

METHOD OF LINES TO NON-LINEAR PARTIAL REACTOR MODEL EQUATIONS

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ABSTRACT

The partial reactor model equations under study evolved with stringent constraints from continuous regeneration reactor plant for upgrade of hydro treated feed naphtha into reformat gasoline. Appropriate rate of feed conversion per time was generated from the principles of material and energy balance maintaining a two-dimensional homogeneous constraint. The partial models were converted to a set of ordinary differential equations applying method of lines MOL of finite difference approximation of the spatial derivatives and integrated with respect to time domain using Mat-lab ode-solver-23. The model results gave the following deviations on reactor R3 outlet stood at naphthene 8.09, paraffin 0.03, aromatics -2.20 and temperature, 0.39. The deviations were most credible and plausible at minimal values suggestive of optimality of the reactors. Finally, open loop sensitivity analysis showed temperature, pressure and catalyst activity are the major variables to striking a balance economically.

Keywords: Reactor-model-equations, method of lines MOL; chemical species, Continuous-catalyst-regenerator-reactors.

INTRODUCTION

This paper deals primarily with the systematic mathematical approach of resolving complex reactions and/or reactor model equations. These are plug flow partial differential equations developed from the operations of a continuous catalyst reactor stacked in series. The reactor units upgrades low fractions feed from the distillations column, after being treated with some solvent chemicals to remove corrosive agents on the feed naphtha, that would have naturally corrode the system condensers, heaters and heat exchangers tubes over some periods. The equation models for the unit reactors were developed from the principles of conservation of mass and energy and neglecting momentum transfer.

Ferchneider and Mege (2004) investigated on fixed bed reactors with a single fluid phase for reaction processes catalyzed by a solid phase. They made use of a one-dimensional model and separately resolved the equation of conservation of mass and energy, and momentum. The calculation was based on the multi-dimensional model and the simultaneous resolution of the local conservation equations. And, in most cases previous research focused on fixed-bed and /or packed bed reactors which involves catalyst activity drop over some time.

Hu and Zhu (2004), presented molecular modeling and optimization for the naphtha catalytic reforming process; the molecular modeling approach also focuses on producing high octane number gasoline by reforming reactions in three sequencing fixed bed reactors. They made use of the naphtha consisting of molecules from C₅ to C₁₀ including paraffin iso-paraffin,

naphthene and aromatic. The molecular kinetic network consisted of paraffin cracking, naphthene side-chain cracking, aromatic side-chain cracking, ring opening, ring closure, paraffin isomerization, dehydrogenation and hydrogenation. Based on this reaction network molecular model for catalytic reforming was formulated.

The (Wordu, 2009); and (Oboho, 2005) developed a system of non-linear intractable reactor equations handy for evaluation using the optimized parameters values of reactor plant obtained after several search for convergence was achieved at 96-iterations.

(Wordu, 2009); (Oboho, 2005) adopted the lumping-chemistry material balance development with respect to naphthenes, paraffins, aromatics, hydrogen gas and enthalpy changes for the four reactions taking place in the reactors. An industrial plug flow reactor operating adiabatically, quantity of heat input Q and heat output Q is equal to zero.

Therefore, the present paper thrives to elucidate the mathematical sequence of resolution of the partial differential reactor equations. The lumped partial differential equations were broken into ordinary differential equations applying Method of lines MOL numerical method. The process of applying MOL to resolve nonlinear equations with lumped parameters stems from the fact that it removes stiffness imposed on the model equations, which analytical techniques should have been faced with.

REACTOR MODEL DEVELOPMENT

Model Formulations/Assumptions

The positive constraints to develop the mathematical model equations for the industrial reactor operations are as follows.

1. The model derivations accounted for the dynamics of the reactors stacked in series; a two-dimensional homogeneous system model.
2. Model formulations are based on reactor systems that maintain a continuous catalyst regeneration which compensates for drop in catalyst functions depletion effects over periods.
3. Radial variations of both temperature and concentrations are neglected.
4. Model developed from the principles of mass and energy does not incorporate catalyst deactivation function
5. An open-loop response system is assumed
6. Finally. Internal and external diffusions are not taken into account.

MATERIALS

The appropriate kinetic parameters are stated tables 1, 2, 3, 4 and 5. The parameters were obtained from optimization search for best value suitable for the reactor plant operations.

Table 1: Kinetic Parameters A_0 , K_p , K_f , K_c and ΔH_R for the reactions

Reactions 1, 2, 3 & 4	Parameters		
	Pre-exponential constant, A_0	Equilibrium Constant, K_p	Heat of Reaction, ΔH_R Kj/Kmol of H_2 liberated
Conversion of naphthenes to Aromatics	1.19×10^8	$1.0404 \times 10^6 \exp(46.15 - 212700/RT)$	70928
Conversion of paraffins to naphthenes	4.170×10^{13}	$9.869 \times 10^3 \exp(36950/RT - 712)$	- 44185
Naphthenes cracking	4.5881×10^{18}	-	- 51860
Paraffins cracking	4.5881×10^{18}	-	- 51860

Table 2: Equilibrium Constants, K_p

Reactions	Parameters
1, 2, 3 and 4	Equilibrium constant, K_p
Conversion of naphthenes to aromatics	$1.0404 \times 10^6 \exp(46.15 - 212700/RT)$
Conversion of paraffins to naphthene	$9.869 \times 10^3 \exp(36950/RT - 712)$
Naphthenes hydrocracking	-
Paraffins hydrocracking	-

Table 3: Heat of Reactions, ΔH_R

Reactions	Parameters
1, 2, 3 and 4	Heat of Reactions, ΔH_R , kJ/Kmol of H_2 liberated
Conversion of naphthenes to aromatics	70928
Conversion of paraffins to naphthene	- 44185
Naphthenes hydrocracking	- 51860
Paraffins hydrocracking	- 51860

Table 3: Arrhenius Constants or Pre-exponential Constants, A_0

Reactions	Parameters
1, 2, 3 and 4	Arrhenius Constants, A_0
Conversion of naphthenes to aromatics	1.19×10^8
Conversion of paraffins to naphthene	4.170×10^{13}
Naphthenes hydrocracking	4.5881×10^{18}
Paraffins hydrocracking	4.5881×10^{18}

METHOD**Material Balance**

Fundamentally, for 1mole of a fresh feed lumped components C_5, C_6, C_7, C_8 are transformed and/or upgraded into products (stable aromatics) will be monitored by the application of the law of conservation of mass, energy and momentum on a differential volume element of the reactors in Nigerian Petroleum Refinery located Alesa-Elleme. But, the law of conservation of momentum has no relevance in this research; hence, it is neglected. Therefore, the law of conservation of mass and energy prevails.

For any given material component i in the reactor, of a cross-sectional area $A_C.dL$ the material balance for 1mole of the species i is stated mathematically as,

$$F_{AO} \rho_i = F_{AO} \rho_i + \partial \rho_i + (-r_i) \rho_i A dL + A \frac{\partial \rho_i}{\partial t} dL \quad (1)$$

Rearranging equation (1) gives

$$-A \frac{\partial \rho_i}{\partial t} - F_{AO} \frac{\partial \rho_i}{\partial L} = (-r_i) \rho_i A \quad (2)$$

But,

$$y_i = \frac{\rho_i}{\rho_{Feed}} \quad (3)$$

$$U_F = \frac{F_{AO}}{A} = \frac{v_o}{A} \quad (4)$$

Where,

U_F = Feed rate or superficial velocity of the Feed (moles/s)

v_o = Volumetric flow rate (moles/s)

A = Cross sectional area of the reactor

Substituting equation (4) into equation (2) gives

$$-\frac{\partial y_i}{\partial t} - U_F \frac{\partial y_i}{\partial L} = (-r_i) \quad (5)$$

But,

$$U_F = \frac{L}{\tau} \quad (6)$$

$$\partial L = U_F \cdot \partial \tau \quad (7)$$

$$-\frac{\partial y_i}{\partial t} - U_F \cdot \frac{\partial y_i}{U_F \cdot \partial \tau} = (-r_i) \quad (8)$$

$$\frac{\partial y_i}{\partial t} + \frac{\partial y_i}{\partial \tau} = -(-r_i) \quad (9)$$

$$\frac{\partial y_i}{\partial t} + \frac{\partial y_i}{\partial \tau} + (-r_i) = 0 \quad (10)$$

$$-\frac{\partial y_i}{\partial t} - \frac{\partial y_i}{\partial \tau} = (-r_i) \quad (11)$$

Equation (11) is the plug flow partial reactor equation for the reactor unit describing the fractional conversion of feed i or the yield of product j along the three reactors in series. Subsequently, the partial model equation is couched in the fashion:

$$-\frac{\partial y_i}{\partial t} - \frac{\partial y_i}{\partial \tau} = (-r_i) \quad (12)$$

$$\frac{\partial y_i}{\partial t} = -\frac{\partial y_i}{\partial \tau} - (-r_i) \tag{13}$$

Energy Equation

The temperature distribution along the reactor can be monitored by applying the law of conservation of energy on a differential volume element of the reactor stated below:

$$N_T C_p \rho T = N_T C_p \rho (T + dT) + (\Delta H_r)(-r_i)_{1 \rightarrow 4} AC_p \rho T dz + \frac{\partial}{\partial t} (AC_p \rho T) dz \tag{14}$$

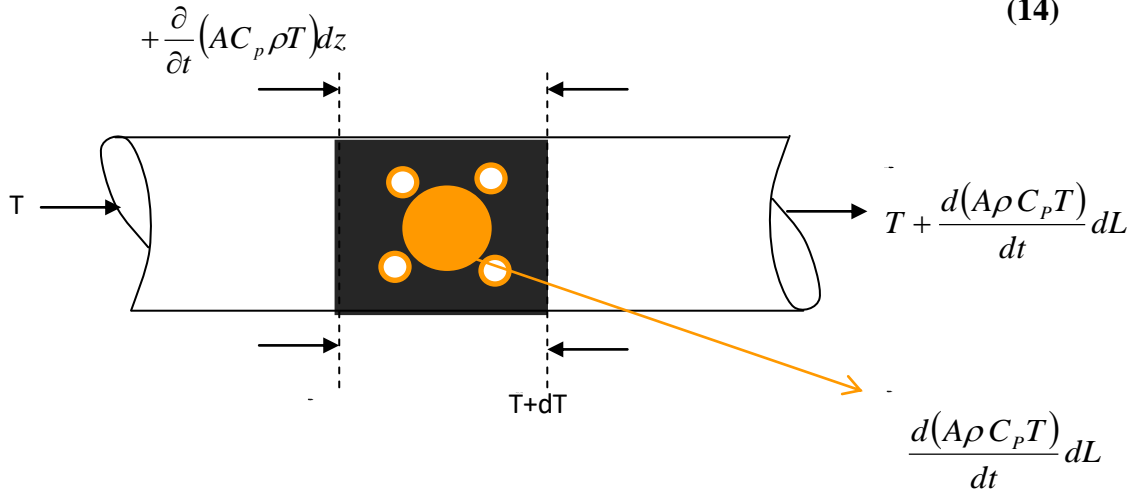


Figure 1 Differential volume reactor for energy balance

Reaction Rate Equation

Mathematically, the reaction rate equation gives an expression for the rate of transformation or depletion of a reactant or formation of desired product in a given chemical process. The rate of transformation, conversion or disappearance of a reactant *i* to form the product *j* through the cracking reactions 1 to 4, $(-r_{i,j})_{1 \rightarrow 4}$, (feed converted per unit fresh feed per unit time) in the reactor maintaining a first-order elementary reactions is given by:

$$(-r_{i,j}) = K_{i,j} y_i^n \phi_{i,y} \tag{15}$$

w.r.t. mole fraction of reaction species

Since catalyst deactivation is negligible, the function $\phi_{i,j}$ is therefore dropped in the rate model. The model is then written w.r.t partial pressure of the components in the vapour phase in the reformer reactors.

$$(-r_{i,j}) = K_{i,j} P_i^n \tag{16}$$

w.r.t. rate of depletion of feed component *i*,

We have,

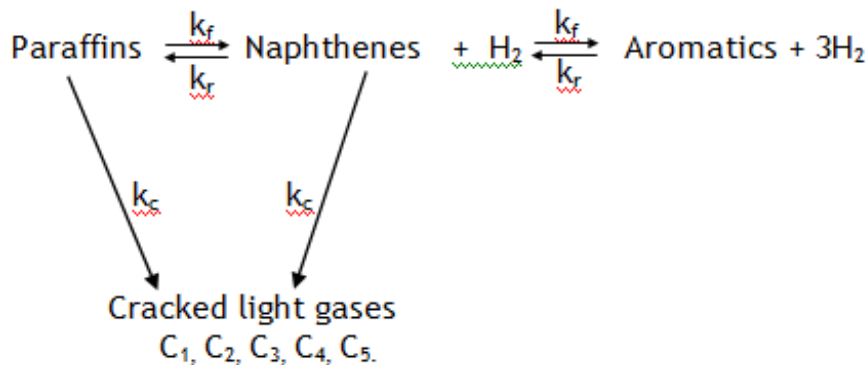
$$(-r_{i,j}) = \left(\frac{dN_i}{dt} \right)_{1 \rightarrow 4} = K_{i,j} P_i^n \tag{17}$$

The introduction of this expression into the model equation makes the model equation intractable non-linear equations and difficult to solve for the reaction rate constants $K_{i,j}$ analytically. Therefore appropriate numerical method i.e method of lines MOL was applied to resolve the models.

Six-Lump Process Chemistry

(Oboho, 2005); (Wordu, 2009) stated at different works that the complex reactions taking place in the reactors follow lumping scheme kinetics of paraffin, naphthenes, and aromatics.

This is true because when crude petroleum is struck during petroleum search the first experimental test carried out is assaying for the hydrocarbon generic fractions inherent in the petroleum i.e PONA and/or PNA, metals percent in the petroleum and non-metals in the crude petroleum.



Lumping model of reforming reactions posited by Oboho, (2005); Wordu (2009)

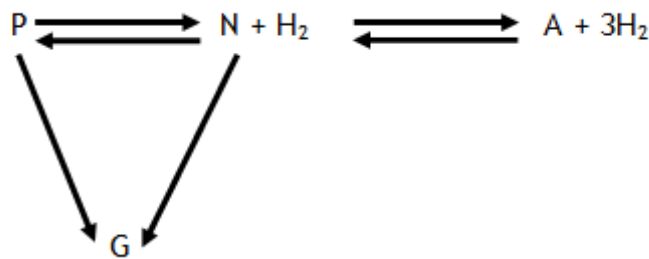


Figure 2: Six-Lump reactions (Oboho, (2005); Wordu (2009))

P – Paraffins, N - Naphthenes, A - Aromatics, H₂ - hydrogen, G – Gases, K_c - rate constant for hydro-cracking, K_f - rate of forward reaction, K_r -rate of reverse reaction.

The target parameter is to establish the sulphur content of the crude petroleum, Which will consequently, decide the refinery type to be design for processing. The rate equations will be derived with respect to the components of the feed naphtha which are Paraffins, Naphthenes, Aromatics, Hydrogen and Cracked Gases.

These are the constituents of the lumping chemistry considered for the research.

Dehydrogenation of naphthenes to form aromatics and hydrogen

Hydrogenation of aromatics to form paraffins and vice versa

Hydro-cracking of naphthenes to gases

Hydrocracking of paraffins to gases and Temperature effects

Estimation of kinetic parameters

The reactor model equations developed contain strong kinetic parameters which are specific for the Nigerian crude oil fractions for simulation of the reactor model equations. These are rate constant, K_f for the forward reaction, and reverse reaction, K_r, frequency / pre – exponential factor, activation energies E_i for the kinetic lumps reactions, equilibrium constant, K_p, rate constant K_c for the naphthene and paraffin hydro-cracking reactions

Objective function

The objective function is therefore defined as follows:

$$S = \sum_1^m \left[\sum_{i=1}^3 (N_{i \text{ calculated}} - N_{i \text{ plant}})^2 + \sum_{j=1}^3 (T_{out \text{ calculated}} - T_{out \text{ plant}})^2 \right]$$

Where, m = number of data sets used, $i = 1, 2$ and 3 for naphthene, paraffin and aromatic hydrocarbon respectively. $j = 1, 2$ and 3 for reactor 1, 2 and 3 respectively. For assumed value of E_i , Equations 1 to 5 (i.e. the five model equations developed for the research) were integrated numerically using mat lab ode–15s solver for stiff ordinary differential equations to obtain calculated values of the yields of naphthene, paraffin and aromatic hydrocarbons at the third reactor outlet and the dimensionless reactor temperatures.

An improved estimate of the activation energies were obtained as described in (Seinfeld and Lepidus, 1974) according to the model,

$$E_i^{(z+1)} = E_i^{(z)} - \gamma' \left. \frac{\partial S}{\partial E_i} \right|_{E=E^{(z)}} \quad (19)$$

The partial differentials $\frac{\partial S}{\partial E_i}$ were evaluated numerically by varying the activation energy over a narrow interval (2 KJ Kmol⁻¹) about the current values and evaluating the correspondence changes in S . A suitable upper and lower bound were specified for the activation energies to avoid convergence to some spurious or false values.

The iteration process was discontinued or terminated when the difference between successive values of the sum of the squares of the deviations ($S^{(z+1)} - S^{(z)}$) became less than 10^{-9} . This was achieved after 96 iterations (Oboho, 2005). The values of the activation energies obtained were as follows: $E_1 = 174500$; $E_2 = 356460$; $E_3 = 394380$. The obtained values lie within the range quoted in (Smith, 1959) and (Bommannan, Srivastava and Sara, 1989) research works.

Solution techniques

The partial differential equations were resolved numerically applying the method of lines MOL. The method converts the partial differential equations into a set of ordinary differential equations using a finite difference approximation of the spatial derivatives and integrates the set of equations with respect to time. First order forward difference was used to approximate the spatial derivatives. The reactor length was divided into 6 sections giving rise to 30 coupled ordinary differential equations. These were integrated applying Mat lab Ode 15s solver simulink for ordinary differential equations. Simulation was effected by varying temperature and pressure in the three reactors, 1, 2, and 3. Therefore, varying the inlet temperature from 812K to 823K at pressure $9.8 * 101.35$ KPa for reactor 1, 2, and 3 to observe the extent of conversion of feed and outlet temperature of the reactors.

Boundary conditions for element of volume of reactor

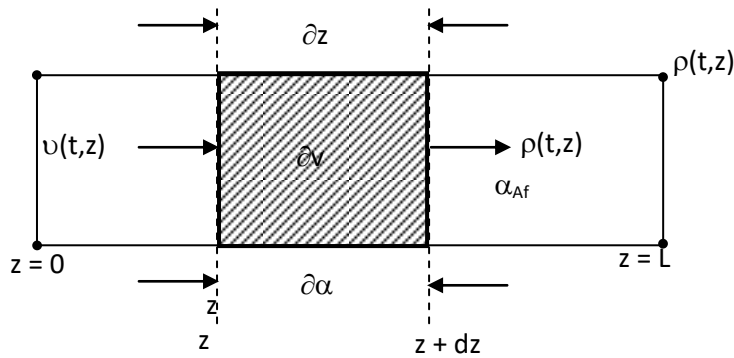


Figure 3: Boundary conditions for the reactor model

1	6	11	16	21	26	Naphthene
2	7	12	17	22	27	Paraffin
3	8	13	18	23	28	Aromatics
4	9	14	19	24	29	Hydrogen
5	10	15	20	25	30	Temperature

Figure 4: Method of generating 30 Odes split reactor length into 6 nodes (sections)

Discretization of feed components mole fractions into a system of Ode

$$\frac{dN_{(0)}}{dt} = -\left(\frac{N_{0,z+1} - N_{0,z}}{\Delta L}\right) - K_{f1}N_1P_T + \frac{K_{f1}}{K_{p1}}N_2N_4^3P_T^4 - K_{f2}N_1P_T^2N_4 + \frac{K_{f2}}{K_{p2}}N_3P_T - K_3N_1 \tag{20}$$

Naphthenes, N_N

$$N = 1 \quad \frac{dN_{(1)}}{dt} = -\left(\frac{N_{1,z+1} - N_{1,z}}{\Delta L}\right) - K_{f1}N_1P_T + \frac{K_{f1}}{K_{p1}}N_2N_4^3P_T^4 - K_{f2}N_1P_T^2N_4 + \frac{K_{f2}}{K_{p2}}N_3P_T - K_3N_1 \tag{21}$$

Aromatics, N_A

$$N = 2 \quad \frac{dN_{(2)}}{dt} = \left(\frac{N_{2,z+1} - N_{2,z}}{\Delta L} \right) + \frac{K_{f1}}{K_{p1}} N_2 N_4^3 P_T^4 - K_{f1} N_1 P_T \quad (22)$$

Paraffins, N_P

$$N = 3 \quad \frac{dN_{(3)}}{dt} = - \left(\frac{N_{3,z+1} - N_{3,z}}{\Delta L} \right) - \frac{K_{f2}}{K_{p2}} N_3 P_T + K_{f2} N_1 N_4 P_T^2 - K_4 N_3 \quad (23)$$

Hydrogen, N_{H2}

$$N = 4 \quad \frac{dN_{(4)}}{dt} = - \left(\frac{N_{4,z+1} - N_{4,z}}{\Delta L} \right) - 3 \left[\left(\frac{K_{f2}}{K_{p2}} N_2 N_4^3 P_T^4 \right) + K_{f1} N_1 P_T \right] -$$

$$K_{f2} N_1 N_4 P_T^2 + \frac{K_{f2}}{K_{p2}} N_3 P_T - \frac{n_c}{3} K_3 N_1 - \frac{n_c - 3}{3} K_4 N_3 \quad (24)$$

Temperature, T

$$N = 5 \quad \frac{dN_{(5)}}{dt} = \left(-N_T C_p \frac{(T_{5,z+1} - T_{5,z})}{\Delta z} \right) + 3 \left(\frac{K_{f1}}{K_{p1}} N_2 N_4^3 P_T^4 + K_{f1} N_1 P_T \right) \Delta H_1 -$$

$$\left(K_{f2} N_1 N_4 P_T^2 + \frac{K_{f2}}{K_{p2}} N_3 P_T \right) \Delta H_2 - \frac{n_c}{3} K_3 N_1 \Delta H_3 - \frac{n_c - 3}{3} K_4 N_3 \Delta H_4 \quad (25)$$

The PDEs were rewritten in terms of the index variable *i*.

For *i* = 1, ... *I* + 1, and

t = 1, 2 ... *t* + 1.

Results and Discussion

The steady state simulation process: open loop system

The model equations (20) to (24) and (25) were solved assuming steady state conditions in the reactors, 1, 2 and 3.

Temperature effects: Temperature 812K, Pressure 9.8 * 101.35 KPa

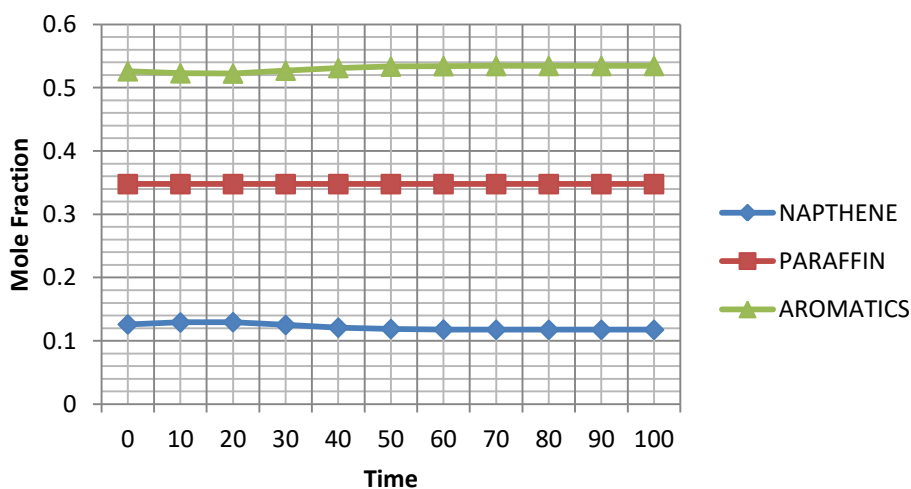


Figure 4 Dependence of mole fractions of naphthene, paraffin and aromatic on time

Table 4 depicts the dynamic response for reactor 3. For a dynamic model simulation temperature of 812K, and pressure of 993 KPa, the mole fractions of naphthene increased from 0.1261 to a steady state value of 0.1372 after 40 seconds. Whereas, that of aromatics decreased from 0.5261 to 0.5149 after about 40 seconds, thus, stability is attained after 40 seconds in reactor 3.

Similarly, from Figure 4.5(d) the temperature of the reactor 3 decreased from 768 to a steady state value of 771 after about 30 seconds to attain stability of the process.

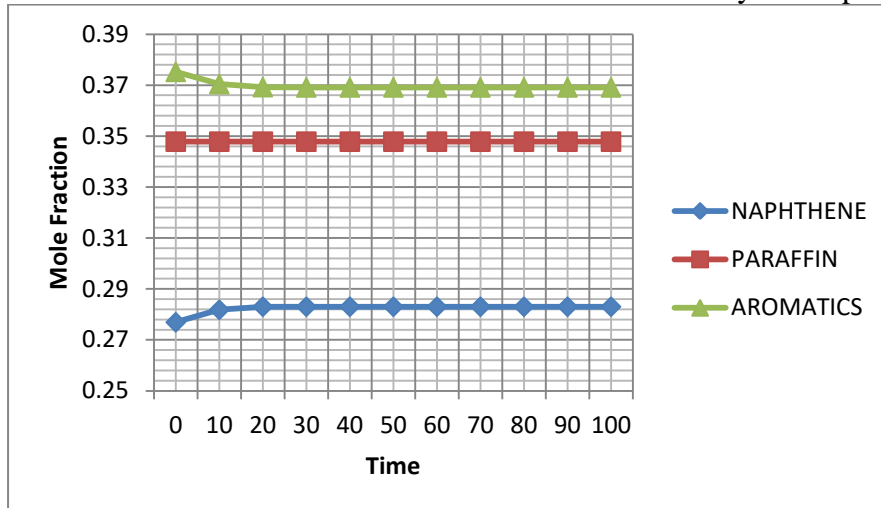


Fig. 4.4(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time

In reactor 2 figure 4.4(a) indicates the changes of mole fractions of naphthene from 0.2769 to a steady state value of 0.2830 while that of aromatics decreases from 0.3752 to 0.3691 after 20 seconds.

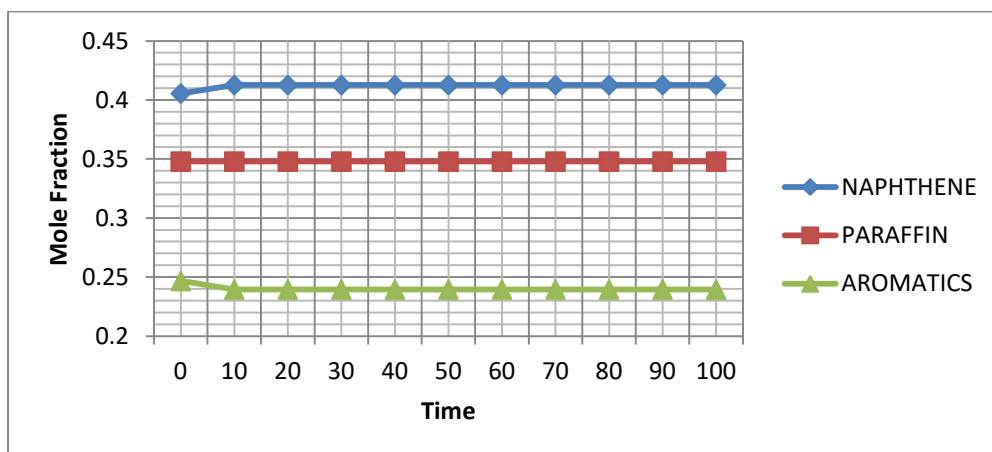


Fig. 4.5(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time

In reactor 1 figure 4.5(a) indicates the increase of mole fractions of naphthene from 0.4055 to a steady state value of 0.4126 while that of aromatics decreases from 0.2467 to 0.2395 after about 10 seconds.

Step increase in temperature from 812K to 833K for pressure of 993 KPa

4.6.2 Step increase in temperature from 812K TO 823K, pressure of 993 KPa

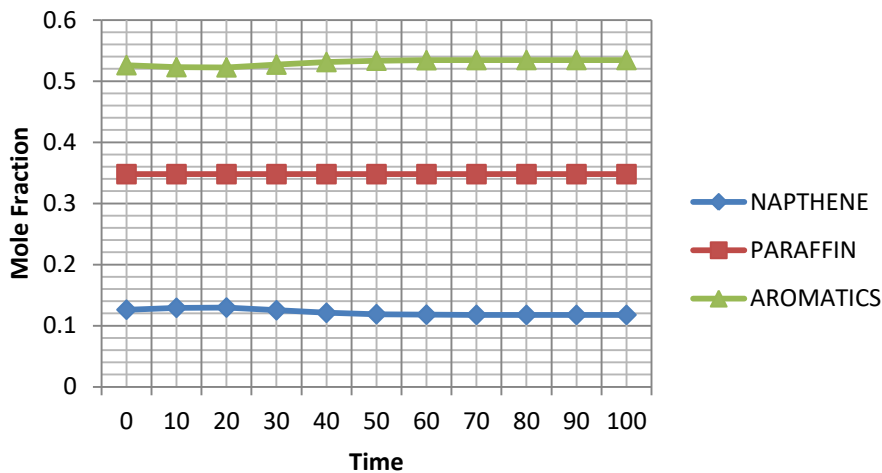


Fig. 4.9(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time

In Figure 4.9(a), the dynamic response of the open loop system for reactor 3 is given in Table 4.14 for a step increase in temperature from 812K to 823K. The mole fraction of naphthene decreases from 0.1261 to a steady state value of 0.1176, whereas, that of aromatics increased from 0.5261 to 0.5345 after about 60 seconds. Thus, steady state is attained after 60 seconds. Also, temperature increased from 768K to 776K and stabilized after 30 seconds.

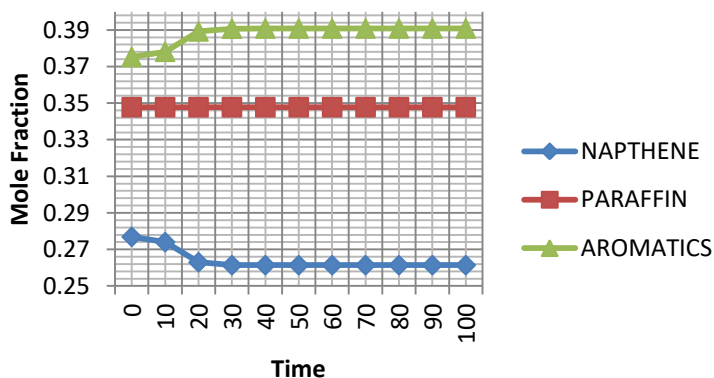


Fig. 4.10(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time
In reactor 2 from figure 4.10(a), Table 4.15 the response is a decrease in the mole fraction of naphthene from 0.2769 to 0.2614 to attain a steady state after 20 seconds, whereas, that of aromatics increase from 0.3752 to 0.3908 after 30 seconds. Thus, temperature of the reaction process increased from 774K to 780K and stabilized after about 10 seconds.

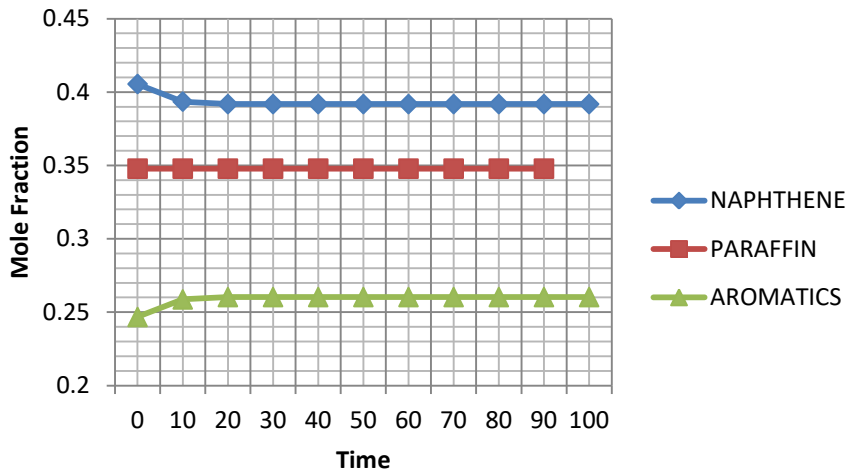


Fig. 4.11(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time

Similarly, for reactor 1, Table 4.16 the mole fraction of naphthenes decreased from 0.4055 to 0.3918 while that of the aromatics increased from 0.2467 to 0.2603, after about 20 seconds steady state is attained. Also, temperature of the reaction process increased from 779K to 786K and stabilized after about few seconds.

4.6.3 Step decrease in temperature from 812K to 783K, pressure of 993 KPa

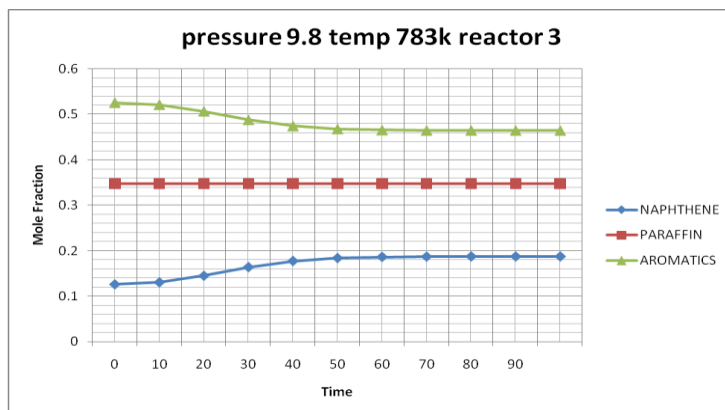


Fig. 4.12(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time

The dynamic response of the open loop system for reactor 3, is given in Figure 4.12(a) for a step decrease in reactor inlet temperature from 812K to 783K, the mole fractions of naphthene increased from 0.1261 to a steady state value of 0.1874, whereas, aromatics decreased from 0.5261 to 0.4647 after about 80 seconds. Thus, steady state is attained at 80 seconds. From table 4.16 it is clearly observed that there is a significant change in the mole fractions of naphthenes and aromatics. This clear change in mole fraction can be attributed to the fact that low temperature does not favor endothermic reactions.

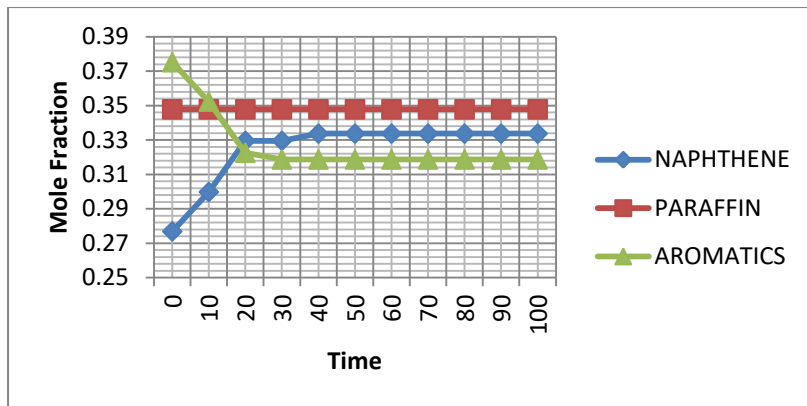


Fig. 4.12(c): Dependence of mole fractions of Naphthene, Paraffin and Aromatics on time.

Figure 4.12(c) depicts the type of dynamic response occurring in reactor 2 when temperature is reduced to 783K. The mole fraction of naphthene increased from 0.2769 to a steady state value of 0.3337 while aromatic decreased from 0.3752 to 0.3187 after 30 seconds to attain stability.

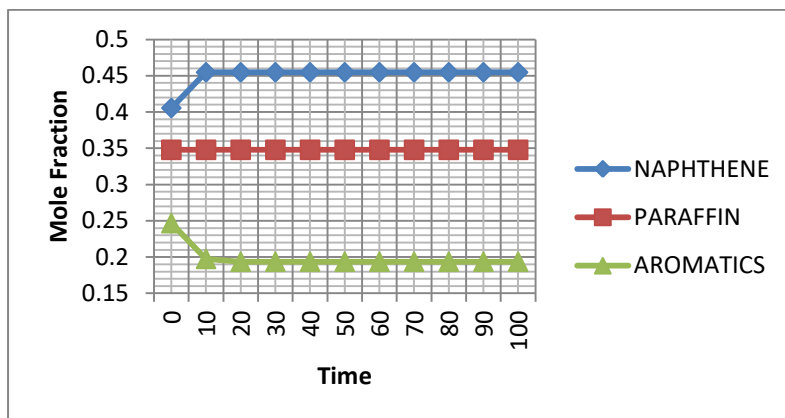


Fig. 4.13(a): Dependence of mole fractions of naphthene, paraffin and aromatic on time

Figure 4.13(a) shows the dependence of mole fractions of naphthene, paraffin and aromatic on time in reactor 1. It is apparent from the figure that the mole fractions of naphthene increase from 0.4055 to a steady state value of 0.4547 whereas that of aromatics decrease from 0.2467 to 0.1935 after 10secs.

4.6.3 Step Decrease in temperature from 812K TO 783K, pressure of 993 KPa

Effect of pressure on the dynamics of the process

Steady state simulation of reactor 3 using the parameters pressure 9.8 x 101.35 KPa, indicates in figure 4.20 the mole fractions of naphthenes and aromatic with temperature 812K increased from 0.1261 to a steady state value of 0.1372, while that of aromatic decreased from 0.5261 to 0.5149 to attain stability of the process. The paraffins as shown in same figure 4.20 maintained a constant value of 0.3478.

Figure 4.20 also shows that the change of the mole fractions of the components with time is quite small as to be considered in industrial practice. Therefore, this is the required pressure range or plant design pressure. Consequently, this pressure value assists in the suppression of coke formation and does not encourage or facilitate equipment wear.

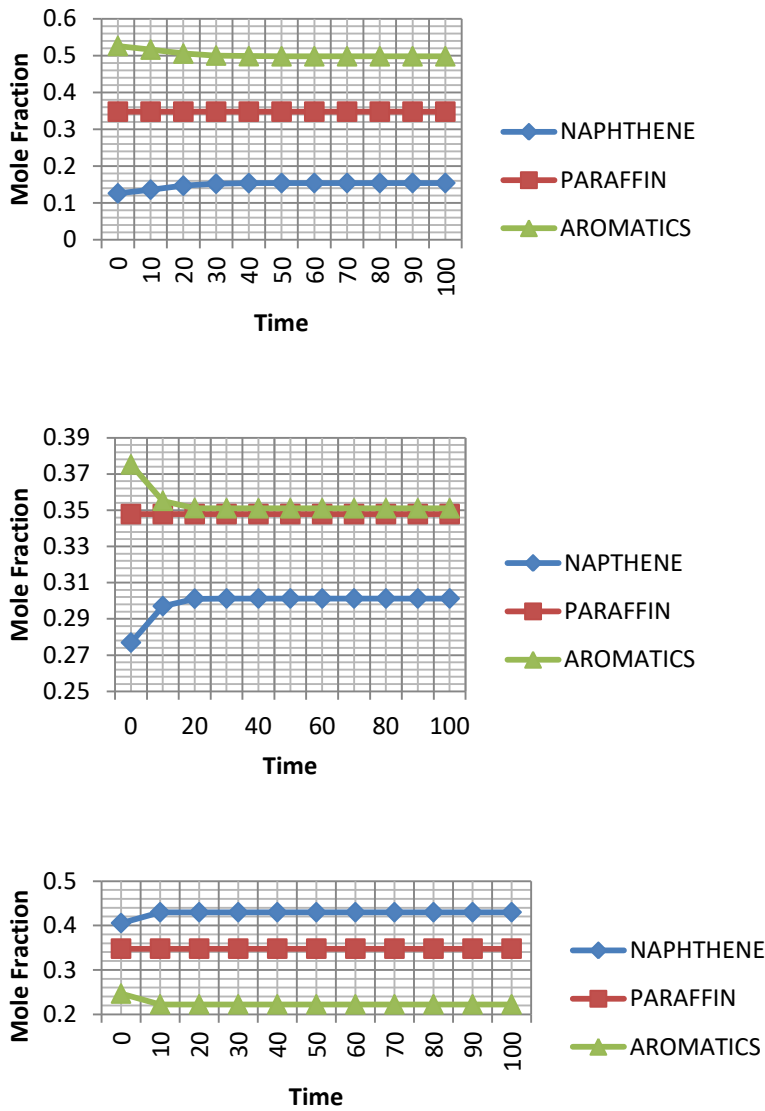


Fig. 4.16(a): Variation of mole fractions of naphthene, paraffin and aromatic on time

The dynamic response for the mole fractions of naphthenes, paraffin and aromatic and the reactor outlet temperature for a step increase in pressure from 993 KPa to 709 KPa is given in figure 4.16 a, b, c .

From table 4.21, the mole fraction of naphthene increases significantly from 0.4055 to a steady state value 0.4299 whereas the aromatics decrease from 0.2467 to 0.2223 after 10secs to attain stability.

NOMENCLATURE

G'_F = Feed rate moles/second
 $-r_i$ = Moles of Feed components per moles of fresh feed per second
 $\frac{\text{moles } N_N}{\text{moles of fresh feed} \cdot \text{sec}}$

N_{H_2} = Moles of Hydrogen in the reaction moles / second
 \bar{U}_F = Superficial velocity of the Feed moles / second
 $v_{o,F}$ = Volumetric flowrate of Feed moles / second

A	=	Aromatics	reactor
A_c	=	Cross sectional areas in meters	moles/ second
C_A	=	Concentration of Aromatic in the Feed moles / second	G = Cracked gases
C^B	=	Concentration of reacting species moles/dm ³	H = Hydrogen gas
C_C	=	Concentration of products moles/dm³	K_p = Equilibrium constant for the reaction.
C_D	=	Concentration of products moles/dm³	K_c = Rate constant hydrocracking reaction
C_F	=	Total concentration of the Feed component moles / second	K_f = rate constant for forward reaction
C_N	=	Concentration of Naphthene in the Feed moles / second	K_r = rate constant for reverse reaction
C_P	=	Concentration of Paraffin in the Feed moles / second	N = Naphthenes
F_A	=	molar flow rate of pure A for fractional conversion α_A .	N_A = Moles of Aromatic component in the Feed moles / second
F_{A_0}	=	molar flow rate of completely unconverted Feed into the	N_N = Moles of Naphthene component in the Feed moles / second
N_{total}	=	Total number of moles	N_p = Moles of Paraffin component in the Feed moles / second
P	=	Paraffins	y = Space-time in the reactor S^{-1}
Pa	=	Pressure in Pa or atmospheres	y_i or N_i = Mole fraction of component i, $N_A, N_p, N_N, N_{H_2}, N_{gases}$
P_A	=	Partial pressure of aromatics Pa	z = Elemental distance in differential volume element meters
P_N	=	Partial Pressure of Naphthenes Pa	α_A = Fractional conversion at inlet of the elemental volume
P_p	=	Partial Pressure of Parafins Pa.	α_{A+d} = Fractional conversion at outlet of the elemental volume
P_{total}	=	Reactor total Pressure or system total pressure	α_{Af} = Final friction at the outlet of reactor
r_2	=	rate of backward reaction moles/seconds	α_{A_0} = Fractional conversion at time = 0
R_A	=	rate of chemical reaction moles/second	$K_{i,j}$ = rate constant for the reaction process i,j (s^{-1})
r_i	=	rate of forward reaction moles/seconds	$(-r_{i,j})$ = rate of reaction
t	=	Element of time in second	y_i^n = mass fraction of the Feed component i
T	=	Temperature °C or K	N_i = mole fraction of the feed components i
V_0	=	Volumetric flow rate m ³ /sec	n = order of reaction i,j
			$\phi_{i,j}$ = deactivation

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