

## Full Paper

# DYNAMIC MODELING AND SIMULATION OF FLUID CATALYTIC CRACKING UNIT RISER

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## ABSTRACT

This study developed and simulated a dynamic mathematical model for a Fluid Catalytic Cracking Unit (FCCU) riser reactor with consideration of coke deposition on the catalyst in the overall mass balance of the system. It also proposed a mathematical model that accounts for the dynamic effect of coke deposition on the hydrodynamics of the FCCU riser. The spatial derivatives are discretized using finite difference to obtain the dependency of the state variables on time.

The resulting ordinary differential equations were simulated using Java Application Programme Interface, ODEToJava. An approach proposed in this study is in good agreement with experimental and numerical data available in the literature.

The results showed an outlet vapor density of 2.76 kg/m<sup>3</sup> which gave a +7.39 % deviation when compared with plant data. Also the temperature outlet of the riser predicted by the model deviated by -5.49% when compared with real plant data. The model also confirmed the acceptability of the general assumption of isothermal condition while modeling the FCCU riser. The model prediction of components yield along the height of the riser is within permissible limit when compared with that reported for industrial riser. The study concluded that the developed model accurately described the dynamic behavior of an FCCU riser and its

predictions when compared with real plant data proved satisfactory.

**Keywords:** Fccu, riser, numerical modeling, simulation.

## 1. INTRODUCTION

The fluid catalytic cracker (Fig. 1.) is the heart of modern refinery because it bridges the gap between the market demand for gasoline and excess of heavy high-boiling range products resulting from the distillation of crude oil (Gary and Handwerk, 2001).

Direct distillation of crude oil is inadequate to meet high demand of octane gasoline Jet fuel and Diesel fuel; so, supplementary means are being developed to combat this inadequacy.

Modeling of riser reactor is very complex due to complex hydrodynamics, unknown multiple reactions coupled with mass transfer and heat transfer resistances. Also, the conditions keep changing all along the riser height due to cracking, which cause molar expansion in the gas phase and influence the axial and radial catalyst density in the riser.

In the literature, numerous models of FCC riser are available with varying degrees of simplifications and assumptions. The importance of the FCCU has led to the development of many models over time, based on varying assumptions regarding component hydrodynamics and reaction kinetics. However, most of these simulations assumed the idealized mixing conditions within the riser reactors and that coke deposited on the catalyst has a negligible effect on the hydrodynamics of the system.

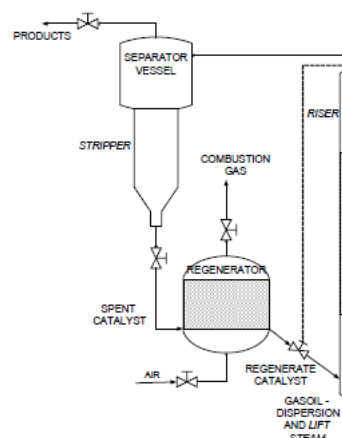


Figure 1. Simplified scheme of a FCC converter

The actual flow structure of gas and solids in a riser flow is very complex, with multidimensional variations in axial, radial and even azimuthal directions (such as near a bend or asymmetric gas-solids feeder inlet); multidirectional flows in core, annulus and wall regions; multi-scaled phase interactions (such as interactions among dispersed solids, clusters, turbulent eddies and pipe wall surfaces in different flow regimes); and other complications from solids cohesion and electrostatic charges. A simple mechanistic model of such a complicated system inevitably requires many assumptions for simplification.

Theologos and Markatos (1993) developed a mathematical model of the flow within the riser using the Weekman and Nace (1970) three lump kinetic model, with emphasis on the analysis of the two-phase flow. A previous one-dimensional analysis of an air-solid flow is made to validate the empirical correlations used for drag force and friction with the wall. Ding and Gidaspow (1990) and Tsuo and Gidaspow (1990) considered models of gas-solid flow based on the Navier-Stokes equation. They showed velocity fields throughout fluidized beds. Kunii and Levenspiel (1997) presented fluidization models and analyzed the formation of beds and the behavior of solid particles in pneumatic transport. Their works had great importance on the determination of void fraction.

Theologos and Markatos (2004) developed a three-dimensional model using a two-phase flow system. Their model ignored the turbulence of gas and solids and characterized the cracking reaction with a 4 lump kinetic model. The model predicted the flow field, heat distribution and concentrations of all species throughout the reactor. Berry et al., (2004) proposed a predictive hydrodynamic model which incorporated the slip factor for the calculation of the cross-sectional average voidage. The model has been coupled with the four-lump kinetic model to predict the effect of operating conditions on profiles of conversion, yield, temperature and pressure in the riser. Martignoni (2000) developed a 1-D model for a FCC riser, using a four lump (gasoil, gasoline, fuel gas, coke) and six lump (LCO, gasoline, GLP, coke, gasoil and fuel gas) approach. In this model, an analysis of the flow is made taking into account the friction with the internal walls, the drag force and the heat transfer mechanisms. You and Zhu (2002) developed a hydrodynamic framework model for the FCCU riser which emphasized simultaneous simulation of a multiphase flow hydrodynamics, cracking reaction and their inter-coupling characteristics in riser reactor. They estimate the total drag force per unit volume by multiplying the drag force on single particle by the number of particle per unit volume. They compensated for the reduction in drag force which occur in the solid acceleration regime (when stabilize wake effect becomes non-negligible) by multiplying the drag force with the coefficient of wake effect of the neighboring particles on the particle-fluid interfacial force.

Feed stocks passing through a cracking unit vary in component species, which are typically a huge amount of different hydrocarbons, beyond the ability of models to account for the kinetics of each one. Overcoming this obstacle involves the introduction of a lumping concept, in which species are grouped together based on their boiling range, where it is thought that their reaction kinetics will be the same. Several catalytic cracking reaction kinetic models for the FCC process have been proposed by different researchers. Blanding (1953) presented the first model of catalytic cracking kinetics using a two-lump approach, where the first lump contained all the components with boiling points above that of gasoline, and the second lump contained those below.

Nearly two decades later, a 3-lump model was proposed; the first lump contained gas oil that was not cracked, the second grouped the components of gasoline, and the third light gas and coke (Weekman and Nace, 1970). This model was distinguished by being a simple model as it has three components resulting in only three reactions, and allowed the yield of gasoline, and conversion of gasoil to be calculated at the same time and is regarded as a

milestone in the lumping technology (Lee et al., 1989). This scheme was further extended to several other kinetic schemes. Among them the four lump models, five lump models, six lump models, ten lump models, eleven lump models, twelve lump models, thirteen lump models, and nineteen lump models are widely used (Gupta et al., 2007).

The concept of lumping feedstock components and products has become well-established and progressed over time. In catalytic cracking models proposed by Yen et al. (1988) and Lee (1998), they modified the three-lump model to a 4-lump model by creating two separate lumps from the coke and gas oil lump. An advance in the area of 5-lump model was presented in the work of Dupain et al. (2006), taking account of thermal cracking in producing coke and gas.

However, despite the simplicity of kinetic models based on products, they are dependent on the feedstock conceptualized as one component. Such dependence on the feedstock in the model kinetics is a significant disadvantage, as new experiments must be performed for any change to the feedstock composition to derive the appropriate kinetic parameters. For simplification and less computational constraints, this present work used the 4-lump kinetic model of cracking reactions, which considers the heavy gas oil, gasoline, light gas and coke.

The current work presents a mathematical model of the gas-solid flow that occurs in FCC risers. For the sake of simplicity, considering the model is to be applied to control systems, the flow is assumed as one-dimensional and the momentum and energy conservation equations are employed to represent the two-phase flow (fluid and solid) and the heat transfer between the phases with a mass balance in the two phase to describe the rate of decomposition of coke on the catalyst. Four lumps are considered in the kinetic of the reaction model.

## 2. MATHEMATICAL MODELING

The complexity inherent in the riser is due to complicated hydrodynamics, heat transfer, mass transfer and catalytic cracking kinetics. Moreover, influential parameters vary along the riser height (Gupta and Rao, 2003). However, the following assumptions will be made to simplify the modeling task:

- Instantaneous vaporization of liquid fluid occurs when it comes in contact with hot regenerated catalyst.
- Vaporization of liquid feed increases gas velocity. Expansion of the vapor phase is however the main driving force.
- Riser is adiabatic. Temperature in the riser falls only due to the endothermicity of the cracking reaction.
- Mass transfer resistances is negligible.
- Both phases are in plug flow condition; hence back mixing is neglected.
- Deposited coke on catalyst has a considerable effect on the hydrodynamics of the system

### 2.1. Mass Conservation

The mass conservation is required to evaluate the dynamic changes that occur in the solid fraction in the riser as well as determining the rate of coke deposition on the catalyst

$$\frac{\partial \varepsilon_i}{\partial t} = -\frac{\partial (V_i \varepsilon_i)}{\partial z} \pm \frac{K_c}{\rho_i} \quad (1)$$

where  $\varepsilon_i$  is the fraction of volume occupied by each phase, defined as



$$\varepsilon_s + \varepsilon_g = 1 \quad (2)$$

$k_c$  is the rate of coke formation,  $V_i$  is the velocity of each phase and  $\rho_i$  is the density of each phase.

## 2.2. Momentum Conservation

The momentum balance is necessary to explain the hydrodynamics behind the transportation of the particle up the riser

$$\frac{\partial(v_i \varepsilon_i)}{\partial t} = - \frac{4\tau_i \varepsilon_i}{D_{riser}} - \varepsilon_i \frac{dP}{dz} - \rho_i \varepsilon_i \frac{\partial(v_i v_i)}{\partial z} - \rho_i \varepsilon_i g \pm F_D \varepsilon_i \quad (3)$$

where  $\tau_i$  is the respective phase-to-wall shear stress and  $F_D$  is the drag force which contributes to the acceleration of the solid phase and retards the vapor phase.  $\tau_i$  is defined as (Han and Chung, 2000; Martignoni, 2000 and Yang, 1978)

$$\tau_i = \frac{1}{2} f_{p,i} \varepsilon_i V_i^2 \quad (4)$$

where  $f_{p,i}$  is the friction factor for the vapor phase for  $2,100 \leq Re \leq 100,000$ .

$$f_{p,g} = \frac{0.0791}{Re^{0.25}} \quad (5a)$$

For Re above 100,000,

$$f_{p,g} = 0.0008 + 0.0552 Re^{-0.237} \quad (5b)$$

For solid,

$$f_{p,s} = \frac{0.051}{V_s} \quad (6)$$

The drag force defined by Markatos and Shinghal (1982) and as:

$$F_D = 0.5 C_D A_p \rho_g |V_g - V_s| (V_g - V_s) \quad (7)$$

The drag coefficient  $C_D$  is defined by Arastoopour and Gidaspow (1979) as

$$C_D = \frac{24}{Re_{CD}} (1 + 0.51 Re_{CD}^{0.687})_{Re_{CD} < 1000} \quad (8a)$$

$$C_D = (0.44)_{Re_{CD} \geq 1000} \quad (8b)$$

$Re_{CD}$  is the Reynolds number based on the relative velocity between the two phases defined as

$$Re_{CD} = \frac{\rho_g \varepsilon_g |V_g - V_s| D_{cat}}{\mu_{gas}} \quad (9a)$$

$A_p$  is the projected area per unit volume given as:

$$A_p = 1.5 \frac{\varepsilon_s}{D_{cat}} \quad (9b)$$

In the vapor phase, the Boussinesq approximation is used to estimate the dependency of the vapor density on temperature to provide for the buoyancy force.

$$\rho_{bar,g} = \rho_g \Big|_{\bar{T}_g} - \rho_g \beta \Big|_{\bar{T}_g} (T_g - \bar{T}_g) \quad (10a)$$

$$\bar{T}_g = \frac{1}{2} (T_g \Big|_{t=t} + T_g \Big|_{t=t-1}) \quad (10b)$$

$$\beta \Big|_{\bar{T}_g} = \frac{1}{\bar{T}_g} \quad (10c)$$

## 2.3. Reaction kinetics

A 4-lump kinetic scheme was employed in the model.

For vacuum gas oil (VGO),

$$r_{vgo} = -\phi \varepsilon_c \rho_c (K_1 + K_2 + K_3) C_{vgo}^2 (A_r \Delta z) \quad (11a)$$

For gasoline,

$$r_{gasoline} = \phi \varepsilon_c \rho_c (a_1 K_1 C_{vgo}^2 - (K_4 + K_5) C_{gasoline}) (A_r \Delta z) \quad (11b)$$

For light gases,

$$r_{gas} = \phi \varepsilon_c \rho_c (a_2 K_2 C_{vgo}^2 + a_4 K_4 C_{gasoline}) (A_r \Delta z) \quad (11c)$$

For coke,

$$r_{coke} = \phi \varepsilon_c \rho_c (a_3 K_3 C_{vgo}^2 + a_5 K_5 C_{gasoline}) (A_r \Delta z) \quad (11d)$$

$a_j$  is the stoichiometric coefficient used in rate equation for each lump. The rate of catalyst deactivation due to coke deposition is expressed as

$$\phi_c = e^{-\delta_c t_c} \quad (12)$$

Where  $t_c$  is the catalyst residence time.

$\delta_c$  is the deactivation coefficient which is defined by the Arrhenius equation based on the vapor phase temperature as

$$\delta_c = \delta_{c0} e^{-\frac{E}{RT_g}} \quad (13)$$

Where E is the activation energy for the deactivation (= 49,000 kJ/kmol) and  $\delta_{c0}$  is the pre-exponential factor (=  $1.1 \times 10^{-5} \text{ m}^6/\text{kgcat.kmol.s}$ ) and T is the absolute temperature of the catalyst.

Table 1: Plant data used for riser simulations given by Ali et al., (1997)

Parameter	Value
Feed flow rate	38 kg/s
Catalyst flow rate	144 kg/s
Riser Pressure	2.9 atm
Catalyst inlet temperature	960.0 K
Riser Height	33 m

Table 2: Parameter used for riser simulations

Parameter	Value	Source
Specific heat of VGO (Liquid)	2.67 kJ/kg.K	Ali et al., 1997
Specific heat of VGO (Vapor)	33 kJ/kg.K	Ali et al., 1997
Latent heat of Vaporization	96 kJ/kg	Gupta and Subba Rao, 2003
Gas phase viscosity	$1.3 \times 10^{-3} \text{ kg/m.s}$	Gupta and Subba Rao, 2003
Catalyst Particle density	1200 kg/m <sup>3</sup>	Gupta et al., 2008
Catalyst Particle diameter	75 $\mu\text{m}$	Gupta and Subba Rao, 2003
Specific heat of Catalyst	1.15 kJ/kg.K	Ali et al., 1997

The rate of change of change of each component in the riser was determined thus:

$$\frac{\partial(C_A \varepsilon_g)}{\partial t} = \varepsilon_g \frac{\partial(C_A V_g)}{\partial z} + R_A \quad (14)$$

Where  $C_A$  is the concentration of each species per unit volume of the riser.  $R_A$  is the rate of formation and or disappearance of each species per unit volume of the riser. The vacuum gas oil source is expected to be only from vaporization of feed stock while its sink is the cracking reaction which will be second order. Gasoline will be formed from the cracking of the feed stock as well as consumed through cracking to fuel gas and coke. The reaction rate for each species was determined by equations 11.  $K_{j,i}$  is the kinetic constant evaluated by Arrhenius equation thus:

$$K_{ji} = K_0 e^{-\frac{E_{ji}}{RT_g}} \quad (15)$$

$K_0$  is the pre-exponential factor and  $E_{ji}$  is the activation energy for each reaction.

#### 2.4. Heat Conservation

Finally, to complete the formulation, two more equations are necessary - the catalyst and vapor energy equations. The catalyst equation is obtained as

$$\rho_c C_{pc} \frac{\partial(\varepsilon_s T_s)}{\partial t} = -h_c A_{gs} (T_s - T_g) - R_{g,i} (\Delta H_i) - \rho_c \varepsilon_c C_{pc} \frac{\partial(V_s T_s)}{\partial z} \quad (16)$$

where  $R_{g,i}(\Delta H_i)$  is the energy lost by the catalyst for the endothermic cracking reaction,  $(\Delta H_i)$  is the heat of reaction of respective reaction specie and  $h_s$  is the convective heat transfer coefficient defined by Kunii and Levenspiel (1997) as:

$$h_s = 0.03 \frac{\kappa_g}{\sqrt[3]{D_{cat}}} \sqrt[6]{\frac{|V_g - V_s| \rho_g \varepsilon_g}{\mu_g}} \quad (17)$$

where  $\kappa_g$  is the thermal conductivity of gas phase defined by API (American Petroleum Institute) technical data book (Technical Data Committee, 1988), cited in Han e Chung (1990):

$$\kappa_g = 10^{-6} [1.9469 - 0.374 M_{wg} + 0.00148 M_{wg}^2 + 0.1028 T_g] \quad (18)$$

$M_{wg}$  is the average molecular mass of the gas phase, calculated as a function of the composition ( $y_i$ ) and the average molecular mass of each lump ( $M_i$ )

$$M_{wg} = \frac{1}{\sum \frac{y_j}{M_j}} \quad (19)$$

The vapor heat balance is given as:

$$\rho_g C_{p,g} \frac{\partial(\varepsilon_g T_g)}{\partial t} = -\rho_g C_{p,g} \varepsilon_g \frac{\partial(V_g T_g)}{\partial t} + h_c A_{gs} (T_s - T_g) \quad (20)$$

where  $\rho_g$  is the average density of the fluid phase and  $C_{p,g}$  which, is consider constant for this work.

Table 3: Parameter used in the model.

Reaction	Pre exponential factor (m <sup>6</sup> /kgcat.kmol.s)	Activation energy(kJ/kmol) (Gupta and Subba Rao, 2003)
VGO to gasoline	946	68316
VGO to gas	11878	89303
VGO to coke	72	64638
Gasoline to gas	0.42043	52768
Gasoline to coke	0	115566

Table 4: Heat of reaction data (Source: Dave and Saraf, 2003)

Reaction	H <sub>r</sub> (KJ/Kmol)
VGO to gasoline	45000
VGO to gas	159315
VGO to coke	159315
Gasoline to gas	42420
Gasoline to coke	42420

### 3. RESULTS AND DISCUSSION

On simulation of the riser reactor using some useful parameters which include: industrial riser operating conditions by Ali *et al.* (1997), plant data used for riser simulation by Ali *et al.* (1997), modified kinetic parameters by Gupta and Subba Rao (2003), thermodynamic properties of the feed by Ali *et al.* (1997) and Gupta and Subba Rao (2003); the results were obtained as presented in Figures 2 to 4.

After vaporization, the liquid feed expands rigorously into the vapor phase and rapidly travels through the riser. Its density dramatically reduces in the process to that of vapor VGO. With VGO being cracked into gasoline and gas oil and coke, the average density of the vapor phase also decreases since the average molecular weight decreases. It should be noted that the rate of change of the density at the lower part of the riser is larger, pointing to the fact that cracking reaction at that part of the riser is more violent than other parts the riser (see Figure 2). The decrease in the gas phase density along the riser height gives rise to increase in the velocity of the phase.

The temperature profile along the length of the riser is presented graphically in Figure 3. The initial sharp rise in the temperature of the feed is due to sensible and latent heat of vaporization gained by the feed from the hot regenerated catalyst which rapidly increases its temperature to its boiling point. This corresponds to the fall in the temperature of the regenerated catalyst which provides heat to the liquid feed. Afterward, isothermal conditions prevails within the riser with both phases exiting the riser at a common temperature of about 488.6 °C which is comparable to the value reported by Ali *et al.* (1997).

At the point when the liquid feed comes in contact with the hot regenerated catalyst, VGO is the only component of the vapor phase. In the first 8 m of the riser length, VGO cracks very rigorously into gasoline, light gas and coke (this is evident from the slope of the curve representing VGO in Figure 4). During this period, the percentage composition of gasoline and light gas in the vapor phase increases; the rate at which that of gasoline increases, however, is more than that of light gas because the rate at which VGO cracks into gasoline is more than that at which it cracks into light gas. The concentration of gasoline however starts to fall towards the end of the riser while that of light gas tends to be on the rise. This likely due to the fact that the cracking of gasoline to



light gas and coke is more noticeable here and tends to overwhelm its production from VGO cracking.

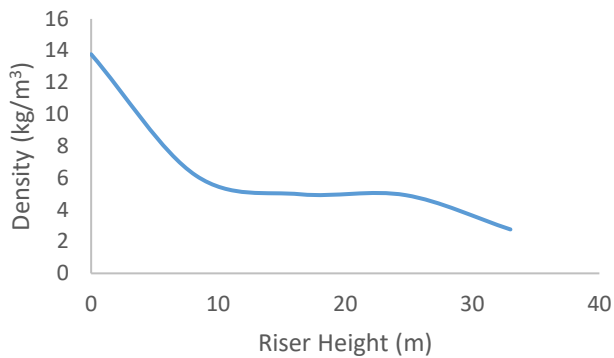


Figure 2. Vapor phase density.

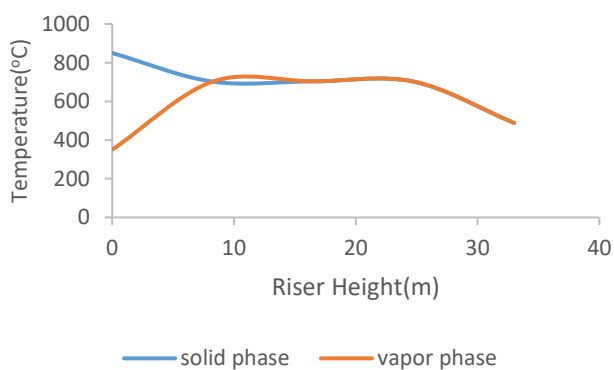


Figure 3. Phase temperature (solid and vapor).

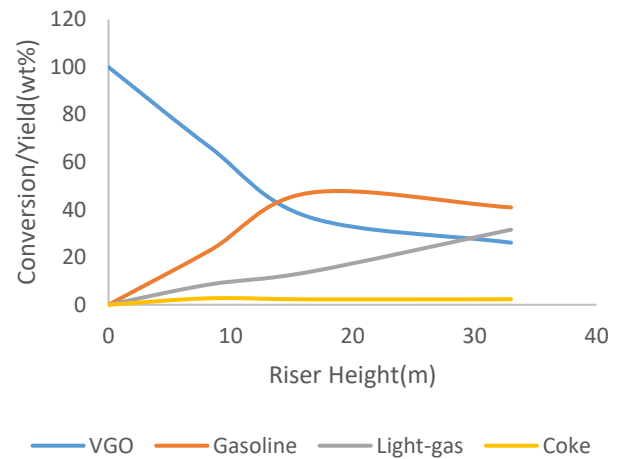


Figure 4. Mass fraction profiles in the riser.

Finally, a general model evaluation was performed based on available plant data reported in literature using some plant variables and parameters with results shown in Table 5. Model performance is determined by calculating the percentage deviation of model predictions from actual plant data using the following equation (Babatope *et al.*, 2013):

$$\% \text{ Dev.} = \left[ \frac{\text{Plant Data} - \text{Model Prediction}}{\text{Plant Data}} \right] \times 100\%$$

The simulation results are as presented above. Table 5 shows the comparison of plant and model data with the results predicted by this model. From these results, we can observe the good agreement between the existing models, the true plant data and the predicted model in this work.

Table 5. Model Evaluation

Comparison	Models	Gasoline Yield (wt%)	Light Gas Yield (wt%)	Coke Yield (wt%)	VGO Yield (wt%)	Temp (K)
Comparison 1	Plant (Ali <i>et al.</i> , 1997)	44	20	6	28	795
	This Model	41	26	2.34	31.6	762
	%Deviation	6.82	-30	61	12.86	4.15
Comparison 2	Model (Gupta <i>et al.</i> , 1997)	43	20	4	30	775
	This Model	41	26	2.34	31.6	762
	%Deviation	4.65	-30	41.5	5.3	1.68
Comparison 3	Model (Lan <i>et al.</i> , 2009)	40	21	4	33	773
	This Model	41	26	2.34	31.6	762
	%Deviation	-2.5	-23.81	41.5	4.24	1.42
Comparison 4	Model (Ahsan <i>et al.</i> , 1997)	41	26	5	26	755
	This Model	41	26	2.34	31.6	762
	%Deviation	0	0	53.2	-21.53	-0.93

Mean values in the same roll followed by different superscripts are significantly different at  $p \leq 0.05$

#### 4. CONCLUSION

In this paper, a dynamic model for the FCCU riser which can be used to simulate the transient behavior of the system is proposed. The model considered the effect of coke deposition on the catalyst on the hydrodynamics of the system. It was found out, according to this study that coke deposition on catalyst affects the dynamics of the FCCU riser and the yield of components is higher near the bottom of the riser due to low coke deposition. The proposed model accurately described the dynamic behavior of FCCU riser and its predictions when compared with real plant data proved satisfactory.

#### NOMENCLATURE

$\epsilon_s$	Fraction occupied by the solid phase.
$\epsilon_g$	Fraction occupied by the vapor phase.
$V_s$	Velocity of the solid phase (m/s)
$V_g$	Velocity of the vapor phase (m/s)
$C_j$	Concentration of lump "j" (kmol/m <sup>3</sup> )
$T_s$	Temperature of the solid phase (°C)
$T_g$	Temperature of the gas phase (°C)



$\Delta z$	Height Increment (m)
$A_r$	Cross sectional area of riser (m <sup>2</sup> )
$D_{riser}$	Diameter of riser (m)
$a_1 - a_5$	Stoichiometry Coefficient of each reaction occurring in the riser
$K_1 - K_5$	Kinetic rate constant of each reaction in the riser (m <sup>6</sup> /kgcat.kmol.s)
$K_{jo}$	Pre-exponential factor for each reaction the riser (m <sup>6</sup> /kgcat.kmol.s)
$E_1 - E_5$	Activation energy for each reaction in the riser (kJ/kmol)
$\phi$	Catalyst activity in riser
$\delta_c$	Deactivation coefficient of catalyst in the riser (m <sup>6</sup> /kgcat.kmol.s)
$\rho_c$	Density of catalyst (kg/m <sup>3</sup> )
$C_s$	Specific heat capacity of catalyst (kJ/kg°C)
$r_{cat}$	Radius of catalyst particle (m)
$C_{vap}$	Specific heat capacity of vapor phase (kJ/kg°C)
$\mu_g$	Viscosity of the vapor phase (kg/ms)
$P$	Pressure in the riser (N/m <sup>2</sup> )
$\rho_g$	Density of vapor phase (kg/m <sup>3</sup> )
$F_D$	Drag force between both phases per unit riser volume in the riser (N/m <sup>3</sup> )
$C_D$	Drag force coefficient between both phases in the riser
$A_p$	Projected area per unit volume (m <sup>2</sup> /m <sup>3</sup> )
$\tau_j$	The shear stress of phase j the in riser (N/m <sup>2</sup> )
Re	Reynolds number
g	Acceleration due to gravity (m/s <sup>2</sup> )
$h_s$	Convective heat transfer coefficient between the catalyst and the vapor phase in the riser
$\kappa_g$	Thermal conductivity of gas phase in the riser
$\Delta H_1 - \Delta H_5$	Enthalpy of each reaction in the riser
$\delta_{co}$	Pre-exponential factor for the deactivation of catalyst (m <sup>6</sup> /kgcat.kmol.s).

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