CHAPTER 3

FIVE LUMP KINETIC MODEL

A steady state model was developed for simulating the performance of an industrial fluid catalytic cracking (FCC) unit which was subsequently used in parametric sensitivity studies. The simulator includes five lump kinetic model for the riser reactor and a two-phase model regeneration system. Mass and energy balances were performed for each of these sections and simulation results were compared with the plant data available in the literature. Model predictions were found to be in close agreement with the reported data. Finally this validated model was used for studying the effects of independent variables such as feed preheat temperature ($T_{feed}$) and feed flow rate ($F_{feed}$) on the unit performance at either fixed regenerated catalyst temp/regenerator temp ($T_{rgn}$) or constant reactor outlet temperature (ROT). The catalyst circulation rate (CCR) was automatically adjusted to keep the ROT constant with varying the independent variables feed preheat temperature while the air rate adjusted for keeping the regenerator temperature constant which consequences the dependency of both dependent and independent variables on the unit performance. The air flow rate to the regenerator was also an independent variable during the parametric sensitivity analysis and its effect on FCC performance was investigated at constant $T_{feed}$, $F_{feed}$ and CCR.

3.1 RISER MODEL

A 5-kinetic lump reaction scheme proposed by Bollas et al. 2007a and shown in Figure 3.1 has been adopted in the present study. The feed is represented by only one lump as gas oil while the products are lumped as gasoline, LPG, Dry Gas and Coke. The total number of kinetic reactions for the five lump kinetic model are nine.
The following assumptions were made for the modeling of FCC riser reactor:

1. Gases and catalyst are in plug flow in the riser reactor.
2. Gas oil cracking is a second order reaction but cracking of gasoline and LPG are first order reactions.
3. There are no radial temperature gradients in the gas and solid phases.
4. As the catalyst particles are very small (20 – 80 µm) and the vaporized gas oil carries catalyst particles at high velocities, slip factor is assumed to be unity.
5. Dry gases produce no coke.
6. Catalyst deactivation is non-selective and related to coke on catalyst only.
7. The solid catalyst particles are in thermal equilibrium with the gaseous mixture at all times.

Tables 3.1 to 3.4 provide plant operating data, design data and thermodynamic and other data (Dave and Saraf, 2003; Kasat et al., 2002)

Table 3.1: Input Data Used in the Simulation

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Numerical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>F_{feed} (kg/sec)</td>
<td>32.14</td>
</tr>
<tr>
<td>F_{rgc} (kg/sec)</td>
<td>208.33</td>
</tr>
<tr>
<td>T_{feed} (K)</td>
<td>625.1</td>
</tr>
<tr>
<td>P_{ris} (atm)</td>
<td>2.546</td>
</tr>
<tr>
<td>P_{rgn} (atm)</td>
<td>2.68</td>
</tr>
<tr>
<td>F_{air} (kmol/sec)</td>
<td>0.57</td>
</tr>
<tr>
<td>T_{air} (K)</td>
<td>493.9</td>
</tr>
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</table>
Table 3.2: Thermodynamic and Other Parameters Used in the Simulation of FCC Unit

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Numerical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{p,c}$ (kJ/kg K)</td>
<td>1.003</td>
</tr>
<tr>
<td>$C_{p,fi}$ (kJ/kg K)</td>
<td>3.430</td>
</tr>
<tr>
<td>$C_{p,v}$ (kJ/kg K)</td>
<td>3.390</td>
</tr>
<tr>
<td>$C_{p,N2}$ (kJ/kg K)</td>
<td>30.530</td>
</tr>
<tr>
<td>$C_{p,O2}$ (kJ/kg K)</td>
<td>32.280</td>
</tr>
<tr>
<td>$C_{p,H2O}$ (kJ/kg K)</td>
<td>36.932</td>
</tr>
<tr>
<td>$C_{p,CO}$ (kJ/kg K)</td>
<td>30.850</td>
</tr>
<tr>
<td>$C_{p,CO2}$ (kJ/kg K)</td>
<td>47.400</td>
</tr>
<tr>
<td>$\Delta H_{evp}$ (kJ/kg)</td>
<td>350.0</td>
</tr>
<tr>
<td>$H_{CO}$ (kJ/kmol)</td>
<td>$1.078 * 10^5$</td>
</tr>
<tr>
<td>$H_{CO2}$ (kJ/kmol)</td>
<td>$3.933 * 10^3$</td>
</tr>
<tr>
<td>$H_{H2O}$ (kJ/kmol)</td>
<td>$2.42 * 10^3$</td>
</tr>
<tr>
<td>$X_{pt}$</td>
<td>0.10</td>
</tr>
<tr>
<td>$\rho_c$ (kg/m$^3$)</td>
<td>1089.0</td>
</tr>
<tr>
<td>$C_H$ (kg H$_2$/kg)</td>
<td>0.165</td>
</tr>
<tr>
<td>$D_p$ (ft)</td>
<td>$2.0 * 10^{-4}$</td>
</tr>
<tr>
<td>$MW_{Gas Oil}$</td>
<td>350</td>
</tr>
<tr>
<td>$MW_{Gasoline}$</td>
<td>114</td>
</tr>
<tr>
<td>$MW_{LPG}$</td>
<td>58</td>
</tr>
<tr>
<td>$MW_{Dry Gas}$</td>
<td>30</td>
</tr>
<tr>
<td>$MW_{Coke}$</td>
<td>12</td>
</tr>
</tbody>
</table>

Table 3.3: Design Data Used for the Simulation of FCC Unit

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Numerical Value</th>
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<tbody>
<tr>
<td>Riser Length (m)</td>
<td>36.965</td>
</tr>
<tr>
<td>Riser Diameter (m)</td>
<td>0.684</td>
</tr>
<tr>
<td>Regenerator Length (m)</td>
<td>19.344</td>
</tr>
<tr>
<td>Regenerator diameter (m)</td>
<td>4.522</td>
</tr>
<tr>
<td>Catalyst Inventory in the Regenerator(kg)</td>
<td>34000</td>
</tr>
<tr>
<td>Height of the cyclone inlet(ft)</td>
<td>49</td>
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</tbody>
</table>

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Table 3.4: Kinetic and Thermodynamic Parameters Used for Reactor Modeling

<table>
<thead>
<tr>
<th>Rate Constant</th>
<th>Reaction</th>
<th>Rate Constant</th>
<th>Reaction</th>
<th>Frequency Factor**</th>
<th>Activation Energy (kJ/kmol)</th>
<th>Heat of Reaction (kJ/kmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>k1</td>
<td>Gas Oil → Gasoline</td>
<td>18579.9</td>
<td>57540</td>
<td>45000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>k2</td>
<td>Gas Oil → LPG</td>
<td>3061.1</td>
<td>52500</td>
<td>159315</td>
<td></td>
<td></td>
</tr>
<tr>
<td>k3</td>
<td>Gas Oil → Dry Gas</td>
<td>532.14</td>
<td>49560</td>
<td>159315</td>
<td></td>
<td></td>
</tr>
<tr>
<td>k4</td>
<td>Gas Oil → Coke</td>
<td>39.04</td>
<td>31920</td>
<td>159315</td>
<td></td>
<td></td>
</tr>
<tr>
<td>k5</td>
<td>Gasoline → 65.4</td>
<td>73500</td>
<td>42420</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>k6</td>
<td>Gasoline → 0.00</td>
<td>45360</td>
<td>42420</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>k7</td>
<td>Gasoline → 0.00</td>
<td>66780</td>
<td>42420</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>k8</td>
<td>LPG → 0.32</td>
<td>39900</td>
<td>2100</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>k9</td>
<td>LPG → 0.19</td>
<td>31500</td>
<td>2100</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**m³/ (kg catalyst) (kmol gas oil) for reactions (1) to (4) and m³/(kg catalyst) (s) for reactions (5) to (9)**

3.1.1. Riser Model Equations

a. The mass balance for the jth lump over a differential element of height dh

$$\frac{dF_j}{dh} = A_{ris}H_{ris}(1 - \epsilon)\rho_c \sum_{i=1}^{9} (\alpha_{k,j})_i r_i$$  (3.1)

Rate equations for each of the nine reactions is as follows:

$$r_i = k_{oi} \exp\left(-\frac{E_i}{RT}\right)C_j^2 \phi$$ for i = 1,2,3,4 and j = 1  (3.2)

$$r_i = k_{oi} \exp\left(-\frac{E_i}{RT}\right)C_j \phi$$ for i = 5,6,7 and j = 2  (3.3)

b. Enthalpy balance across the same differential element of the riser

$$\frac{dT}{dh} = \frac{A_{ris}H_{ris}\rho_c(1-\epsilon)}{F_{rgC_{pc}} + F_{feedC_{pv}}} \sum_{i=1}^{9} r_i(-\Delta H_i)$$  (3.5)

$$T(h = 0) = \frac{F_{rgC_{pc}}(T_{rgn}-10.0) + F_{feedC_{pv}}T_{feed} - \Delta H_{evp}F_{feed} - Q_{loss,ris}}{F_{rgC_{pc}} + F_{feedC_{pv}}}$$  (3.6)

c. Gas oil properties in the riser reactor are calculated by the following equations:
Stripper Modeling

\[ \rho_v = \frac{P_{\text{ris}} MW_g}{RT} \quad \text{and} \quad \varepsilon = \frac{F_{\text{feed}}/\rho_v}{F_{\text{feed}}/\rho_v + F_{\text{rgc}}/\rho_c} \]  

3.1.2 Catalyst Deactivation

The catalyst activity (\( \phi \)) was related to coke concentration on the catalyst and proposed by Yingxun (1991) for catalytic cracking of vacuum gas oil is as follows:

\[ \phi = (1 + 51C_c)^{-2.78} \]  

where \( C_c \) is the weight percent carbon and is dependent on catalyst residence time (Voorhies et al, 1945):

\[ C_c = m \theta^n \]  

\( \theta \) is the catalyst residence time in minutes and \( m \) and \( n \) are the constants and depend on the feed. The exponent of \( \theta \) is close to 0.5.

3.2 REGENERATOR MODEL

The regenerator has two regions, a dense and dilute phase. The deactivated catalyst, after steam stripping of hydrocarbons, enters the regenerator where all
hydrogen in the coke is converted into steam. Carbon can be converted to either CO or CO2. The heat of combustion raises the temperature of the catalyst recycling from the regenerator. The heat of combustion released in the regenerator is therefore the most critical item in any such simulation. The following assumptions are made in the development of the regenerator model (Dave and Saraf, 2003; Kasat et al, 2002; Krishna et al 1985; De Lasa, 1979, McFarlane et al 1995).

1. The gases are in plug flow through bed and in thermal equilibrium with surrounding bed.
2. Catalyst in dense bed is well mixed and isothermal with uniform carbon on catalyst.
3. Kinetics of the coke combustion assumes catalyst particles to be of 60 μm size.
4. Resistance to mass transfer from gas to catalyst phase is negligible.
5. Mean heat capacities of gases and catalyst are assumed to remain constant over the temperature range encountered.
6. All entrained catalyst is returned via cyclones.

The coke combustion, reactions 3.13 and 3.14 are proportional to Crgc and Po2. The CO combustion, reactions 3.15 and 3.16, are proportional to Po2 and Pco and take place through two parallel paths, heterogeneous and homogeneous. The hydrogen combustion, reaction 3.17 is complete and immediate and the hydrogen weight fraction in the coke is constant. The main combustion reactions in the regenerator are as follows:

\[
\begin{align*}
\text{C} + \frac{1}{2} \text{O}_2 & \xrightarrow{k_{11}} \text{CO} \\
\text{C} + \text{O}_2 & \xrightarrow{k_{12}} \text{CO}_2
\end{align*}
\]
CO + $\frac{1}{2} O_2 \xrightarrow{k_{13c}} CO_2$  \hspace{1cm} \text{Heterogeneous CO Combustion} \hspace{1cm} (3.15)

CO + $\frac{1}{2} O_2 \xrightarrow{k_{13h}} CO_2$  \hspace{1cm} \text{Homogeneous CO combustion} \hspace{1cm} (3.16)

$H_2 + \frac{1}{2} O_2 \xrightarrow{k_{14}} H_2O$ \hspace{1cm} (3.17)

The following rate expressions for the combustion reactions in the regenerator in kmol / (m$^3$.sec) are:

\[
r_{11} = (1-\epsilon)\frac{\rho c k_{11}}{MW_c} P_{O_2} = (1-\epsilon)\frac{\rho c k_{11}}{MW_c} \frac{C_{rgc} f_{O_2}}{f_{tot}} p_{rgn} \tag{3.18}
\]

\[
r_{12} = (1-\epsilon)\frac{\rho c k_{12}}{MW_c} P_{O_2} = (1-\epsilon)\frac{\rho c k_{12}}{MW_c} \frac{C_{rgc} f_{O_2}}{f_{tot}} p_{rgn} \tag{3.19}
\]

\[
r_{13} = k_{13} P_{O_2} P_{CO} = (X_{pt}(1-\epsilon)\rho c k_{3h} + \epsilon k_{13h} P_{O_2}) P_{CO} = (X_{pt}(1-\epsilon)\rho c k_{13c} + \epsilon k_{13h}) \frac{f_{O_2} f_{CO}}{f_{tot} f_{rgn}} \tag{3.20}
\]

where $X_{pt}$ is the relative combustion rate simulating the addition of promoter.

The CO2/CO ratio in the gas leaving the dense bed is a function of the bed temperature, residence time, carbon- on-catalyst, and equilibrium metals on catalyst. The presence of CO promoter catalyzes CO oxidation and raises CO2/CO ratio. The CO in the dense bed exit is also oxidized in the dilute bed in presence of entrained catalyst.

The initial ratio of CO/CO2 at the catalyst surface is given by equation 3.21 (Weisz, 1966) and $k_c$ is the overall coke combustion rate.

\[
\left(\frac{CO}{CO_2}\right)_{Surface} = \frac{k_{11}}{k_{12}} = \beta_c = \beta_c \exp\left(-\frac{E_{beta}}{RT}\right) \tag{3.21}
\]

\[
k_c = k_{11} + k_{12} = k_{co} \exp\left(-\frac{E_{c}}{RT}\right) \tag{3.22}
\]

\[
k_{11} = \frac{\beta_c k_c}{\beta_c + 1} = \beta_c \frac{k_{co} \exp\left(-\frac{E_{c}}{RT}\right)}{\beta_c + 1} \tag{3.23}
\]

\[
k_{12} = \frac{k_c}{\beta_c + 1} = \frac{k_{co} \exp\left(-\frac{E_{c}}{RT}\right)}{\beta_c + 1} \tag{3.24}
\]


\[ k_{13c} = k_{13c0} \exp \left( -\frac{E_{13c}}{RT} \right) \]  \hspace{1cm} (3.25)

\[ k_{13b} = k_{13b0} \exp \left( -\frac{E_{13b}}{RT} \right) \]  \hspace{1cm} (3.26)

### 3.2.1. Dense Phase Model Equations

The regenerator dense bed consists of two phases, the gases phase and catalyst phase (solid phase), where as the gases are assumed to be moving in plug flow, the catalyst phase is assumed to be well mixed. In this model it is assumed that there is no resistance to mass transfer of gaseous components between gas phase and catalyst phase (Krishna and Parkin, 1985).

#### a. The Gas Phase Material Balance:

The material balances across a differential elemental of height, \( dz \), of dense bed are as follows:

\[ \frac{dF_{\text{O}_2}}{dz} = -A_{\text{rgn}} \left( \frac{r_{11}}{2} + \frac{r_{12}}{2} + \frac{r_{13}}{2} \right) \]  \hspace{1cm} (3.27)

\[ \frac{dF_{\text{CO}}}{dz} = -A_{\text{rgn}} (r_{13} - r_{11}) \]  \hspace{1cm} (3.28)

\[ \frac{dF_{\text{CO}_2}}{dz} = A_{\text{rgn}} (r_{12} + r_{13}) \]  \hspace{1cm} (3.29)

\[ \frac{dF_{\text{N}_2}}{dz} = 0 \]  \hspace{1cm} (3.30)

Initial Conditions (at \( z=0 \)) for Dense Bed Modeling:

\[ F_{\text{H}_2\text{O}} = \left( C_{\text{sc}} - C_{\text{rgc}} \right) \frac{C_{\text{H}}}{\text{MW}_{\text{c}}} \]  \hspace{1cm} (3.31)

\[ F_{\text{O}_2} = 0.21F_{\text{air}} - \frac{1}{2}F_{\text{H}_2\text{O}} \]  \hspace{1cm} (3.32)

\[ F_{\text{CO}} = F_{\text{CO}_2} = 0 \]  \hspace{1cm} (3.33)

\[ F_{\text{N}_2} = 0.79F_{\text{air}} \]  \hspace{1cm} (3.34)

\[ F_{\text{tot}} = F_{\text{O}_2} + F_{\text{CO}} + F_{\text{CO}_2} + F_{\text{H}_2\text{O}} + F_{\text{N}_2} \]  \hspace{1cm} (3.35)

#### b. Carbon Mass Balance:
Under the assumption that all the entrained catalyst returns to the dense bed, it is possible to write an overall carbon balance for the regenerator.

\[
\frac{dC_{rgc}}{dt} = \frac{1}{W_{rgn}} \left[ (F_{sc} C_{sc} - F_{rgc} C_{rgc})(1 - C_{H}) + (F_{CO}(2\text{bed}) + F_{CO_2}(2\text{bed})) MW_c \right] \tag{3.36}
\]

For constant Crgc in dense bed, \( \frac{dC_{rgc}}{dt} = 0 \), as catalyst is in CSTR.

\[
C_{rgc} = \frac{[F_{sc} C_{sc}(1-C_H) - (F_{CO}(2\text{bed}) + F_{CO_2}(2\text{bed})) MW_c]_{F_{rgc}(1-C_H)}} \tag{3.37}
\]

**c. Energy Balance**

Similar to the carbon mass balance, the catalyst temperature is also constant (catalyst is in CSTR and \( \frac{dT_{rgn}}{dt} = 0 \)) in dense bed, so overall heat balance in the dense bed is given by the following equation:

\[
\frac{dT_{rgn}}{dt} = \frac{1}{W_{rgn} C_p} \left[ (Q_C + Q_H + Q_{air} + Q_{sc} + Q_{ent}) - (Q_{rgc} + Q_{sg} + Q_{loss,rgn}) \right] \tag{3.38}
\]

Heat balance across the regenerator dense bed is given by the following equation:

\[
Q_C + Q_H + Q_{air} + Q_{sc} + Q_{ent} = Q_{rgc} + Q_{sg} + Q_{loss} \tag{3.39}
\]

Where,

\[
Q_C = F_{CO}(2\text{bed}) C_{CO} + F_{CO_2}(2\text{bed}) C_{CO_2} \tag{3.40}
\]

\[
Q_H = F_{H_2O} C_{H_2O} \tag{3.41}
\]

\[
Q_{air} = F_{air} C_{air}(T_{air} - T_{base}) \tag{3.42}
\]

\[
Q_{sc} = F_{sc} C_{sc}(T_{sc} - T_{base}) \tag{3.43}
\]

\[
Q_{rgc} = F_{rgc} C_p(T_{rgn} - T_{base}) \tag{3.44}
\]

\[
Q_{sg} = F_{CO_2}(2\text{bed}) C_{CO_2} + F_{CO}(2\text{bed}) C_{CO} + F_{O_2}(2\text{bed}) C_{O_2} + F_{H_2O} C_{H_2O} + F_{N_2} \tag{3.45}
\]

\[
Q_{ent} = F_{ent} C_p(T_{dil(2\text{bed})} - T_{base}) \tag{3.46}
\]

The final equation for the dense bed temperature is:

\[
T_{rgn} = T_{base} + \frac{F_{CO}(2\text{bed}) C_{H_2O} + F_{CO_2}(2\text{bed}) C_{H_2O} + F_{air} C_{air}(T_{air} - T_{base}) + F_{en} C_p(T_{base} - T_{dil(2\text{bed})}) + Q_{loss,rgn}}{F_{rgc} C_p + F_{CO_2}(2\text{bed}) C_{CO_2} + F_{en} C_p + F_{CO}(2\text{bed}) C_{CO} + F_{O_2}(2\text{bed}) C_{O_2} + F_{H_2O} C_{H_2O} + F_{N_2}} \tag{3.47}
\]
d. Evaluation of Bed Characteristics:

\[ \rho_g = \frac{P_{\text{rgn}}}{RT_{\text{rgn}}} \quad (3.48) \]

\[ u = \frac{F_{\text{air}}}{\rho_g A_{\text{rgn}}} \quad (3.49) \]

\[ \varepsilon_{\text{den}} = \frac{0.305u_{1+1}}{0.305u_{1+2}} \quad \text{Ewell and Gadmer, 1978} \quad (3.50) \]

\[ \rho_{c,\text{dense}} = \rho_c (1 - \varepsilon_{\text{den}}) \quad (3.51) \]

\[ \rho_{c,\text{dilute}} = \text{Max}[0, (0.582u1 - 0.878)] \quad \text{(lb/ft3), from McFarlane et al., 1995} \quad (3.52) \]

Void fraction in the dilute phase:

\[ \varepsilon_{\text{dil}} = \frac{\rho_{c,\text{dil}}}{\rho_c} \quad (3.53) \]

\[ F_{\text{ent}} = \rho_{c,\text{dil}} A_{\text{rgn}} u \quad (3.54) \]

Dense Bed Height:

The regenerator dense bed height is calculated by the given correlation McFarlane et al., 1995

\[ z_{\text{bed}} = \min \left[ z_{\text{cyc}} \left( 2.85 + 0.8u + \frac{W_{\text{reg}} - \rho_{c,\text{dilute}} A_{\text{rgn}} z_{\text{cyc}}}{A_{\text{rgn}} \rho_{c,\text{dense}}} \right) \frac{1}{1 - \frac{\rho_{c,\text{dilute}}}{\rho_{c,\text{dense}}}} \right] \]

3.2.2 Dilute Phase Model Equations

The Dilute bed is described as a lean phase where entrained catalyst particles and gases evolve in a plug flow pattern. The material and energy balance equations from Kasat et al., 2002 for the dilute bed regenerator are presented as follows:

a. Material Balance

\[ \frac{dF_{\text{O}_2}}{dz} = -A_{\text{rgn}} \left( \frac{r_{11}}{2} + r_{12} + \frac{r_{13}}{2} \right) \quad (3.55) \]

\[ \frac{dF_{\text{CO}}}{dz} = -A_{\text{rgn}} (r_{13} - r_{11}) \quad (3.56) \]

\[ \frac{dF_{\text{CO}_2}}{dz} = A_{\text{rgn}} (r_{12} + r_{13}) \quad (3.57) \]

\[ \frac{dF_C}{dz} = -A_{\text{rgn}} (r_{11} + r_{12}) \quad (3.58) \]
b. Energy Balance

\[
\frac{dT_{\text{dil}}}{dz} = \frac{1}{C_{\text{P, tot}}} \left( H_{\text{CO}} \frac{dP_{\text{CO}}}{dz} + H_{\text{CO}_2} \frac{dP_{\text{CO}_2}}{dz} \right) = \frac{A_{\text{rgn}}}{C_{\text{P, tot}} f_{\text{tot}}} \left[ H_{\text{CO}}(r_{11} - r_{12}) + H_{\text{CO}_2}(r_{11} - r_{12}) \right]
\]  

(3.59)

\[
C_{\text{P, tot}} = \frac{C_{\text{P, N}_2} F_{\text{N}_2} + C_{\text{P, O}_2} F_{\text{O}_2} + C_{\text{P, CO}} F_{\text{CO}} + C_{\text{P, CO}_2} F_{\text{CO}_2} + C_{\text{P, H}_2\text{O}} F_{\text{H}_2\text{O}} + C_{\text{P, ent}} F_{\text{ent}}}{f_{\text{tot}}}
\]

3.3 SIMULATION PROCEDURE FOR CONTINUOUS REACTOR - REGENERATOR OPERATION

A simulator has been developed where the coupled riser reactor and regenerator model equations have been assembled along with solution procedures. These have been computer coded using C programming language. The ordinary differential equations and nonlinear algebraic equations for material and energy balance are solved by using a Runge Kutta fourth order integration scheme and Successive Substitution methods respectively. The solution of these equations starts with initially guessed values of regenerated catalyst temperature \((T_{\text{rgn}})\) and coke on regenerated catalyst \((\text{Cr}_\text{gc})\), the product yields are, then, calculated at the outlet of the reactor. Subsequently the temperature of spent catalyst and coke on spent catalyst are calculated. The regenerator consists of the two beds: dense bed and dilute bed. The spent catalyst enters into the regenerator dense bed where it regenerates in presence of air and produces flue gases (see Figure 1.1). The dense bed calculations provide the new values of catalyst temperature \((T_{\text{cal}})\) and coke on regenerated catalyst \((\text{C}_\text{cal})\) which are compared with the initial value of \(T_{\text{rgn}}\) and \(\text{Cr}_\text{gc}\). If \(T_{\text{cal}}\) and \(\text{C}_\text{cal}\) do not match with assumed \(T_{\text{rgn}}\) and \(\text{Cr}_\text{gc}\) then one needs to start the reactor calculation with newly calculated values of \(T_{\text{rgn}}\) and \(\text{Cr}_\text{gc}\) by using the successive substitution method. Finally all the reactor and regenerator equations are solved with converged
value of Trgn and Crgc. The tolerance for the convergence of Trgn and Crgc used are $1^\circ C$ and $10^{-4}$ kg of coke/kg of catalyst respectively.

3.4 MODEL VALIDATION AND PARAMETRIC SENSITIVITY ANALYSIS FOR FIVE LUMP KINETIC MODEL

A complete reactor regenerator FCC unit has been simulated using the reactor model equations given by Dave and Saraf, (2003) and the regenerator model equations from different literature sources (Kasat et al., 2002; Avidan et al., 1990; Krishna and Parkin, 1985; De Lasas and Grace, 1979). The data on activation energies, frequency factors and heat of reaction (Table 3.4) are also used from the literature Dave and Saraf, 2003. The plant data and the model predicted data are compared in Table 3.5 and the match was found to be satisfactory. This validated model was used for the parametric sensitivity of the model to operating conditions. The coupled reactor and regenerator models were used to study the effect of different independent and dependent parameters on the plant performance. In order to study the effect of changing one independent variable on the reactor performance, all others must be held constant. However, it is important that the reactor operates under steady state conditions at all times, and this may require some other variable to be varied simultaneously. The feed flow rate ($F_{\text{feed}}$) and feed preheat temperature ($T_{\text{feed}}$) are the two key independent variables in the FCC process. The effects of these operating variables on steady state FCC unit performance are calculated by varying air flow rate ($F_{\text{air}}$) and catalyst circulation rate (CCR) to keep either regenerated catalyst temp ($T_{\text{rgn}}$) or ROT constant. The air flow rate to the regenerator was also used as an independent variable and its effect on conversion and yield studied.
Table 3.5: Comparison of Plant Measured and Models Prediction Data

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Plant Measured</th>
<th>Model Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactor Outlet Temp (K)</td>
<td>768.8</td>
<td>769.1</td>
</tr>
<tr>
<td>Gas Oil (wt %)</td>
<td>45.6</td>
<td>42.5</td>
</tr>
<tr>
<td>Gasoline (wt %)</td>
<td>34.0</td>
<td>36.7</td>
</tr>
<tr>
<td>LPG (wt %)</td>
<td>12.4</td>
<td>13.2</td>
</tr>
<tr>
<td>DG (wt %)</td>
<td>3.4</td>
<td>3.6</td>
</tr>
<tr>
<td>Coke (wt %)</td>
<td>4.6</td>
<td>4.0</td>
</tr>
<tr>
<td>Regenerator Temp(K)</td>
<td>937.5</td>
<td>937.2</td>
</tr>
<tr>
<td>Dense Bed Height(m)</td>
<td>-</td>
<td>6.5</td>
</tr>
<tr>
<td>Coke on Regenerated Catalyst (wt %)</td>
<td>-</td>
<td>0.12</td>
</tr>
<tr>
<td>O₂ (Vol %)</td>
<td>-</td>
<td>1.4</td>
</tr>
<tr>
<td>CO (Vol %)</td>
<td>-</td>
<td>10.3</td>
</tr>
<tr>
<td>CO₂ (Vol %)</td>
<td>-</td>
<td>6.4</td>
</tr>
<tr>
<td>N₂ (Vol %)</td>
<td>-</td>
<td>81.9</td>
</tr>
<tr>
<td>Flue Gas Temp(K)</td>
<td>-</td>
<td>939.0</td>
</tr>
<tr>
<td>Entrained Cat Flow Rate (kg/sec)</td>
<td>-</td>
<td>13.6</td>
</tr>
</tbody>
</table>

3.4.1 Effect of Feed Preheat Temperature on FCC Performance at Constant Feed Flow Rate ($F_{feed}$)

a) At Constant CCR and Constant Regenerator Temperature ($T_{rgn}$)

Feed preheat temperature plays an important role in controlling the temperature in the riser reactor and hence the cracking reactions (see Figures 3.2 and 3.3). Gas oil conversion as well as yield of all the products were found to increase linearly with increase in $T_{feed}$ (Figure 3.2). Figure 3.3 shows that reactor outlet temperature (ROT) increases nearly linearly with $T_{feed}$ but air flow rate to the regenerator decreases linearly. This is to be expected in view of the fact that with increased ROT, air flow rate must decrease in order to keep $T_{rgn}$ fixed.
Figure 3.2: Effect of feed preheat temperature on gas oil conversion and product yields at fixed \( F_{\text{feed}} \) (32.14 kg/sec) and fixed regenerator temperature (937.5K)

Figure 3.3: Effect of feed preheat temperature on riser outlet temperature (ROT) at fixed \( F_{\text{feed}} \) (32.14 kg/sec) and fixed regenerator temperature (937.5K)

b) At Constant Air Flow Rate (Fair) and Constant Reactor Outlet Temperature (ROT)

For ease of operation often the reactor outlet temperature is kept constant with the help of a controller. When feed preheat temperature is increased, regenerated catalyst flow rate (FrGC) must decrease to hold ROT constant (Figure 3.4). At constant feed
rate, this amounts to decreasing cat/oil ratio which leads to decrease in conversion and product yields (Figure 3.5). Figure 3.4 also shows that with increasing $T_{\text{feed}}$, regenerator temperature increases initially rapidly and latter gradually. The change in slope seems to occur at feed preheat temperature 625K perhaps indicating an optimal condition of operation. At low $T_{\text{feed}}$ the catalyst circulation rate is high giving rise of high conversion and high rate of coke formation. In view of this, regenerator temperature must increase rapidly, explaining the early sharp rise.

**Figure 3.4: Effect of Feed Preheat Temperature on Regenerator Temperature ($T_{\text{rgn}}$) at Fixed Feed Flow Rate (32.14 kg/sec) and Fix ROT (769 K)**

From Figure 3.5 one can conclude that the effect of catalyst circulation rate (or cat/oil) is more pronounced as compared to that of $T_{\text{feed}}$. Increasing $T_{\text{feed}}$ alone would have led to increase in conversion. The analysis showed that a decrease in feed preheat temperature by 10 K at fixed ROT and fixed feed could possibly result in 4% increase in gas oil conversion and 3.9% gasoline yield. This corresponds to an increase in catalyst circulation rate from 208 to 220 kg/sec or an increase in cat/oil ratio from 6.5 to 6.9.
Figure 3.5: Effect of feed preheat temperature on gas oil conversion and product yields at fixed feed flow rate (32.14 kg/sec) and fix ROT (769 K)

3.4.2 Effect of Feed Flow Rate on FCC Performance at Constant $T_{feed}$

a) At Constant CCR and Constant Regenerator Temperature ($T_{rgn}$)

As feed flow rate is increased keeping regenerator temperature and catalyst flow rate constant, the cat/oil ratio decreases which leads to decreased cracking activity and lower conversion and product yields (Figure 3.6).

Figure 3.6: Effect of feed flow rate on the conversion and product yields at fixed feed preheat temperature (625K) and fixed regenerator temperature (937.5K)
Figure 3.7 shows that ROT decreases with increase in feed rate. While lower cat/oil ratio decreases conversion leading to less absorption of endothermic heat, higher feed absorbs more heat. The effect of feed rate being more pronounced as compared to cat/oil ratio, there is net decrease in ROT, which is to be expected since $T_{\text{rgn}}$ is fixed. To keep $T_{\text{rgn}}$ constant, air flow rate must increase since sensible heat brought in the regenerator by the catalyst is less at lower ROT.

![Figure 3.7: Effect of feed flow rate on the reactor outlet temperature (ROT) at fixed feed preheat temperature (625K) and fixed regenerator temperature (937.5K)](image)

**b) At Constant Air Flow Rate and Constant Reactor Outlet Temperature (ROT)**

Figure 3.8 shows effect of change in feed rate on conversion and product yields at constant ROT and air flow rate. Under these conditions, $T_{\text{rgn}}$ is expected to decrease because of extra amount of carbon coming in the regenerator (Figure 3.9). Catalyst circulation rate must increase to keep ROT constant. In the present case both catalyst flow rate and feed rate are increasing, the cat/oil ratio increasing gradually. This should lead to increase in conversion. However, Figure 3.8 shows a decreasing trend
in conversion as well as product yields. This can be explained in terms of sharp decrease in $T_{rgn}$ amounting to less heat being available for endothermic cracking reactions, particularly when reactor outlet temperature must be maintained constant.

Figure 3.8: Effect of feed flow rate on the conversion and product yields at fixed reactor outlet temperature (768.8K) and fixed feed preheat temperature (625K)

Figure 3.9: Effect of feed flow rate on the regenerator temperature ($T_{rgn}$) at fixed feed preheat temperature (625K) and fixed reactor outlet temperature (768.8K)

3.4.3 Effect of Air Flow Rate ($F_{air}$) on FCC Performance at Constant $T_{feed}$, $F_{feed}$ and CCR:

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Figure 3.10 shows that ROT as well as $T_{\text{rgn}}$ increase initially with increasing air rate but become constant at higher air rates. More air rate leads to better coke combustion and hence higher $T_{\text{rgn}}$ which in turn, increases ROT. Both $T_{\text{rgn}}$ and ROT level off once coke combustion is nearly complete.

**Figure 3.10: Effect of air flow rate on the regenerator temperature ($T_{\text{rgn}}$) and reactor outlet temperature (ROT)**

**Figure 3.11: Effect of air flow rate on the conversion and product yields.**
Figure 3.12: Effect of regenerated catalyst temperature \( (T_{\text{rgn}}) \) on the conversion and product yields.

Figure 3.13: Effect of regenerated catalyst temperature \( (T_{\text{rgn}}) \) on reactor outlet temperature \( (\text{ROT}) \)

Higher regenerated catalyst temperature provides higher reactor temperature and hence increased conversion and product yields (Figure 3.11). These plots suggest that it will be advantageous to increase \( \text{ROT} \) by 14 K, \( T_{\text{rgn}} \) by 24 K by increasing air rate to 0.06 kmol/sec. The result of Figures 3.10 and 3.11 have been cross plotted in Figures
3.12 and 3.13 which show variation of conversion, product yields and reactor outlet temperature as a function of $T_{\text{reg}}$.

Combining some of these observations as referred in Table 3.6, a decrease of say, 10K, in the feed preheat temperature ($T_{\text{feed}}$) and corresponding increase in air rate ($F_{\text{air}}$) and catalyst circulation rate ($F_{\text{rgc}}$) was found to increase gas oil conversion and product yields by 5 to 6 percent at constant reactor outlet temperature (ROT) and regenerated catalyst temperature ($T_{\text{rgc}}$). The economic visibility of such changes on the operating conditions can be explored by the refiners.

Table 3.6: Comparison of FCC Performance at Three Different Feed Preheat Temperatures with Increased Cat/Oil Ratio and Air Flow Rate

<table>
<thead>
<tr>
<th>$T_{\text{feed}}$ (K)</th>
<th>625.1</th>
<th>615.1</th>
<th>605.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_{\text{rgc}}$ (kg/sec)</td>
<td>208.3</td>
<td>220.3</td>
<td>232.3</td>
</tr>
<tr>
<td>$F_{\text{air}}$ (kmol/sec)</td>
<td>0.57</td>
<td>0.63</td>
<td>0.63</td>
</tr>
<tr>
<td>ROT (K)</td>
<td>769.1</td>
<td>769.9</td>
<td>771.9</td>
</tr>
<tr>
<td>Gas oil conversion (wt %)</td>
<td>57.5</td>
<td>60.6</td>
<td>64.2</td>
</tr>
<tr>
<td>Gasoline (wt %)</td>
<td>36.8</td>
<td>38.8</td>
<td>41.2</td>
</tr>
<tr>
<td>LPG (wt %)</td>
<td>13.2</td>
<td>13.9</td>
<td>14.7</td>
</tr>
<tr>
<td>DG (wt %)</td>
<td>3.6</td>
<td>3.8</td>
<td>4.0</td>
</tr>
<tr>
<td>Coke (wt %)</td>
<td>4.0</td>
<td>4.2</td>
<td>4.4</td>
</tr>
<tr>
<td>$T_{\text{rgc}}$ (K)</td>
<td>937.2</td>
<td>936.1</td>
<td>937.2</td>
</tr>
</tbody>
</table>

3.5 CONCLUDING REMARKS

An industrial FCC unit has been simulated by integrating kinetic models for the riser reactor and the regenerator. The model equations were solved using a computer based code in C-language. The calculated model results are compared with the plant data, which are found to be in agreement. This validated model is used to study parametric sensitivity such as effects of feed preheat temperature, feed flow rate and air flow rate (independent variables) on the FCC performance. Catalyst
circulation rate has stronger influence on gas oil conversion as compared to feed preheat temperature for a fixed reactor outlet temperature. On the other hand feed flow rate affects conversion more than catalyst circulation rate. Increase in air flow rate with other important parameters remaining constant leads to increased conversion. From above discussion of sensitivity analysis it appears that decreasing Tfeed and increasing catalyst circulation rate and air flow rate should lead to higher conversion and product yields. Table 3.6 shows the result of such computations. At given feed flow rate, a decrease in feed preheat temperature and increase in air flow rate may lead to increased conversion and product yields. However, this will require increased catalyst circulation rate. Trgn and ROT were found to remain essentially constant. The sensitivity analysis is useful for the refiners to understand the effects of individual parameters on the FCC performance for better productivity of the unit.