


Figure 4.5 Plot of Reactor Duty (kJ/hr) against Reactor Length (m) for Reactor (RO2) Design Parameters

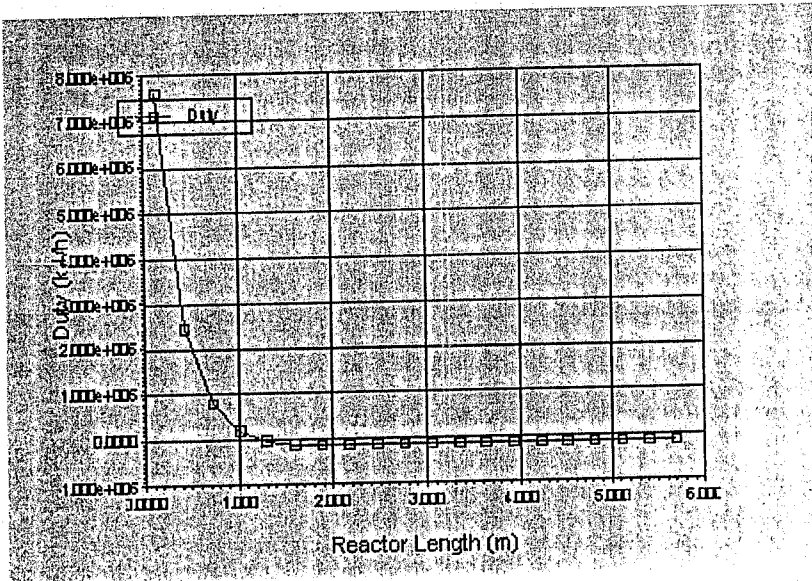


Figure 4.6 Plot of Reactor Duty (kJ/hr) against Reactor Length (m) for Reactor (RO2) Operating Parameters

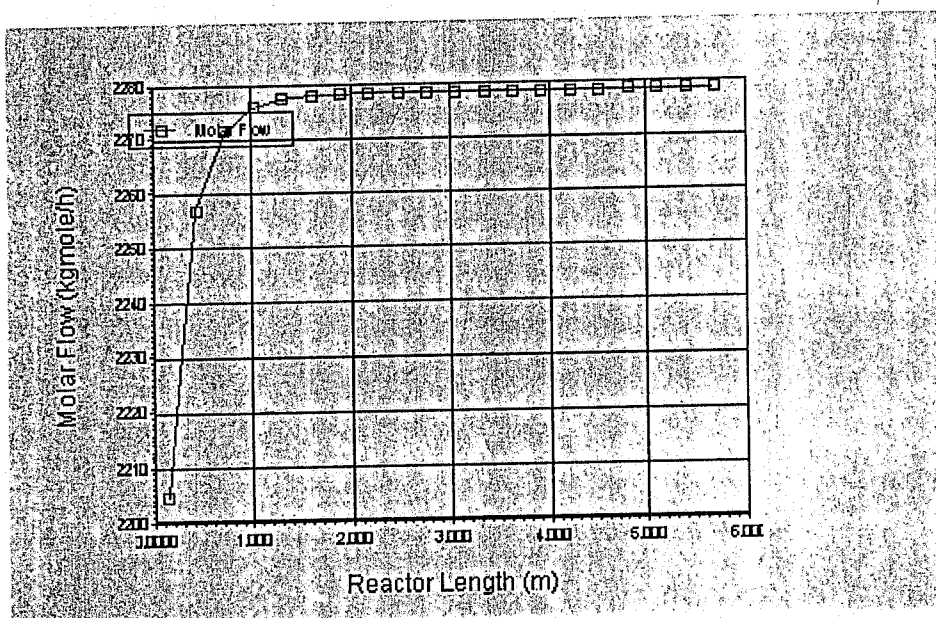


Figure 4.7 Plot of Molar Flow (kgmol/h) against Reactor Length (m) for Reactor (RO2) Design Parameters

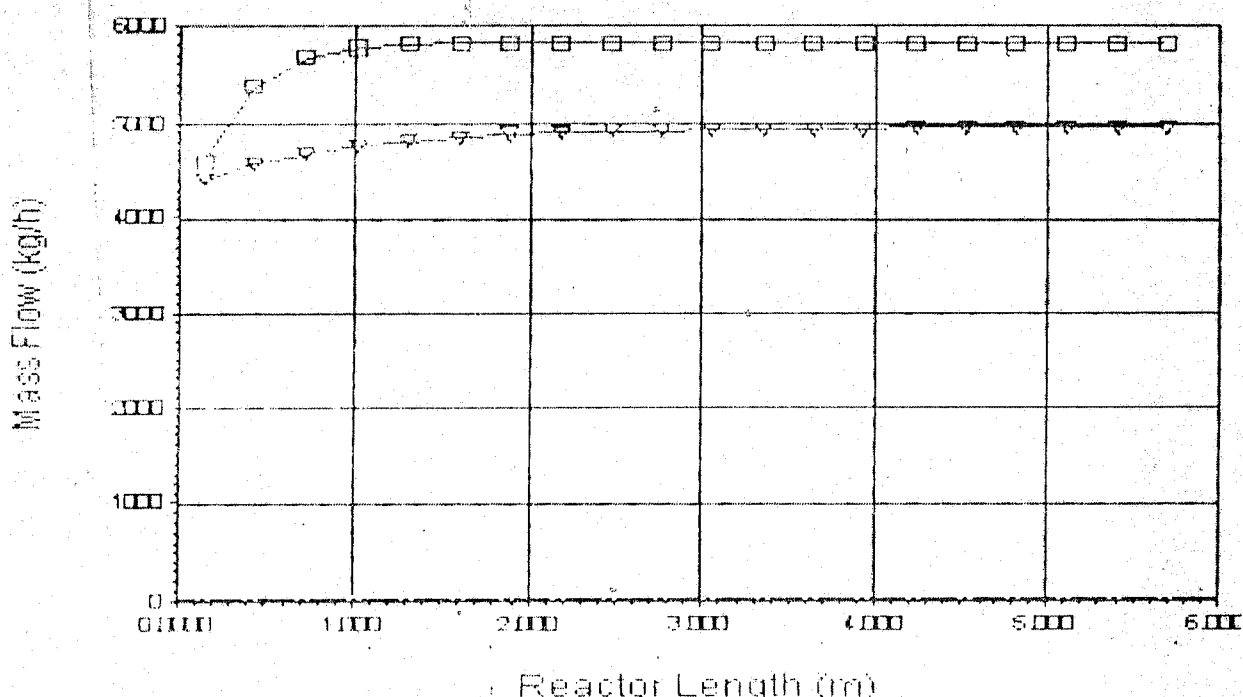


Figure 4.8 Plot of Mass Flow (kg/h) against Reactor Length (m) for Reactor (R02) Operating Parameters

4.2.1 Discussion of Results

Figure 4.1 shows the plot of reactor tube surface temperature against reactor length. The plot shows that the reactor tube surface temperature decreases from 530°C to 517°C from reactor length of 0 m to 0.8 m and increased from 517°C to 558°C from reactor length of 0.8 m to 5.8 m.

The plot of pressure against reactor length is shown in figure 4.2 the plot shows that the reactor pressure dropped from 1913 kPa to 1880 kPa from reactor length of 0 m to 5.8m.

This result conforms with literature which states that pressure drop across a tube due to effect of resistance to flow canes by frictional forces. Figure 4.3 shows the effect of enthalpy change across the reactor length. There was a sharp increase in the find enthalpy from 1700 kJ/kg mole to 5250 kJ/kg mole from reactor length of 0.15 m to 1.00 m and a gradual decrease from an enthalpy of 5250 kJ/kgmole to 3000kJ/kgmole from reactor length of 1.00 m to 5.70 m

length of 0.2 m to 0.7 m then a gradual decrease from 151.3 kJ/kg mole-c to 146.3 kJ/kg mole-c corresponding to a reactor length of 0.7 m to 5.7 m.

The plot of reactor duty against reactor design parameters shown in figure 4.5 the plot shows that there was a sharp drop in reactor duty from 1.280×10^7 kJ/h to 1.800 kJ/h corresponding to a reactor length of 0.2 m to 1.0 m from a reactor length of 1.0 m to 5.7 m the reactor duty was constant at -1.80×10^6 kJ/h.

Figure 4.6 shows the plot of reactor duty against reactor length for reactor operating parameters. There was a sharp decrease in reactor duty from 7.700×10^6 kJ/hr to -0.200×10^6 kJ/hr from reactor length of 0.2 m to 1.3 m. From a reactor length of 1.3 m to 5.7 m, the reactor duty was constant at -0.200×10^6 kJ/hr.

Figure 4.7 shows the plot of molar flow from 2205 kgmole/hr to 2278 kgmole/hr from reactor length of 0.15 m to 1.6 m. From a reactor length of 1.6 m to 5.7 m, the mole flow constant at 2278 kg mole/hr Figure 4.8 shows the plot of mass flow against reactor operating parameters. Mass flow rose sharply from 4600 kg/hr to 5800 kg/hr from a reactor length of 0.1 m to 1.6 m.

The result obtained from simulation of the thermal hydrodealkylation unit

using Hysys for both the design and operating parameters are tabulated in Table 4.1. the operating parameters used in running the plant in the year 1993 and 2005 respectively.

As it can be observed, the inlet and outlet temperature in the years 1993 is 517⁰C and 530⁰C while that of year 2005 is 517⁰C and 558⁰C respectively.

The inlet and outlet pressure is 1913kpa and 1880kpa while that of year 2005 is 150.6kpa and 450kpa respectively.

From literature (Chiyoda, 1979) the temperature required for the thermal hydrodealkylation reaction is 517⁰C - 530⁰C.

The results obtained above shows that the performance of the reactor (TFR) from the period it was commissioned to the present state has dropped significantly and the plant is due for maintenance or complete replacement.

In support of this observation is regular starting and shut down of the plant.

CHAPTER 5

5.0 CONCLUSION AND RECOMMENDATIONS:

5.1 Conclusion

The following conclusions could be drawn based on these designs;

1. Steady state simulation of tubular flow reactor using Hysys process simulator has been carried out.
2. The tubular flow reactor temperature dropped from 540°C to 480°C across a reactor length of 5.6m
3. An optimum enthalpy of 800 kJ/hr is achieved at reactor length of 6.0m.

5.2 Recommendations

Following the desire to carry out steady state simulation of a tubular flow reactor, the following recommendation can be made:

1. Dynamic simulation of tubular flow reactor should be carried out
2. Research work should be carried out to determine the steady state and dynamic simulation of other process equipments.

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