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COMPUTER MODELING OF PLATINUM REFORMING REACTORS

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ABSTRACT

Usually, the reformate that is leaving any stage of the platinum reforming reactors in terms of hydrocarbon composition is assessed by laboratory analysis. The ideal composition can only be tested through theoretical means, which in most cases is avoided because of long computation time involved. This paper, instead of using a theoretical approach has considered a computer model as means of assessing the reformate composition for three-stage fixed bed reactors in platforming unit. This is done by identifying many possible hydrocarbon transformation reactions that are peculiar to the process unit, identify the operating data, mathematically model and programme their reaction rate equations using QBasic language. In this article outlet product rate of 311363.59 kg/hr in the first, second and third reactor was obtained by modeling 275 m³/h inlet feed rate of Bayton Rouge Naphtha in the Kaduna Refinery. A manual or theoretical calculated value of 311145.22 kg/hr of outlet product rate was obtained showing a slight deviation of 0.9%. The authors are convinced that the written computer model could be applied in the process unit because it is accurate and less time **consuming.**

Keywords: *modeling, platimun reforming, reformate, reaction rate equations, operating data*

1. INTRODUCTION

It is well known that reforming processes were developed for the purpose of converting low octane heavy gasoline fractions (naphthas) into product with a high ignition quality, in terms of octane number [1], for blending into motor and aviation gasoline. This conversion involves subjecting the compounds in the naphtha to complex chemical reactions, at high temperature and pressure, with the aim of producing primarily aromatics and isoparaffins. In these processes by-products are also formed, mainly as a result of breakdown reactions yielding, cokes, petroleum gas (propane-butane), light hydrocarbon gases and hydrogen [2].

By process design, the various forms of reforming operations that are available in refineries worldwide are platforming, Iso Plus Houdri Forming, Rhein Forming, Power Forming, selectoforming, Ultra forming and Rex Forming. Primarily, they are all designed to perform the same function, i.e. to produce reformate that is rich in monocyclic aromatic hydrocarbons for blending with PMS and for petrochemical feed stocks. Their major differences lie in the operating conditions, nature of catalysts, product slates, feed range, etc., [2].

In this study, only platinum reforming process with fixed bed reactors would be focused upon. This is because, apart from the fact that it is the only type employed in the four refineries in Nigeria, Bhaskara Rao reported in [3] that its types are also, the most prevalent (about 90 %) in crude reforming units of the refineries worldwide.

The use of modeling tools to describe the trends and extent of products transformation in chemical engineering practices has been well studied [4, 5]. Therefore, the aim of this work is to model platinum reforming in order to assess the reformate composition in the reactors.

2. LITERATURE BACKGROUND

Usually for any chemical processing, the first and foremost step is to identify as many as possible the chemistry of the process itself, represent the reactions by their rate equations reaction(s) in differential form, solve the mathematical equations, then use the results as the input data for modeling the design. Same procedure was employed here.

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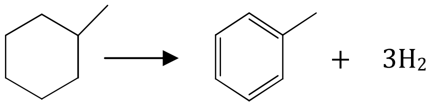
2.1 Chemistry of Platforming Reactions

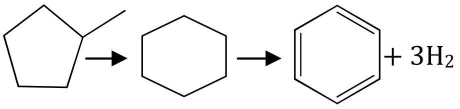
The main reactions occurring in catalytic reforming processes have been well studied [2, 3]. According to [6] the followings are the major ones:

a. Dehydrogenation of naphthenic hydrocarbons yielding aromatics and hydrogen



(1)

b. Dehydro-isomerisation of alkylcyclopentanes



(2)

c. Dehydrocyclisation of alkanes

$$C_7H_{16} \longrightarrow C_6H_5CH_3 + 4H_2 \qquad (3)$$

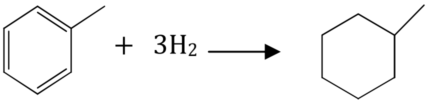
d. Cyclodehydrogenation of alkenes

$$C_7H_{14} \longrightarrow C_6H_5CH_3 + 3H_2 \qquad (4)$$

Nelson in [7] cited that other reactions that are related to platforming are:

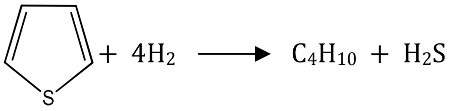
e. Hydrogenation of unsaturates

$$C_4H_8 + H_2 \longrightarrow C_4H_{10} \qquad (5)$$



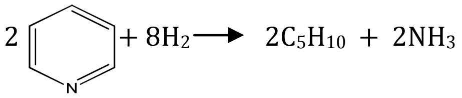
(6)

f. Hydrodesulphurisation



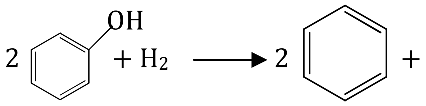
(7)

g. Denitrogenation



(8)

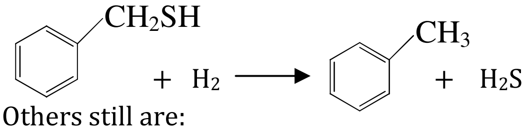
h. Deoxidation



(9)

i. Combination reactions

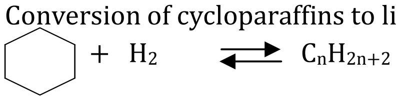
$$2RSO_3 + 3H_2 \longrightarrow 2RH + 2SO_2 + 2H_2O \qquad (10)$$



(11)

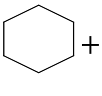
Others still are:

j. Conversion of cycloparaffins to linear paraffins



(12)

k. Hydrocracking of naphthenic hydrocarbon



$$+ \frac{n}{3}H_2 \longrightarrow \frac{n}{15}(CH_4+C_2H_6+C_3H_8+C_4H_{10} + C_5H_{12}) \qquad (13)$$

l. Hydrocracking of paraffinic hydrocarbons

$$C_nH_{2n+2} + \frac{n-3}{3}H_2 \longrightarrow \frac{n}{15}(CH_4 + C_2H_6 + C_3H_8 + C_4H_{10} + C_5H_{12}) \qquad (14)$$

Where n is the number of carbon atoms in the molecule.

However, of all the reactions listed above, those of 1, 12, 13, 14 are enough to model platforming reaction process [7] and [8] because these four reactions majorly involve the conversion of paraffins and naphthenes into branch-chained and aromatic hydrocarbons respectively. The resultant effect is the increment in octane rating and net production of hydrogen in the process [8].

According to [6] these reactions occur under the condition that the feed must be fairly free of sulphur, nitrogen and oxygen; of course, this would have been taken care of in the desulphurisation unit.

Other reactions apart from 1, 12, 13, and 14 take place concurrently and to a large extent sequentially, therefore, their reaction mechanisms and kinetics do not play significant role in the process [9].

2.2 Catalysts and Operating Conditions

Depending on the reforming processes type which may be semi-regenerative, or fully-regenerative or continuously regenerative, normally mono metallic or bimetallic catalysts types are employed [6] and [9]. Examples of such catalysts include platinum, platinum-rhenium, molybdenium oxide (MoO_3) supported on alumina, etc, [3, 9].

Normally reforming reactions overall, is endothermic [6] and proceed at economic rates in the temperature range of 450-530 ^oC to limit the catalyst performance decline rate due to coke deposition. In [7] and [8], the reaction pressure is in the range of 10 – 40 bar, leading to hydrogen partial pressures in the range of 5 – 35 bar [7].

The circulation ratio of the hydrogen containing gas to the feed, as specified by [8] is about 900 – 1850 m^3/m^3 feed. The fractional feed cut is normally 62-180^{o}C, while the space velocity of the feed is between 1-3 hr^{-1} and the volumetric percentage composition of hydrogen in the hydrogen containing gas is 85 – 93 % [7].

Therefore, if one can establish the reaction mechanisms of Equations 1, 12, 13 and 14 using optimal operation conditions, a mathematical model of the reaction rate equations can be programmed so that reformate composition can be obtained for process and reactor design.

3. PROCEDURE

The steps that are employed in the programming are:

(a) Representation of the hydrocarbon transformation and their respective reaction kinetics.
(b) Mathematical and computer modeling of the reaction mechanisms.

3.1 Representation of the Hydrocarbon Transformation

As earlier mentioned, only rate reactions for reaction Equations 1, 12, 13 and 14 are respectively considered in this work, which are:

I. Conversion of cycloalkanes to aromatics:

$$C_nH_{2n} \rightleftharpoons C_nH_{2n-6} + H_2 \qquad (15)$$

II. Conversion of cycloparaffins to normal paraffins:

$$C_nH_{2n} + H_2 \rightleftharpoons C_nH_{2n+2} \qquad (16)$$

III. Hydrocracking of the naphthenic hydrocarbons to lighter fractions:

$$C_nH_{2n} + \frac{n}{3}H_2 \rightarrow \frac{n}{3}(CH_4 + C_2H_6 + C_3H_8 + C_4H_{10} + C_5H_{12}) \qquad (17)$$

IV. Hydrocracking of paraffinic hydrocarbons:

$$C_nH_{2n+2} + \frac{n-3}{3}H_2 \rightarrow \frac{n}{15}(CH_4 + C_2H_6 + C_3H_8 + C_4H_{10} + C_5H_{12}) \qquad (18)$$

3.2 Reaction kinetics of the Transformation

The four differential reaction rate equations for the four hydrocarbon transformation reactions above can be respectively represented as in [8] and they are:

$$-\frac{dN_n}{dV_r} = K_1P_n - \frac{K_1}{K_{E1}}P_A(P_H)^3 \qquad (19)$$

$$-\frac{dN_n}{dV_r} = K_2P_nP_H - \frac{K_2}{K_{E2}} \qquad (20)$$

$$-\frac{dN_n}{dV_r} = K_3\frac{P_n}{\pi} \qquad (21)$$

$$-\frac{dN_p}{dV_r} = K_4\frac{P_p}{\pi} \qquad (22)$$

Where, N_n and N_p are molar concentrations of the naphthenic and paraffinic hydrocarbons respectively in the feed;

V_r – Reciprocal of the volumetric flow rate of the feed, (kg catalyst/kmol.hr); K_1, K_2, K_3 and K_4 – Rate constants of the four reactions respectively, kmol. /(h. Pa. kg catalyst); K_{E1} and K_{E2} – Constants of chemical equilibrium as reported [8] and can be expressed as the following:

$$K_{E1} = 9.81^3 * 10^{12} * e^{46.15-25600/T}\text{, Pa}^3 \qquad (23)$$

$$K_{E2} = 9.81^{-1} * 10^{-3} * e^{4450/T-7.12}\text{, Pa}^{-2} \qquad (24)$$

T is expressed in degree Kelvin; P_n, P_A, P_P and P_{H2} – are partial pressures of naphthenic, aromatic, paraffinic hydrocarbons and hydrogen in the process, Pa.

3.2 Mathematical and Computer Modeling of the Reaction Mechanisms

All the expressions above were used as the basis for the mathematical modeling of the process. The next step involved the sub-routine programming of the model, which was debugged in such a manner that it could be simple and well interactive. The debugged sub-routine programmes employed include AddRec, DataScreen, Processing, Report, Reportintro and Wipe. Their meanings are explained thus:

1. AddRec is for 'Y' to save the input records and 'N' to re-enter the correct data especially if the input data was wrong.
2. DataScreen is to input data.
3. Processing which is the most important routine in the modeling is for the programming. See Appendix 1
4. Report is for the generation of the result output.
5. Reportintro serves the purpose of requesting the particular reformate record that one wishes to generate and at the same time send that record to the screen for viewing and printout if desired.
6. Wipe is to convey educative message that one is dealing with generation of result in the main menu which is boldly captioned Reformate Composition.

The following input data are required to run the programme:

Enter the Code/Record Number for the Crude = Baton Rouge (See Table 1)
Feed Rate, m^3/h =275 m^3/h. (as in [10])
Specific Gravity = 0.740 (See Table 1)
Temperature in First Reactor, K = 803 (as in [8])
Temperature in Second Reactor, K = Depends on the output from the programme.
Temperature in Third Reactor, K = Depends on the output from the programme.
Pressure in First Reactor, Pa = 3.43 x 10^6 (as in [7])
Pressure in Second Reactor, Pa = Depends on the output from the programme.
Pressure in Third Reactor, Pa = Depends on the output from the programme.
Space Velocity, 1/h = 1.5 (as in [7])
Hydrogen - Containing Circulation Ratio, m^3/m^3 = 1500 (as in [2])
Paraffinic content, wt. %. (See Table 1 for Baton Rouge)

Naphthenic content, wt. % (See Table 1 for Baton Rouge)

Aromatic content, wt. % (See Table 1 for Baton Rouge)

ASTM distillation Temp of 50 % feed, K (See Table 1 for Baton Rouge)

Bulk Density of Alumnoplatinium Catalyst = 600 kg/m^3 (as in [8]).

Meanwhile Table 1 displays the physical properties of naphthas that were obtained from five different crudes. These properties partly act as the source of input data as requested above

Table 1: Properties of Naphtha Obtained from Five Crudes

Crude type→ Properties↓	Baton Rouge	Arabian Light	Arabian Heavy	Pona	Baytown
Paraffin, vol.%	53	66.3	70.3	50.4	38.1
Naphthenes, vol. %	39.9	20.0	21.4	39.2	42.6
Aromatics, vol. %	10.1	13.7	8.3	10.4	19.3
Specific gravity	0.740	0.744	0.737	0.745	0.767
ASTM Distillation, °C					
IBP	85	100	100	70	99
10 %	92	105	107	79	115
50 %	102	125	124	110	134
90 %	128	145	146	142	157
FBP	159	150	150	150	177

Source: Reforming Unit, Kaduna Refinery and Petrochemical Company, KRPC (2002)

Table 2: Summary of the Result Obtained for Reforming Baton Rouge Naphtha Using the QBasic programming

The first reactor , kg/h		
	Inflow	Outflow
Aromatics	20207.5492	86971.7358
Naphthenes	75111.8545	8639.4837
Paraffins	108180.6032	96885.1518
Hydrogen	107863.5796	118867.2152
Total	311363.5865	311363.5865
The second reactor , kg/h		
Aromatics	86971.7358	90682.7894
Naphthenes	8639.4837	0
Paraffins	96885.1518	87633.1051
Hydrogen	118867.2152	133047.6920
Total	311363.5865	311363.5865
The third reactor , kg/h		
Aromatics	90682.7894	90682.7894
Paraffins	87633.1051	88515.8367
Hydrogen	133047.6920	132164.9604
Total	311363.5865	311363.5865

4. RESULTS

Baton Rouge naphtha was employed for the mathematical model as well as for the

Programming. Though oversimplified the result or material balance obtained as in [8] and [11] is displayed in Table 2:

4.1 Discussion

The result obtained above is based on the feed rate of the reactor at 275 m^3/h, which is in conformity with [10].

Suffice to say that the model was equally employed for other naphthas that were obtained from the other sources and results obtained were of the same pattern as in Table 2.

With regards to the values obtained in Table 2, it can be observed that the naphthenic content of the naphtha drastically reduced in the first reactor. This is expected because aromatization of the naphthenes is highly favored in the first reactor [8], [12] and [13]. Meanwhile, the hydrogen produced has gone ahead to enrich the hydrogen -containing gas that was initially charged into the reactor as seen in the outflow of hydrogen in the first reactor. In the second reactor, hydrogen again has increased through the aromatization of the remaining naphthenes. But in the last reactor the hydrogen content has reduced because part of it has been utilized for the hydrocracking of paraffinic contents of the feed. The paraffinic content initially reduced in the first and second reactor due to hydrocracking but again picked up in the third reactor because this process enhances production of paraffinic hydrocarbon gases.

5. CONCLUSION

The use of the modeling tools to describe the trends in the platinum reforming of naphtha has been demonstrated. The authors are convinced that this computer modeling and simulation of platinum reforming process is very efficient and the data obtained are reliable. As a result it can be used to assess and monitor the reformate composition as it leaves one stage of the reactors to another. In essence, the data obtained from it can act as a check to the information obtained from theoretical approach and laboratory.

The model is equally highly recommended for prototype and industrial design of platinum reforming reactors.

6. REFERENCES

[1] Peer, R.L. Bennett, R.W. Felch, D.E. and Kabza, R.G. (1990): PLATFORMING. Leading Octane Technology into The 1990's. UOP Partnership For The 1990's, pp.1-2.

[2] Erikh, V.N. Rasina, M.G. and Rudin, M.G. (1988): The Chemistry and Technology of Petroleum and Gas, Moscow. pp.234-252.

[3] Bhaskara Rao, B.K. (2007): *Modern Petroleum Refining Processes,* 5th edition, published by Oxford and IBH Publishing, Co.PVT. Ltd, New Delhi, pp.344-360.

[4] N.A. Amenaghawon, E.I. Osagie, S.O. Osemwengie, S.E. Ogbeide and C.O. Okieimen (2013): Modeling and Simulation of the Batch Hydrolysis of Acetic Anhydride to Produce Acetic Acid. *Nigerian Journal of Technology*, Vol. 32, No. 3, pp 386- 392.

[5] M.C. Ndukwu, S.I. Manuwa, O.J. Olukunle and I.B. Oluwalana (2013): Mathematical Model for Direct Evaporative Space Cooling Systems. *Nigerian Journal of Technology*, Vol. 32, No. 3, pp. 403- 409.

[6] Baxendell, P. (1983)*: The Petroleum Handbook,* 6th Edition, compiled by staff of the Royal Dutch/Shell Group of Companies Elsevier, pp.268-276.

[7] Nelson W.L. (1969): *Petroleum Refinery Engineering, Catalytic Cracking and Reforming*; 4th Edition, McGraw-Hill Book Company, New York, USA. pp. 810-818.

[8] Kuznyesov, A.A., Kagermanov, S.M. and Sudakov, E.N., (1974): *Calculations of Unit Operations in Petroleum Industries.* Leningrad: Khimia. pp.251-288.

[9] Speight, J. G. (1999): The Chemistry and Technology of Petroleum, 3rd edition, New York Based, pp.684-693.

[10] Reforming Unit Record, (2002). Kaduna Refinery and Petrochemicals Company, KRPC Ltd, Kaduna State, Nigeria

[11] Coulson, J.M., Richardson, J.F. and Peacock, D.G. (1979): *Chemical Engineering* Vol.3, Chemical Reactor Design; Biochemical Reaction Engineering including computational techniques and control. 2nd ed. (SI units). Pergamon Press. Oxford. Britain, pp.12-14.

[12] Van Dyke K. (1997): *Fundamentals of Petroleum; Catalytic Reforming*, 4th edition. Published by Petroleum Extension Services, Continuing & Extended Education. The University of Texas at Austin; Austin, Texas, USA, p. 281.

[13] http://chemcases.com/converter/converter-f.htm (1998), accessed March 15, 2006.

Appendix 1

```
SUB Processing
 Mf = 105
 n = 7.4538
 Hydro = .86
 Methane = .04
 Ethane = .05
 Propane = .03
 Buthane = .01
 Penthane = .01
 Ma = (14 * n) - 6
 Mn = 14 * n
 Mp = (14 * n) + 2
 Ya = (Mf / Ma) * FileRec.AW
 Yn = (Mf / Mn) * FileRec.NW
 Yp = (Mf / Mp) * FileRec.PW
 RRC2 = 2.398 * 10 ^ -15
 RRC1 = .0000003145#
 RRC3 = .1
 RRC4 = RRC3
 SecRRC1 = 290.5 * 10 ^ (-9)
 SecRRC4 = .0714
 ThirdRRC4 = .06178
 GF = FileRec.SPgravity * 1000 * FileRec.FeedRate
 TotalMoleOfFeed = GF / Mf
 TMMOfAromatic = TotalMoleOfFeed * Ya
 TMMOfParafin = TotalMoleOfFeed * Yp
 TMMOfNaphthene = TotalMoleOfFeed * Yn
 TotalMolarMass = TMMOfAromatic + TMMOfParafin +
TMMOfNaphthene
 GH = (GF * FileRec.HCCR) / (1000 * FileRec.SPgravity)
 NH = GH / 22.4
 MMHydrogen = 2
 MMMethane = 16
 MMEthane = 30
 MMPropane = 44
 MMButhane = 58
 MMPentane = 72
 MRHydrogen = Hydro * MMHydrogen
 MRMethane = Methane * MMMethane
 MREthane = Ethane * MMEthane
 MRPropane = Propane * MMPropane
 MRButhane = Buthane * MMButhane
 MRPentane = Penthane * MMPentane
 TotalMR = MRHydrogen + MRMethane + MREthane +
MRPropane + MRButhane + MRPentane
 NHHydro = NH * Hydro
 NHHydro = NH * Hydro
 NHMethane = NH * Methane
 NHEthane = NH * Ethane
 NHPropane = NH * Propane
 NHButhane = NH * Buthane
 NHPentane = NH * Penthane
 TotalNHi = NHHydro + NHMethane + NHEthane +
NHPropane + NHButhane + NHPentane
 KMolePerHour = TotalNHi - NHHydro
 TotalAmount = TMMOfAromatic + TMMOfParafin +
TMMOfNaphthene + NHHydro + KMolePerHour
 MfAromatic = TMMOfAromatic / TotalAmount
 MfNaphthene = TMMOfNaphthene / TotalAmount
 MfParafin = TMMOfParafin / TotalAmount
 MfHydro = NHHydro / TotalAmount
 MfKMolePerHour = KMolePerHour / TotalAmount
 PpOfAromatic = FileRec.PFR * MfAromatic
 PpOfNaphthene = FileRec.PFR * MfNaphthene
```

```
 PpOfParafin = FileRec.PFR * MfParafin
 PpOfHydro = FileRec.PFR * MfHydro
 PpOfKmolePerHour = FileRec.PFR * MfKMolePerHour
 TotalPp = PpOfAromatic + PpOfNaphthene + PpOfParafin + PpOfHydro + PpOfKmolePerHour
 VC = GF / (FileRec.SPgravity * 1000 * FileRec.SV)
 GC = VC * FileRec.BDAC
 VolOfFirstReactor = VC / 7
 VolOfSecondReactor = (2 * VC) / 7
 VolOfThirdReactor = (4 * VC) / 7

 REM FIRST REACTOR COMPUTATION
 KP1 = 14.866 * 10 ^ 20
 Nn = (RRC1 * PpOfNaphthene) - (RRC1 / KP1) * PpOfAromatic * PpHydro
 GCAromatic = FileRec.BDAC * VolOfFirstReactor
 VRi = GCAromatic / TotalMolarMass
 REM now computes the total amount of naphthene converted into Aromatic
 Nni = Nn * VRi
 REM to compute the remaining amount of Naphthene left in the First Reactor
 NleftinFirstReactor = (Yn - Nni) * TotalMolarMass
 REM to compute the amount of naphthene converted to aromatic in the first reactor
 NconvertedtoA = TMMOfNaphthene - NleftinFirstReactor
 REM using reaction rate constant 2 for the first reactor
 Kp2 = 2.103 * 10 ^ (-6)
 DNni2 = (RRC2 * PpOfNaphthene * PpOfHydro) - (RRC2 * PpOfParafin) / Kp2
 Nni2 = DNni2 * VRi
 IncrementInNNi2 = ((Yn - Nni) + Nni2) * TotalMolarMass
 MQNaphtheneToParafin = IncrementInNNi2 - NleftinFirstReactor
 REM computing for reaction rate constant 3 for the first reactor
 DNni3 = RRC3 * PpOfNaphthene / FileRec.PFR
 Nni3 = DNni3 * VRi
 MQofNaphtheneRem = ((Yn - Nni) + (Nni2 - Nni3)) * TotalMolarMass
 MQNHydrocracking = IncrementInNNi2 - MQofNaphtheneRem
 REM computing for reaction rate constant 4 for the first reactor
 DNp1 = RRC4 * PpOfParafin / FileRec.PFR
 Np1 = DNp1 * VRi
 Np14 = (Yp - Np1) * TotalMolarMass
 Npgi = TMMOfParafin - Np14
 AmtOfGasInFirstReactor = (MQNHydrocracking + Npgi) * n / 15
 ProductAromatic = TMMOfAromatic + NconvertedtoA
 ProductNaphthene = (TMMOfNaphthene - NconvertedtoA) + (MQNaphtheneToParafin - MQNHydrocracking)
 ProductParafin = TMMOfParafin - MQNaphtheneToParafin - Npgi
 TotProduct = ProductAromatic + ProductNaphthene + ProductParafin
 Musty = NconvertedtoA * 3
 Adams = (MQNHydrocracking * n) / 3
 Onimisi = (Npgi * (n - 3)) / 3
 HCG = NHHydro + Musty + MQNaphtheneToParafin - Adams - Onimisi
 MCG = NHMethane + AmtOfGasInFirstReactor
 ECG = NHEthane + AmtOfGasInFirstReactor
 PCG = NHPropane + AmtOfGasInFirstReactor
 BCG = NHButhane + AmtOfGasInFirstReactor
 PentCG = NHPentane + AmtOfGasInFirstReactor
 TotCG = HCG + MCG + ECG + PCG + BCG + PentCG
 Gtotal = TotCG + TotProduct
 HCGMF = HCG / TotCG
 MCGMF = MCG / TotCG
 ECGMF = ECG / TotCG
 PCGMF = PCG / TotCG
 BCGMF = BCG / TotCG
 PentCGMF = PentCG / TotCG
 MYHydro = HCGMF * MMHydrogen
 MYMethane = MCGMF * MMMethane
 MYEthane = ECGMF * MMEthane
 MYPropane = PCGMF * MMPropane
 MYButhane = BCGMF * MMButhane
 MYPenthane = PentCGMF * MMPentane
 TotMY = MYHydro + MYMethane + MYEthane + MYPropane + MYButhane + MYPentane
 AmtOfHydroRichGas = TotCG * TotMY

 REM THIS SHOULD BE MY INLET OUTPUT-----------------------
 FileRec.GiAromatic = TMMOfAromatic * Ma
 FileRec.GiNaphthene = TMMOfNaphthene * Mn
 FileRec.GiParafin = TMMOfParafin * Mp
 GiHydro = NHHydro * TotalMR / .86
 FileRec.GiHydroParaf = (KMolePerHour + NHHydro) * TotMY
 TotalGinlet = FileRec.GiAromatic + FileRec.GiNaphthene + FileRec.GiParafin + GiHydro
 TotOrganicCG = MCG + ECG + PCG + BCG + PentCG
 FileRec.GoHydroParaf = (HCG + TotOrganicCG) * TotMY
 QtyHCLeavingReactor = TotalGinlet - FileRec.GoHydroParaf
 ZZ = 6 * ProductAromatic
 KKZ = 2 * ProductParafin
 XXX = ProductAromatic + ProductNaphthene + ProductParafin
```

```
FirstN = ((QtyHCLeavingReactor + ZZ) - KKZ) / (14 * XXX)
FirstMa = (14 * FirstN) - 6
FirstMn = 14 * FirstN
FirstMp = (14 * FirstN) + 2

REM THIS SHOULD BE MY OUTLET OUTPUT ---------------------
FileRec.GoAromatic = ProductAromatic * FirstMa
FileRec.GoNaphthene = ProductNaphthene * FirstMn
FileRec.GoParafin = ProductParafin * FirstMp
'chy = HCG * TotMY / HCGMF
TotalMoleOutlet = ProductAromatic + ProductNaphthene + ProductParafin + HCG + TotOrganicCG
MFOutletAromatic = ProductAromatic / TotalMoleOutlet
MFOutletNaphthene = ProductNaphthene / TotalMoleOutlet
MFOutletParafin = ProductParafin / TotalMoleOutlet
MFOutletHydro = HCG / TotalMoleOutlet
MFOutletOrganic = TotOrganic / TotalMoleOutlet
TotANP = FileRec.GoAromatic + FileRec.GoNaphthene + FileRec.GoParafin
TotGoutlet = TotANP + FileRec.GoHydroParaf
PFR2 = 3130000
TFR2 = 793
PpAromatic2 = FileRec.PFR2 * MFOutletAromatic
PpNaphthene2 = FileRec.PFR2 * MFOutletNaphthene
PpParafin2 = FileRec.PFR2 * MFOutletParafin
PpHydro2 = FileRec.PFR2 * MFOutletHydro
PpOrganic = FileRec.PFR2 * MFOutletOrganic
REM REACTION RATE CONSTANT FOR SECOND REACTOR
SecRxtMFAroma = ProductAromatic / TotProduct
SecRxtMFNaph = ProductNaphthene / TotProduct
SecRxtMFParaf = ProductParafin / TotProduct
KPSecRxtor = 9.94 * 10 ^ 20
HPower = PpHydro2 ^ 2
DNn2 = (SecRRC1 * PpNaphthene2) - ((SecRRC1 * PpAromatic * HPower) /   KPSecRxtor)
GC2 = FileRec.BDAC * VolOfSecondReactor
VR2 = GC2 / TotProduct
NnSecondRxtor = DNn2 * VR2
NewVolNaph = SecRxtMFNaph / DNn2
NCatalystQty = NewVolNaph * TotProduct
RedCat = GC2 - NCatalystQty
NnSecondRxtor = SecRxtMFNaph
FileRec.NRemAromatize = (NnSecondRxtor - SecRxtMFNaph) * TotProduct
REM USING REACTION RATE CONSTANT 4 FOR THE FIRST REACTOR
DNp2 = (SecRRC4 * PpParafin2) / FileRec.PFR2
NpSecondReactor = DNp2 * NewVolNaph
NPHydrocracking = (SecRxtMFParaf - NpSecondReactor) * TotProduct
AmtPconToGas = ProductParafin - NPHydrocracking
SecRxtOutletAroma = ProductAromatic + ProductNaphthene
SecRxtOutletParaf = ProductParafin - AmtPconToGas
TotSecRxtOutlet = SecRxtOutletAroma + SecRxtOutletParaf
AmtGasLeavSecRxt = AmtPconToGas * (n / 15)
HCG2 = HCG + (ProductNaphthene * 3) - AmtPconToGas * (n - 3) / 3
MCG2 = MCG + AmtGasLeavSecRxt
ECG2 = ECG + AmtGasLeavSecRxt
PCG2 = PCG + AmtGasLeavSecRxt
BCG2 = BCG + AmtGasLeavSecRxt
PentCG = PentCG + AmtGasLeavSecRxt
TotOrgCG2 = MCG2 + ECG2 + PCG2 + BCG2 + PentCG2
TotCG2 = HCG2 + TotOrgCG2
MFYG2Hydro = HCG2 / TotCG2
MFYG2Methane = MCG2 / TotCG2
MFYG2Ethane = ECG2 / TotCG2
MFYG2Propane = PCG2 / TotCG2
MFYG2Buthane = BCG2 / TotCG2
MFYG2Pentane = PentCG2 / TotCG2
MyG2Hydro = MMHydrogen * MFYG2Hydro
MyG2Methane = MMMethane * MFYG2Methane
MyG2Ethane = MMEthane * MFYG2Ethane
MyG2Propane = MMPropane * MFYG2Propane
MyG2Buthane = MMButhane * MFYG2Buthane
MyG2Pentane = MMPentane * MFYG2Pntane
TotMYG2 = MyG2Hydro + MyG2Methane + MyG2Ethane + MyG2Propane + MyG2Buthane + MyG2Pentane
HCRGIncreasedBy = HCG2 + TotCG2 * TotMYG2
HCLeavSecRxt = TotGoutlet - HCRGIncreasedBy
MFOutletSecRxtA = SecRxtOutletAroma / TotCG2
MFOutletSecRxtP = SecRxtOutletParaf / TotCG2
MFOutletSecHydro = HCG2 / TotCG2
MFTotOrganicCG = TotOrganicCG / TotGoutlet
nSec = (HCLeavSecRxt - (6 * SecRxtOutletAroma) - (2 * SecRxtOutletParaf)) / (14 * (SecRxtOutletAroma + SecRxtOutletParaf))

SecMa = (14 * nSec) - 6
SecMp = (14 * nSec) + 2
FileRec.MFR2Aromatic = SecRxtOutletAroma * SecMa
FileRec.MFR2Parafin = SecRxtOutletParaf * SecMp
FileRec.MFR2Hydroparaf = (HCG2 + TotOrgCG2) * TotMYG2
TotMFR2 = FileRec.MFR2Aromatic + FileRec.MFR2Parafin + FileRec.MFR2Hydroparaf
PFR3 = 3 * 10 ^ 6

TotThirdRxt = SecRxtOutletAroma + SecRxtOutletParaf
```

```
 MFThirdRxtAroma = SecRxtOutletAroma / TotThirdRxt
 MFThirdRxtParaf = SecRxtOutletParaf / TotThirdRxt
 ThirdRxtPpAroma = MFOutletSecRxtA * FileRec.PFR3
 ThirdRxtPpParaf = MFOutletSecRxtP * FileRec.PFR3
 ThirdRxtPpHydro = MFOutletSecHydro * FileRec.PFR3
 ThirdRxtPpOrganicCG = MFTotOrganicCG *
FileRec.PFR3
 TotThirdPp = ThirdRxtPpParaf + ThirdRxtPpAroma +
ThirdRxtPpHydro + ThirdRxtPpOrganicCG
 DNn3 = ThirdRRC4 * ThirdRxtPpParaf / FileRec.PFR3
 Gc3Alone = FileRec.BDAC * VolOfThirdReactor
 Gc3 = Gc3Alone + RedCat
 VR3 = Gc3 / TotThirdRxt
 ThirdRxtNn3 = DNn3 * VR3
 NPRemHydrocrack = (MFThirdRxtParaf - ThirdRxtNn3)
* TotThirdRxt
 NPgThirdRxt = SecRxtOutletParaf - NPRemHydrocrack
 ThirdOutletAroma = SecRxtOutletAroma
 ThirdOutletParaf = SecRxtOutletParaf - NPgThirdRxt
 TotOutletPA = ThirdOutletAroma + ThirdOutletParaf
 AmtGhirdRxt = (NPgThirdRxt * nSec) / 15
 HCG3 = HCG2 + (NPgThirdRxt * ((nSec - 3) / 3))

 MCG3 = MCG2 + AmtGhirdRxt
 ECG3 = ECG2 + AmtGhirdRxt
 PCG3 = PCG2 + AmtGhirdRxt
 BCG3 = BCG2 + AmtGhirdRxt
 PentCG3 = PentCG2 + AmtGhirdRxt
 TotCG3 = HCG3 + MCG3 + ECG3 + PCG3 + BCG3 +
PentCG3
 MFYG3Hydro = HCG3 / TotCG3
 MFYG3Methane = MCG3 / TotCG3
 MFYG3Ethane = ECG3 / TotCG3
 MFYG3Propane = PCG3 / TotCG3
 MFYG3Buthane = BCG3 / TotCG3
 MFYG3Pentane = PentCG3 / TotCG3
 MyG3Hydro = MMHydrogen * MFYG3Hydro
 MyG3Methane = MMMethane * MFYG3Methane
 MyG3Ethane = MMEthane * MFYG3Ethane
 MyG3Propane = MMPropane * MFYG3Propane
 MyG3Buthane = MMButhane * MFYG3Buthane
 MyG3Pentane = MMPentane * MFYG3Pntane
 TotMYG3 = MyG3Hydro + MyG3Methane +
MyG3Ethane + MyG3Propane + MyG3Buthane +
MyG3Pentane
 TotOrganicCG3 = MCG3 + ECG3 + PCG3 + BCG3 +
PentCG3
 ThirdHCRGIncBy = (HCG3 + TotOrganicCG3) *
TotMYG3
 QtyHCleavThirdRxt = TotMFR2 - ThirdHCRGIncBy

 MFOutletThirdRxtA = ThirdOutletAroma
 MFOutletThirdRxtP = ThirdOutletParaf
 MFThirdOutletHydro = HCG3
 MFThirdTotOrgCG = TotOrganicCG3
 TotThirdOutlet = MFOutletThirdRxtA +
MFOutletThirdRxtP + MFThirdOutletHydro +
MFThirdTotOrgCG
 TotDen = MFOutletThirdRxtA + MFOutletThirdRxtP
 nThird = (QtyHCleavThirdRxt + (6 *
MFOutletThirdRxtA) - (2 * MFOutletThirdRxtP)) / (14 *
TotDen)
 ThirdMa = (14 * nThird) - 6
 ThirdMp = (14 * nThird) + 2
 FileRec.MFR3Aromatic = SecRxtOutletAroma * ThirdMa
 FileRec.MFR3Parafin = SecRxtOutletParaf * ThirdMp
 FileRec.MFR3HydroParaf = (HCG2 + TotOrganicCG3) *
TotMYG3
 TotMFR3 = FileRec.MFR3Aromatic +
FileRec.MFR3Parafin + FileRec.MFR3HydroParaf
 ThirdMa = 14 * (nThird) - 6
 ThirdMp = 14 * (nThird) + 2

END SUB
```