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Computer Aided Design and Modeling of FCCU Processing Iraqi Feed Stock

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Abstract

The relationships between the process variables for a Fluid Catalytic Cracking unit (FCCU), processing vacuum gas oil (VGO) feedstock from Kirkuk crude oil, were studied depending on material and energy balance calculations. Computer programs written in Visual Basic (6.0) are developed to evaluate all the process variables. The steady state models is used to design the reactor, regenerator, fractionator and slurry settler. A hydrodynamic model for the complete description of the FCCU is developed. The model simulates the riser and the regenerator and incorporates operating conditions, feed properties and catalyst effects. The effect of the selection of the input (manipulated variables) on the output (measured variables) for the reactor and regenerator is also studied.

Keywords: Fluid Catalytic Cracking, Process Variables, Hydrodynamics of Riser and Regenerator.

الخلاصة

يتضمن البحث دراسة العلاقات بين المتغيرات التي تتحكم بعمل وحدة التكسير المحفز و المميع والتي تعمل على زيت الغاز الفراغي الناتج من تقطير نفط كركوك الخام حيث تم تطوير برامج بلغة بيسك (٦,٠)لتقييم هذه المتغيرات وتصميم اجهزة الوحدة (المفاعل , المنشط , عمود التقطير والمرسب).

تم اعداد موديل هيدروديناميكي يمثل توصيف متكامل لعمل الوحدة.هذا الموديل يحا كي عمل الماسورة الصاعدة (المفاعل) و المنشط ويتضمن تاثيرخصائص مادة التغذية والعامل المساعد. كما تمت دراسة تاثير المدخلات (المتغيرات المعالجة) على المخرجات (المتغيرات المقاسة) للمفاعل والمنشط.

Nomenclature

Symbol	***Definition***	***Units***
A	cross sectional area	m^2
A_d	area of downcomer	m^2
A_N	net tray area for vapor	m^2
API	american Pet. Inst.	---
Cp	specific heat	kJ/kg.°C
D	column diameter	m
d_p	particle diameter	m
F	mass flow rate	kg/s
F_{45}	fraction of cat. Below 45 micron	---
H	enthalpy	kJ/kg

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K	steady state gain	^oC
L	liquid flow rate	kg/s
M	mass	kg
NHV	net heating value	kJ/kg
Q	volumetric flow rate	m^3/h
T	temperature	^oC
t	time	s
U_{mb}	min. bubbling velocity	m/s
U_{mf}	min. fludization velocity	m/s
U	superficial velocity	m/s
V	total vapor rate	kg/s
ΔH_R	heat of reaction	kJ/kg
ΔH_C	heat of combustion	kJ/kg
ρ	density	kg/m^3
τ	time constant	s

1. Introduction:

Since the middle of the 1940s, catalytic cracking has been the most important and widely used process to break complex hydrocarbons into simpler molecules in order to increase the quality and quantity of lighter, more desirable products and decreases the amount of residual.(1)

Originally cracking was accomplished thermally but the catalytic process has almost completely replaced thermal cracking because more gasoline having a higher octane number and less heavy fuel oils and light gases are produced.(2)

The catalytic cracking process is very flexible, and the operating parameters can be adjusted to meet the changing product demand. FCC is the most common catalytic cracking process in which the oil is cracked in the presence of a finely divided catalyst which is maintained in an aerated or fluidized state by oil vapors. The fluid cracker consists of a catalyst section and a fractionating section that operate together as an integrated processing unit. The catalyst section contains the reactor and regenerator, which with the standpipe and riser, form the catalyst circulation unit. The fluid catalyst is continuously circulated between the reactor and the regenerator using air, oil vapors, and steam as the conveying media(1).

Raul et al.,(3) developed a mathematical model of the gas-solid flow that takes place in FCC risers. The flow is assumed as one-dimensional and the momentum and energy conservation equations have been applied to solid and gas phases. Four lumps, representing feedstock charge, naphtha, flue gas and coke, were employed to approach the kinetic of reactions.

On the other hand, Pashne et al.,(4) developed an integrated FCC simulator that can be used for studying the performance of the reactor (riser) and the regenerator and also the interactions between them. For the cracking reactions in the riser they have chosen the 4-Lump method. In an article presented by Wei Fei et al.(5), a dispersion reactor model of both riser and downer reactor for the FCC is proposed. The model combines the 4- lump cracking kinetics, the hydrodynamic model for both riser and downer and the dispersion mixing model to predict the fluid catalytic cracking reaction performance.

Ranade V.V.$^{(6)}$ used a two-fluid framework with the kinetic theory of granular flows to simulate fully developed gas-solid flows in vertical risers. The computational model was used to simulate the available experimental data over a wide range of operating and design parameters. In addition, several numerical experiments were carried out to understand the influence of riser diameter, particle size, gas and solid flux, solids and gas density on the simulated flow characteristics. The presented result and analysis will be useful for further development of modeling of gas-solid flows in riser reactors.

An integrated dynamic model for the complete description of the fluid catalytic cracking unit (FCCU) was developed by Bollas G. M. et al.$^{(7)}$, the model simulates successfully the riser and the regenerator of FCC and incorporates operating conditions, feed properties and catalyst effects. The simulator can be utilized as a basis for a model based control of FCC units.

Osman A. M. (2002) $^{(8)}$ developed a kinetic model to simulate the riser of a residue fluid catalytic cracking unit (RFCC) processing residue from Sudanese crude oil. She used the matlab environment to solve and analyze the kinetic model and process variables.

2. Process Specifications and Variables

The proposed FCC unit is processing 251.75 m^3/h of vacuum gas oil (VGO) obtained from the vacuum distillation of Kirkuk crude oil.$^{(9)}$ The properties of Kirkuk crude oil and the vacuum gas oil are given in Appendix (A).

Most often controlling the feed is not enough to get the maximum yields of FCC. Some of the major process variables that can either increase or hinder the yield are cracking temperature, catalyst to oil ratio, space velocity, and catalyst type. For many normal operations, an increase in the reaction temperature, catalyst /oil ratio, catalyst activity and contact time will increase the conversion.$^{(10)}$ The process variables are defined as follows$^{(2)}$:

$$\text{Activity}=\frac{\text{conversion}}{100-\text{conversion}} \quad \text{--- (1)}$$

$$\text{Conversion}=\left(\frac{\text{volume of feed}-\text{volume of cycle stock}}{\text{volume of feed}}\right)\text{x}100 \quad \text{---(2)}$$

$$\text{Yield}=\frac{\textit{moles of produced}\times\textit{stoichiometric factor}}{\textit{moles of reagent conveted}} \quad \text{---(3)}$$

$$\text{Efficiency}= \eta=\left(\frac{\%\,\text{gasoline}}{\%\,\text{conversion}}\right)\times 100 \quad \text{--- (4)}$$

$$\text{Severity factor}=\frac{\text{Cat./Oil ratio, lb/lb}}{\text{Space Velocity, lb oil per hr/lb cat.in bed}} \quad \text{---(5)}$$

$$\text{Residence time} = t = \frac{1}{\text{Space Velocity}\times\text{Cat. / Oil ratio}} \quad \text{---(6)}$$

3-Design Calculations

The data of the process variables needed in the calculation of the material balance and the calculated total material balance are given in Appendix-B.

3-1 Riser $^{(11,12)}$

Total volumetric flow rate in the riser = volume rate of catalyst + steam + vapors ---(7)

Cross sectional area of the riser =

$$\frac{\text{Volumetric rate of flow}}{\text{Velocity}} \quad \text{---(8)}$$

$$\text{Diameter of the riser} = \sqrt{\frac{4 \times \text{Area}}{\pi}} \quad \text{---(9)}$$

The riser is sized for a very short contact time with minimal catalyst back mixing. So the reaction time was taken = 1 second.

Then volume hold-up in the riser = volume rate × time ---(10)

3-2Regenerator (13)

The coke of cracking reaction on spent catalyst is oxidized by combustion and the regenerated catalyst return to the reactor base and the cycle continued again. The regenerator is a fluidized bed, so before investigation of regenerator performance as a reactor, it is investigated as a fluidized bed in cold flow model.

Minimum fluidization velocity $\cong U_{mf}$

$$= \frac{9.0\times10^{-4}\, dp^{1.8}\left[\left(\rho_s - \rho_{air}\right)g\right]^{0.934}}{\rho_{air}^{0.066}\quad \mu_{air}^{0.87}} \quad \text{---(11)}$$

Minimum bubbling velocity $\cong U_{mb}$ =

$$\frac{2.07\, dp\, \rho_{air}^{0.06}\, \exp\left[0.176\, F_{45}\right]}{\mu_{air}^{0.347}} \quad \text{---(12)}$$

where: F_{45}=Fraction of catalyst below 45 microns=18% wt (catalyst distribution)

when bed velocities for dilute and dense phases are calculated, together with total volumetric rate of the bed (catalyst + steam+ air), the diameter of dilute and dense phases are calculated for the regenerator.

3-3 Fractionator (14)

Total weight of top product = wt. gases + wt. reflux +wt. gasoline + wt. water vapor --- (13)

Total volume of top product =

$$\mathbf{V} = \frac{nRT}{p} \quad \text{---(14)}$$

where :

n = total Ibmol of top product.

T = Top temperature (R) or (K)

P = Top pressure (psia) or (kPa)

R = Gas constant

Q_L = volumetric rate of liquid

$$(m^3/s.) = \frac{L}{\rho_L} \quad \text{---(15)}$$

Q_V = volumetric rate of vapor

$$(m^3/s.) = \frac{V}{\rho_V} \quad \text{--- (16)}$$

Liquid-vapor flow parameter, P_f

$$P_F = \frac{L}{V}\left(\frac{\rho_V}{\rho_L}\right)^{0.5} \quad \text{---(17)}$$

The capacity factor Pc is given by Van Winkle (14) for 100% of flooding.

The net vapor velocity (U_{VN}) =

$$\frac{P_C}{\left(\dfrac{\rho_V}{\rho_L - \rho_V}\right)^{0.5}} \quad \text{---(18)}$$

The flooding percent = 70-75% (for foaming system)

Take flooding percent =72.5%.

select A_d/A =0.12.

where

A_d = Area of downcomer, m^2

A =Cross-sectional area of column, m^2

A_N = Net tray area for vapor flow $=A-A_d$.

$A_N = A-0.12\, A = 0.88\, A$.

$$\mathbf{A} = \frac{A_N}{0.88} = \frac{Q_N}{0.88\, U_{VN}} \quad \text{--- (19)}$$

$$\text{Column diameter, } D = \sqrt{\frac{4 \times \text{Area}}{\pi}} \quad \text{---(20)}$$

4. Modeling

FCCUs present challenging multivariable control problems. Fig. (1) shows a simplified PID for a typical FCC unit. The selection of good inputs (manipulated variables) and outputs (measured variables) is an important issue, as is the pairing of chosen controlled and manipulated variables for decentralized control. In this case, the important measured variables are chosen to be the reactor temperature /riser outlet temperature (T_1), the regenerator gas temperature (T_{cy}) and the regenerator bed temperature (T_{rg}). The manipulated variables are the catalyst recirculation rate (F_s) and the regenerator air rate (F_a).(14)

4-1 Reactor

The energy balance around the reactor can be written as:

Input stream –[Output stream-Heat of reaction] = Accum. ---(21)

Reg. catalyst + Feed + Steam – Effluent – Spent catalyst + Heat of reaction= Accumulation ---(22)

$$F_s Cp_s T_s + F_o Cp_o T_o + F_{st.} H_{st.} - F_g Cp_g T_1 - F_G Cp_s T_1 + \Delta H_R = (M_{pro.} Cp_{pro.} + M_{cat.} Cp_{cat}) \frac{dT_1}{dt} \quad \text{---(23)}$$

Taking the Laplace transform of equation (23), and rearranging the equation, the transfer function of T_1 (s) is:

$T_1(s) =$

$$\frac{CP_s\ T_s}{F_g\ CP_g + F_G CP_s + s(M_{pro.} CP_{pro.} + M_{cat.} CP_{cat.})} F_s(s) +$$

$$\frac{F_o\, CP_o\ T_o}{F_g\ CP_g + F_G CP_s + s(M_{pro.} CP_{pro.} + M_{cat.}\ CP_{cat.})} +$$

$$\frac{\Delta H_R}{F_g\ CP_g + F_G CP_s + s(M_{pro.} CP_{pro.} + M_{cat.} CP_{cat.})} \quad \text{--- (24)}$$

The main reason for deriving system response equations is to investigate the effects which a change in an input variable with respect to time will have on a particular output variable. It should be noted that the analysis of the system response can be applied to a change in only one variable at a time and that if the system has more than one input variable, all other input variables apart from the one being considered must be regarded as constant. Since each variable is measured from a datum corresponding to its normal steady state value, this is equivalent to making the unchanged variables equal to zero; the appropriate terms then disappear from the equation, leaving for a first order system the first order equation which has only one input and one output variable.(15)

For a step of magnitude 5 kg/s for input Fs (regenerated catalyst flow rate) as recommended by Bequtte(16), then:

$$T_1(t) = 5\ k\ (1 - e^{-t/\tau}) \quad \text{---(25)}$$

Where:

$$k = M_s\, Cp_s\, T_s / (F_g\, Cp_g + F_G\, Cp_s) \quad \text{---(26)}$$

$$\tau = \frac{M_{pro.} CP_{pro.} + M_{cat.}\ CP_{cat.}}{F_g\ CP_g + F_G CP_s} \quad \text{-- (27)}$$

Input (Manipulated Variable)

Regenerated catalyst feed rate (F_s) : steady state value = 454.79 kg/s

Output (Controlled variable)

Riser outlet temperature (T_1) : steady state value = 503 °C.

4-2 Regenerator *:*

The energy balance around the regenerator can be written as;

Input stream–[Output Stream + Heat of Combustion] = Accum. ---(28)

Spent catalyst + Air – Heat of Combustion – Reg.Catalyst – Flue gases = Accum. --- (29)

$$F_G\, Cp_s\, T_1 + F_a\, Cp_a\, T_a - \Delta H_c - F_s\, Cp_s\, T_{rg} - F_{cy}\, Cp_{cy}\, T_{cy} = M_s\, Cp_s \frac{dT_{rg}}{dt} + M_{cy}\, Cp_{cy} \frac{dT_{cy}}{dt} \qquad \text{--- (30)}$$

Taking the Laplace transform for equation (30), and rearranging the equation, the transfer function of $T_{rg}(s)$ is:

$$T_{rg}(s) = \frac{F_G\, CP_s\, T_1}{F_s\, CP_s + M_s CP_s\, s} + \frac{T_a\, CP_a}{F_s\, CP_s + M_s CP_s\, s} F_a(s) + \frac{N.H.V\, F_{coke}}{F_s\, CP_s + M_s CP_s\, s}$$

---(31)

For a step of magnitude 0.1 kg/s for the input F_a (air flow rate) (16), then

$$T_{rg}(t) = 0.1\, k_1(1 - e^{-t/\tau}1) \qquad \text{--- (32)}$$

where : $k_1 = M_a\, T_a\, Cp_a / F_s\, Cp_s$ and $\tau_1 = M_s/F_s$

The regenerator gas temperature (T_{cy}) in equation (30) becomes :

$$T_{cy}(s) = \frac{F_G\, Cp_s\, T_1}{F_{cy}\, Cp_{cy} + M_{cy} Cp_{cy}\, s} + \frac{T_a\, Cp_a}{F_{cy}\, Cp_{cy} + M_{cy} Cp_{cy}\, s} F_a(s) - \frac{N.H.V\;\; F_{coke}}{F_{cy}\, Cp_{cy} + M_{cy} Cp_{cy}\, s}$$

---.(33)

and

$$T_{cy}(t) = 0.1\, k_2(1 - e^{-t/\tau}{}_2) \qquad \text{....(34)}$$

where **:**

$k_2 = M_a\, T_a\, Cp_a / F_{cy}\, Cp_{cy}$ ---(35)

$\tau_2 = M_{cy}/F_{cy}$ … (36)

Input (Manipulated Variable)

Air rate (F_a): steady state value = 66.41 kg/s

Output (Controlled variable)

Regenerator cyclone temperature (T_{cy}) : steady state value = 715.5 °C

Regenerator bed temperature (T_{rg}) : steady state value = 692.4 °C

5. Results and Discussion

5-1 Process Variables Simulation:

Equations (2) to (7) are used to calculate the process variables (efficiency, activity, yield, severity factor ,and the residence time). The relation between process variables were estimated using the developed computer programs using Visual Basic by changing input variables (%conversion, C/O ratio, space velocity). Fig. (2) shows the relation between efficiency and conversion. The %efficiency decreases with increasing %conversion. The best value of cracking efficiency is obtained when conversion values range between (75-85%). On exceeding the conversion above these values a convergence in the computer program results was obtained .

The effect of activity on conversion is clear, where the % conversion increases with increasing activity as shown in Fig. (3).

Yield calculations depend on °API of feed stock, %conversion and the catalyst used (2). Changing conversion will affect gasoline and gases yield slightly. Fig. (4) indicates that increasing % conversion will increase gasoline and gases yield, but it does not necessarily mean an increase in the gasoline yield because coke and gases yield increase at the expense of gasoline yield. This agrees with the results Gary(2), and Wei Fei et al.,(5)

Fig. (5) indicates that the severity of the operation increases as the catalyst/oil ratio increases for constant space velocity of 2 hr^{-1}. This is due to the fact that the increase in catalyst/oil increases the rate of reaction and for a certain conversion this leads to a decrease in the residence time required in the riser as shown in Fig. (6).

Fig. (7) indicates that the severity of the operation decreases as the space velocity increases for constant value of catalyst/oil ratio.

The relation between residence time and space velocity is shown in Fig.(8). The residence time decreases with increasing the space velocity for constant value of catalyst/oil ratio.

5-2 Design Simulation

The effect of catalyst rate on riser diameter (calculated as given by equations (7-9)), is shown in Fig. (9). The trend of the curve indicates an increase in the riser diameter as the catalyst rate increases to quantify the increase in the volume of the catalyst.

For the regenerator, the diameters of both the dense and dilute phases as given in section 3-2) increase as the catalyst and air rates increase . The results are shown in Figs. (10, 11) and (12, 13) respectively.

Fig. (14) indicates that as the %conversion increases, the yield of top product increases and this in turn increases the fractionator diameter which is estemated using the Equations (13-27) given in section (3-3). Full details of the design calculations are given by Hassan, S. (17)

5-3 Fluidized Catalytic Cracking Unit Model Simulations :

The behavior of the regenerator dominates both the dynamic and steady state behavior of the system. This is due to the adiabatic nature of the system in which the need to balance coke formation and combustion is the overriding force. The riser residence times are much shorter compared to the response time of regenerator, hence at any instance the riser reactor can be described by a set of steady state relations, which simplifies the dynamic analysis, equations (21-26).

The response of the system has been evaluated for a hypothetical step change in the regenerated catalyst flow rate (Fs) and the combustion air feed rate (Fa).

Fig. (15) shows the response of the riser outlet temperature (T_1) for a step of 5 kg/s in the regenerated catalyst flow rate (Fs). The trend of the curve indicates that the increase in T_1 was instantaneous and a new steady state soon established within 5 seconds. This results agrees well with the findings of Bollas et al .(7)

For the regenerator and as shown in Figs. (16) and (17) an increase in the air flow rate (F_a) with a step of 0.1 kg/s and 0.3 kg/s respectively leads to an increase in the regenerator bed temperature (T_{rg}) and regenerator cyclone temperature (T_{cy}). On the contrary, decreasing the air feed rate (F_a) with a step of 0.3 kg/s leads to a decrease in the regenerator bed temperature and regenerator cyclone temperature. However, after the immediate new state is reached, the regenerator lead the system to a new steady state in much longer time of about 10 seconds. The results are in excellent agreement with the real-time operation of FCC unit. (7)

5. Conclusions

An evaluation of the process variables affecting the performance of FCC unit processing VGO of (20.65) ^{o}API is presented. Computer programs written in Visual Basic (6.0) are developed to fulfill this task and to design the main equipments of the unit (riser, regenerator , fractionator, and the slurry settler). The nonlinear hydrodynamic and multivariable model developed is verified with the operating variables of the unit, showing its complex behavior as response to typical disturbances. The simulator can be utilized as a basis for a model based control of FCC unit.

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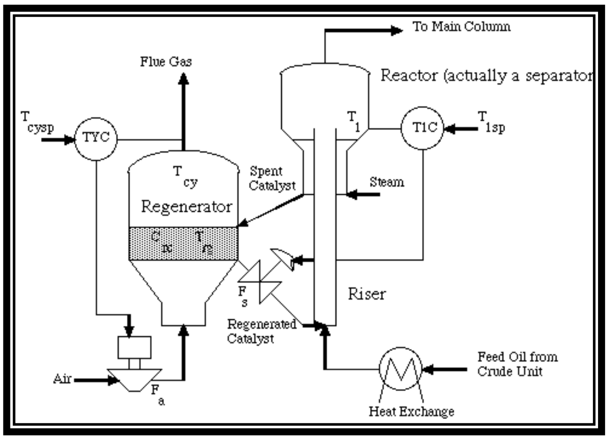

Figure (1): Schematic Diagram of FCCU(15)

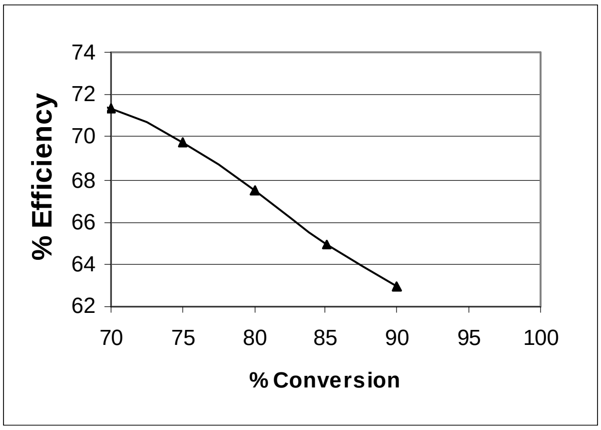

Fig.(2):Efficiency vs. Conversion

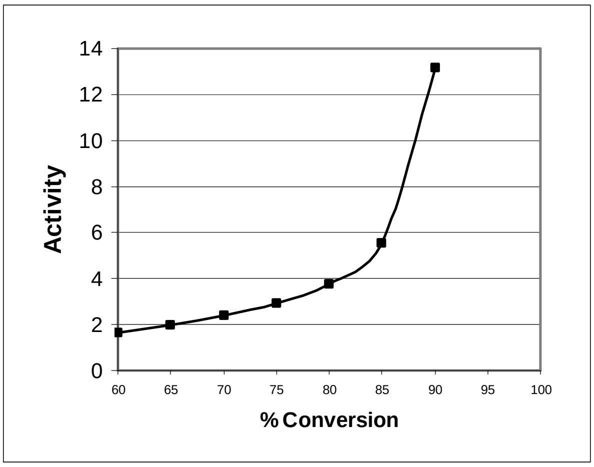

Fig.(3):Activity vs. Conversion

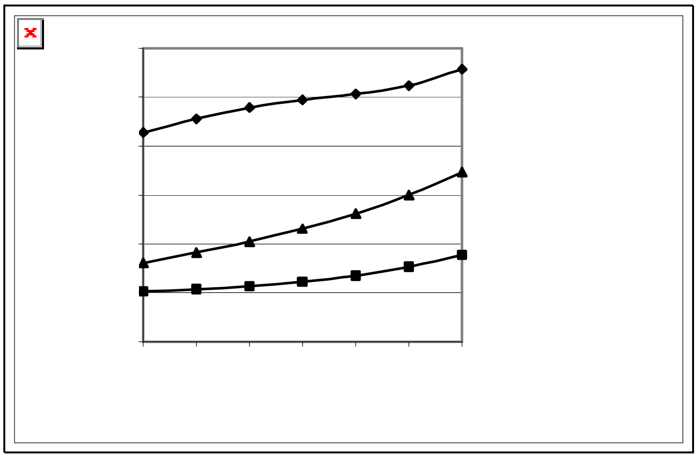

Fig.(4):Product rate vs. Conversion

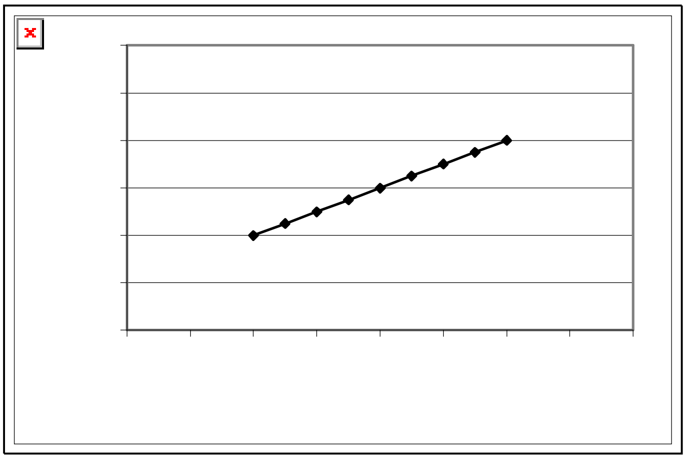

Fig.(5):Severity Factor vs. C/O Ratio

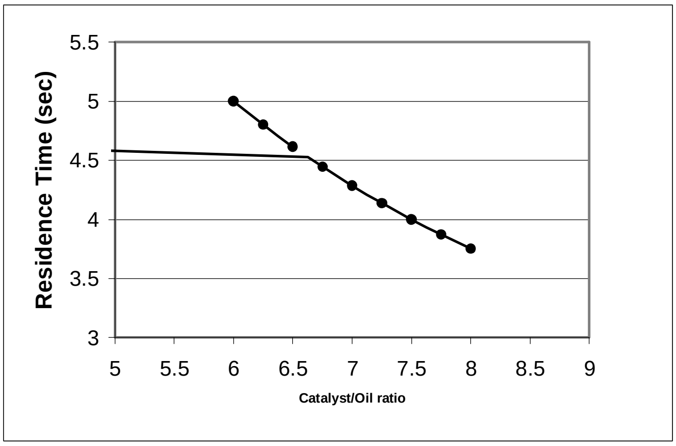

Fig. (6):Residence Time vs. C/O Ratio

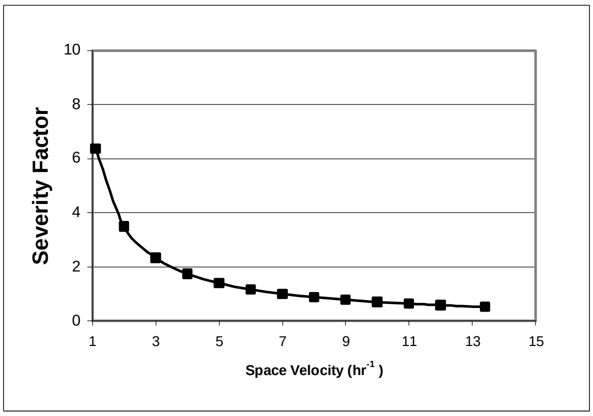

Fig.(7):Severity Factor vs. Space Velocity

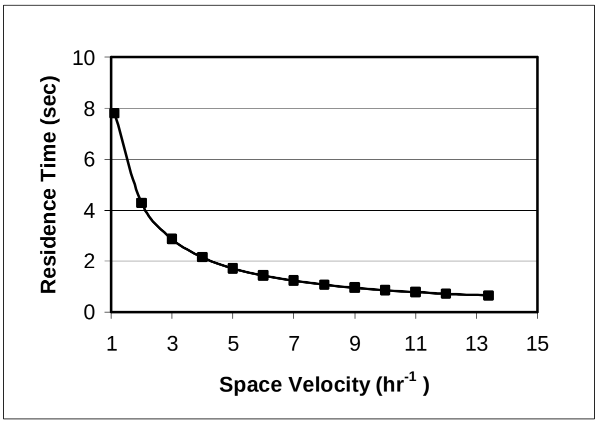

Fig.(8):Residence Time vs. Space velocity

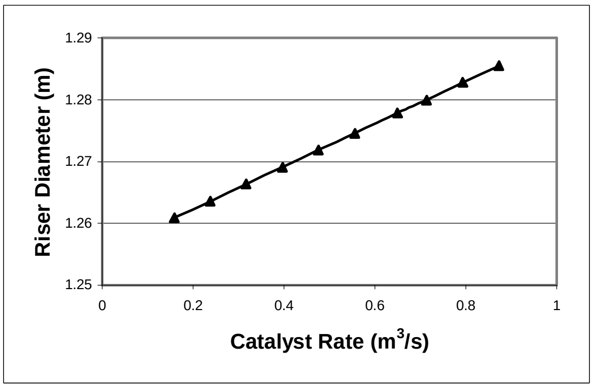

Fig. (9) : Riser Diameter vs. Catalyst Rate

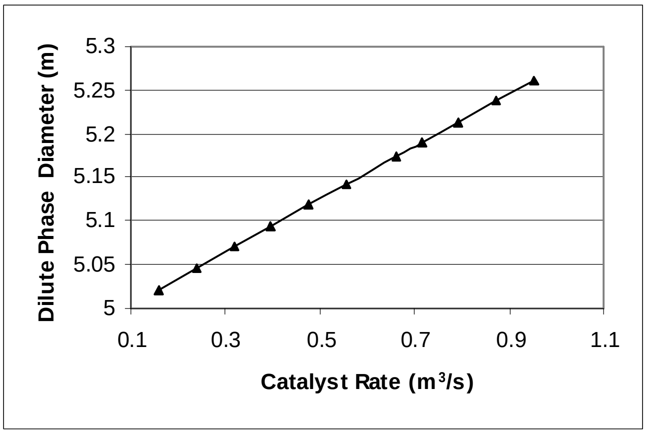

Fig.(10):Reg. Dense phase Diameter vs. Catalyst rate

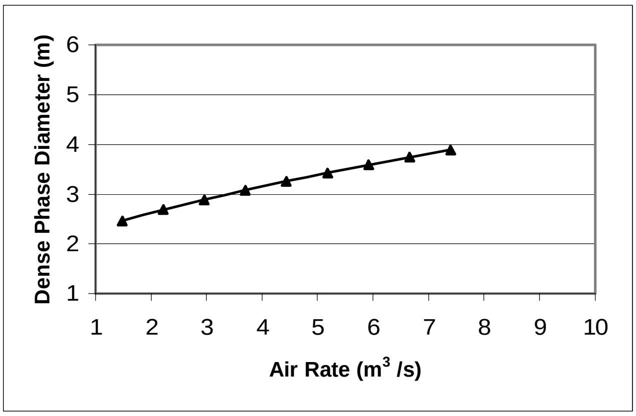

Fig.(11):Reg. Dilute phase Diameter vs. Catalyst Rate

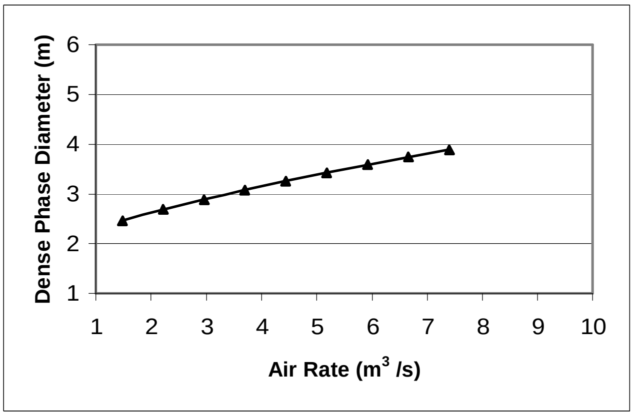

Fig.(12):Reg. Dense phase Diameter vs. Air Rate

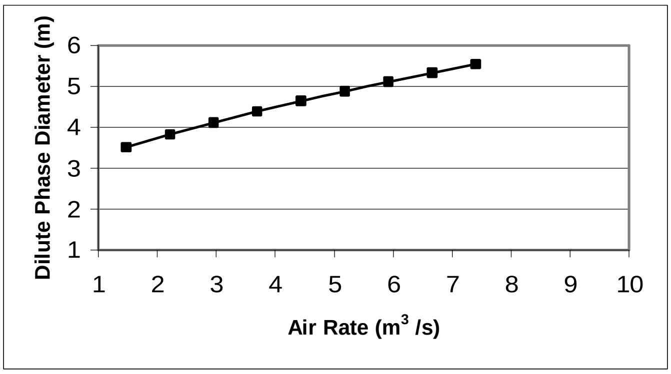

Fig. (13): Reg. Dilute phase Diameter vs. Air Rate

(14) : Fractionator Diameter vs. Top Product

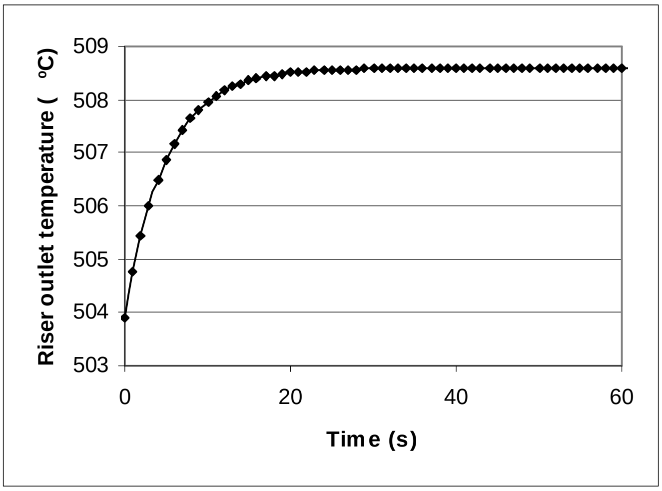

Fig. (15) : Riser Outlet Temperature vs. Time

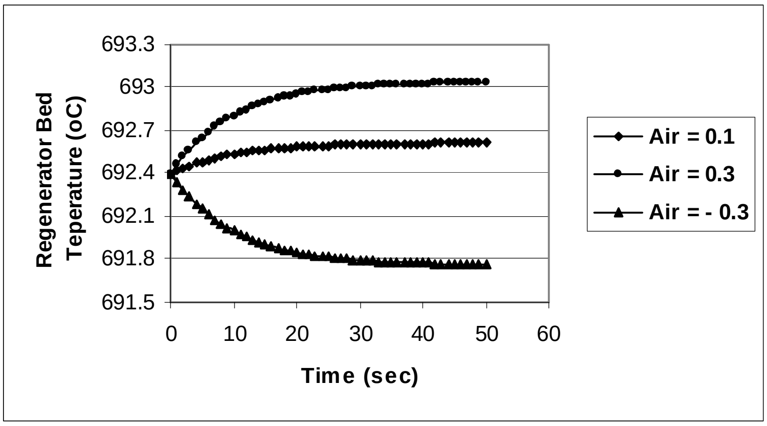

Fig. (16) : Reg. Bed Temperature vs. Time for Different Step Changes in Air Flow Rates in kg/s

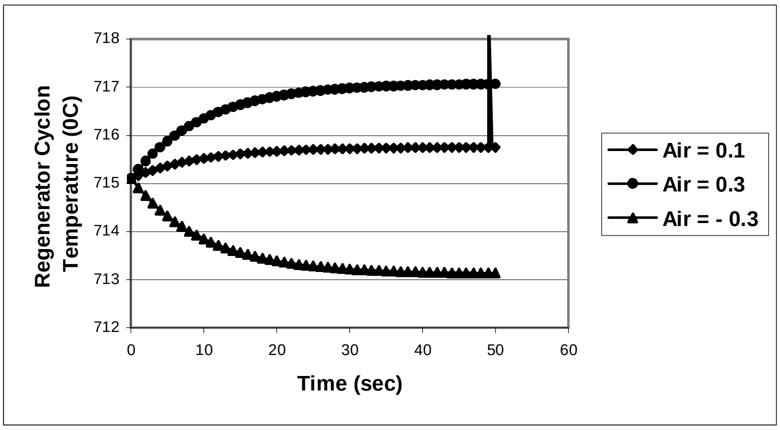

Fig. (17) : Regenerator Cyclone Temperature vs. Time for Different Step Changes in Air Flow Rates in kg/s

Appendix (A)
Properties of Kirkuk Crude Oil and vacuum gas oil(VGO)

Property	Crude oil	VGO
Gravity, degrees API	35.1	20.65
Specific Gravity (60 F / 60 F)	0.8493	0.93
Total sulfur, wt. Pct.	1.97	3.50
Total Nitrogen, wt. Pct.	0.12	0.126
Pour point, degrees F	8.0	83.9
Viscosity at 70 deg. F, CS	7.45	-----
Viscosity at 100 deg. F, CS	4.61	53.04
Vanadium, ppm wt.	29.00	-----
Nickel, ppm, wt.	11.00	-----
Aniline point deg. F		188.1

Appendix(B)

B-1 Process variables

Cracking efficiency	70%
Conversion	75%
Catalyst activity	2.923
Severity factor	3.500
Space velocity	$2.0.h^{-1}$
Catalyst / Oil ratio	7
Catalyst residence time	4.286 min.
Catalyst flow rate	1638892.5 kg/h
Catalyst circulation rate	1.0189 ton catalyst /bbl total feed

B-2 Total material balance :

Item	***Wt.%***	***kg/hr***	***S, wt.%***	***S, kg/hr***
A. Feed	100	234127.5	3.5	8194.46
B. Output				
Coke	10.4030	24356.2838	24	1966.67
C_2 & ltr	5.667	13268.0054	37	3031.95
$C_3^=$, vol%	4.838	6357.78513		
C_3, vol%	2.544	3259.90068		
$C_4^=$, vol%	8.126	12294.7802		
i-C_4, vol%	5.359	7595.59205		
n-C_4, vol%	2.304	3387.38688		
C_5^+ gasoline,vol%	51.959	98889.9276	5	409.72
TCGO, vol%	25.488	64717.8382	34	2786.12
Total		234127.5		8194.46
C. Steam				
Dispersion	5	11706.375		
Stripping	0.4% wt of cat.	6555.570		
Miscellaneous	1.5	3511.9125		
Total steam		21773.8575		