

DYNAMIC SIMULATION OF INDUSTRIAL FCC UNIT

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***Abstract.** In this work a mathematical model for the dynamic simulation of the Fluidized-bed Catalytic Cracking (FCC) Reactor, to be used in the analysis, control, and optimization of this system is developed. Based on the full range of published data in FCC performance and kinetic rates, and adapted to the industrial unit of the PETROBRAS' Alberto Pasqualini Refinery (REFAP), an integrated dynamic model is built up. The model is sufficiently complex to capture the major dynamics effects that occur in this system. The regenerator is modeled as emulsion and bubble phases that exchange mass and heat. The riser is modeled as an adiabatic plug flow reactor. The fluid dynamic is taking into account for the catalyst circulation, and the dynamics of the gas phase and the riser are also considered into the model. The model, represented by a non-linear system of differential-algebraic equations, was written in language C and implemented in MATLAB / SIMULINK. The results are compared with the data obtained from the industrial plant of REFAP.*

***Keywords:** Fluidized-bed catalytic cracking, Dynamic model, Ten lumps kinetic model*

1. INTRODUCTION

The catalytic cracking is a refine process that seeks to increase the gasoline and LPG production, through the heavy vacuum gas oil and residue conversion in lighter fractions. Because of its impact on overall refinery economics, the FCC is the best unit to apply advanced control and optimization strategies, and the base for these is always a good mathematical model. The model has to be able to reproduce reasonably well the main dynamics and stationary gains of the system, without compromising the computational load.

There are many static mathematical models for the FCC in the literature, some of them use a very simplified cracking process description, and few of them present integration between regenerator and riser. Among the cracking kinetic models, it is pointed out the 3 lumps (pseudo-components) model of Weekman (1968), a 10 lumps by Jacob et al. (1976),

and more recently Pitault et al. (1994) developed a model with 19 lumps, approximating the reactants and products according to the crude oil cuts composition. Among the integrated models, McFarlane et al. (1993) published a well-detailed model based on the obsolete Exxon Model IV with a realistic description of the regenerator fluid-dynamic behavior, but the combustion reactions were not considered. It also lacks detailed description from cracking kinetics, making the riser useless for dynamic or stationary control. More recently Arbel et al. (1995) developed a model that makes detailed description of the combustion and cracking kinetics, using the 10 lumps model of Jacobs et al. (1976) to represent the mixture in the riser. Neumann et al. (1999) presented a dynamic simulator with many important FCC steps, but the regenerator performance, using an ideal mixture reactor, was not satisfactory to describe the heat transfer between gas and solid. The important limitation in most of these models is the fact that they ignore the complex two-phase nature of the fluidized bed in the regenerator.

The objective of this work is to develop FCC mathematical model, override the above limitations, to be used for dynamic analysis, control, and optimization of this system. It also shows a comparison between regenerator dense phase modeling like CSTR and emulsion-bubble bed.

2. THE FCC PROCESS

The heavy molecules cracking process occurs in a riser tubular reactor, at high temperatures, building up fuel gas, LPG, cracked naphtha (gasoline), light cycle oil, decanted oil, and coke. The coke deposits on the spent catalyst surface causing its deactivation. The catalytic activity is reestablished by the coke combustion in a fluidized bed reactor, denominated regenerator.

Figure 1 shows a schematic representation of typical catalytic section for heavy vacuum gas oil. Steam lift the heated regenerated catalyst to be combined with the oil in the riser such that the oil-catalyst mixture rises in ascending dispersed stream to the separator. TCV control valve manipulates the quantity of hot regenerated catalyst from the standpipe (a) to the riser in order to maintain a predetermined outlet riser temperature. On the top of the separator, the cyclones (b) separate catalyst particles from the vapor products. The stream (c) transfers the reaction products overhead to the products recovery section. The standpipe (d) transfers spent catalyst continuously from the separator to the regenerator by the LCV control valve. In the regenerator, the spent catalyst particles are burned in the presence of air. The air flow rate to regenerator is controlled by a control valve that vents portion of the air to the atmosphere. On the top of the regenerator, cyclones (e) make the catalyst separation from the flue gas stream. The PdCV control valve regulates the flue gas flow in order to vary the internal regenerator pressure maintaining the desired pressure difference between separator and regenerator. The flue gas goes to carbon monoxide boiler (not shown) where the carbon monoxide is converted to carbon dioxide. There is a recycle stream around the wet gas compressor (not shown) to control the suction pressure, which maintain the converter pressure at its desired value.

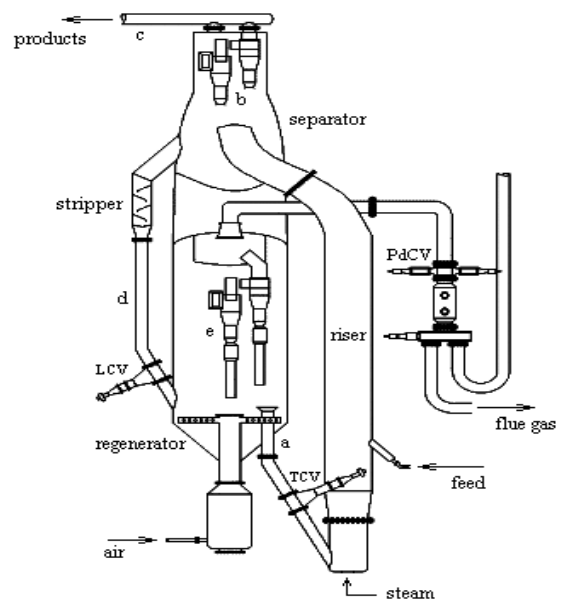


Figure 1 - FCC UOP Stacked.

The measured variables are riser temperature, regenerator temperatures (all phases), wet gas compressor suction pressure, separator-stripper catalyst level, separator-regenerator differential pressure and regenerator flue gas temperature. The manipulated variables are feed flow rate, preheated feed temperature, catalyst circulation rates (in TCV and LCV), combustion air flow rate and wet gas compressor recycle rate. The measured disturbances are feed characteristics, feed temperature, and air temperature.

3. MODELING OF FLUID CATALYTIC CRACKING

The mathematical model describes the UOP Stacked Fluidized-bed Catalytic Cracking (FCC) System adopted by the PETROBRAS' Alberto Pasqualini Refinery (REFAP) in its industrial unit. The model is sufficiently complex to capture the major dynamics effects that occur in this system. The regenerator is modeled as emulsion and bubble phases that exchange mass and heat. The riser is modeled as adiabatic plug flow reactor. The fluid dynamic is taking into account for the catalyst circulation, and the dynamics of the gas phase and the riser are also considered into the model.

3.1 The Riser

The Riser is modeled as adiabatic plug flow reactor, with the kinetics described by the ten lumps model of Jacob et al. (1976), using catalyst deactivation and coke formation tendency functions. The feed is characterized by the methodology developed by Lansarin (1999), using available data at REFAP (oil density and viscosity, ASTM or TBP curves, and sulfur content), which determines the lumps concentration and their thermodynamic properties required by the kinetic model. The fresh feed is considered to be completely and instantaneously vaporized by the hot regenerated catalyst at the bottom of the riser. Then, the bottom temperature is obtained by a stationary energy balance around a mixer of the regenerated catalyst, lift steam, and feed streams. The catalyst/oil mixture is transported in a dilute phase upward across the riser. A mass balance for each lump and for the coke results in:

$$\frac{\partial w_n}{\partial t} = -\frac{F_{ff}}{\epsilon_{ris} A_{ris} \rho_{ov}} \frac{\partial w_n}{\partial z} + R_n \quad (1)$$

where w_n is the weight fraction of lump n or coke [(kg of n)/(kg of oil)], F_{ff} is the total feed flow rate to the riser [kg/s], ϵ_{ris} is the riser bed void fraction, A_{ris} is the riser cross-sectional area [m²], ρ_{ov} is the oil vapor density [kg/m³], and R_n is the formation rate of lump n [s⁻¹].

The lump rate formation, using the kinetic model showed in the Fig. 2, is given by:

$$R_n = A_{cat} \phi \frac{(1-\epsilon_{ris})}{\epsilon_{ris}} \frac{1}{1+k_h w_{CAh}} \rho_c \sum_{i=1}^9 K_{ni} w_i \quad (2)$$

where A_{cat} is the relative catalyst activity, ϕ is the deactivation function, k_h is the adsorption rate constant of heavy aromatics lump (CAh), ρ_c is the catalyst density [kg/m³], and K_{ni} is the temperature- dependent coefficient matrix of the reaction rates [m³/((kg of catalyst).s)] (Arbel et al., 1995).

The coking rate ($n = ck$) is given by the overall rate equation, based on the Voorhies

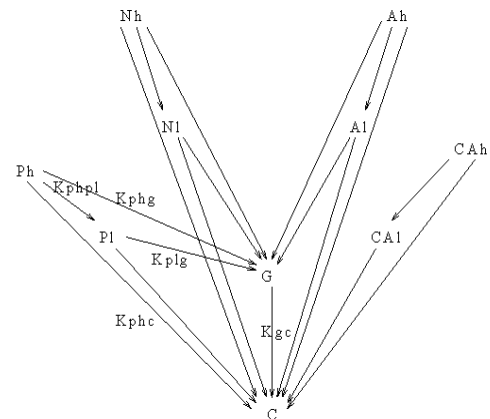


Figure 2 - Ten lumps kinetic model.

relation (Krambeck, 1991):

$$R_{ck} = A_{cat} z_{cat} \phi b \left(\frac{\phi}{100} \right)^{1/b} \frac{F_{rc}}{F_{tf}} K_{ck} \quad (3)$$

where z_{cat} is the relative catalyst coking rate, b is a parameter, ϕ is the feed coking tendency function (Gross et al., 1976), F_{rc} is the regenerated catalyst flowrate [kg/s], and K_{ck} is the coking rate constant [kg of coke/((kg of catalyst).s)]. The deactivation function is given by (Krambeck, 1991):

$$\phi = \left((w_{ck} + f_{ck} RCR) \frac{F_{tf}}{F_{rc}} + C_e \right)^{(1-1/b)} \quad (4)$$

where w_{ck} is the weight fraction of coke, RCR is the Ramsbottom carbon residue (the coke content in the feed), f_{ck} is the RCR factor, representing the RCR fraction deposited on the catalyst, and C_e is the coke on regenerated catalyst [(kg of coke)/(kg of catalyst)].

The energy balance results in:

$$\frac{\partial T_{rx}}{\partial t} = - \frac{F_{tf}}{\epsilon_{ris} A_{ris} \rho_{ov}} \frac{\partial T_{rx}}{\partial z} - \frac{F_{tf}}{(F_{rc} + F_{tf}) C_{p_m}} \sum_{n=1}^{10} R_n \Delta H_n \quad (5)$$

where T_{rx} is the riser temperature [K], C_{p_m} is the average heat capacity of catalyst/oil mixture [kJ/K] (Watson-Fallon, 1944), and ΔH_n is the heat of reaction of the n -th lump [kJ/kg] (Lansarin, 1997).

The riser bed void fraction is obtained by:

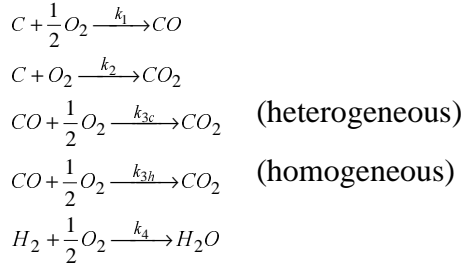
$$\epsilon_{ris} = \frac{F_{tf} / \rho_{ov}}{\left(\frac{F_{tf}}{\rho_{ov}} + \frac{F_{rc}}{\rho_c} \right)} \quad (6)$$

The separator and stripper are assumed to be continuous stirred tanks, where catalyst and vapor products are separated. The wet gas compressor is modeled as a single stage centrifugal compressor, driven by a constant speed. It is assumed that the compressor is pumping against a constant pressure in the gas recover unit. The compression performance equation relates suction flow to polytropic head (McFarlane et al., 1993). There is a recycle stream around the compressor to control the suction pressure. See Neumann et al. (1999) for details.

3.2 The Regenerator

The fluidized bed regenerator is modeled as emulsion and bubble phases that exchange mass and heat. The bubble phase is assumed to be at the pseudo steady-state condition. The disengagement section is modeled as two serial continuous well-mixed tank reactors, corresponding to the diluted and flue gas phases, according to the Fig. 3.

The kinetic model was built with the following assumptions: the coke and carbon monoxide combustion reactions occur at emulsion, diluted and gas phases; the hydrogen combustion is instantaneous; there is no reaction in the bubble phase; the coke has a constant carbon-hydrogen ratio; the CO combustion reaction takes place in two parallel paths, heterogeneous and homogeneous. The following five reactions are considered to take place in the regenerator:



The catalyst circulation rate (F_{cc} , [kg/s]) among the regenerator phases, estimated by an empirical correlation taken from Zenz and Wei (1958), tends to minimise their temperature differences.

The approximate solutions to the pseudo steady-state mass and energy balances in the bubble phase, considering mean properties along the bed height, are given by:

$$C_{i,b}(z) = C_{i,e} + (C_{i,0} - C_{i,e}) \exp\left(-\frac{K_{be}}{u_b} z\right) \quad \text{and} \quad T_b(z) = \frac{T_e T_{ar}}{T_{ar} + (T_e - T_{ar}) \exp\left(-\frac{H_{be}}{\rho_e u_b c_{pe}} z\right)} \quad (7)$$

where z is the height coordinate, the subscripts $i = O_2, CO, CO_2, H_2O$, b : bubble phase, e : emulsion phase, and 0 : income conditions, $C_{CO,0} = C_{CO_2,0} = C_{H_2O,0} = 0$ [(kmol of i)/(m³ of gas)], K_{be} is the mass transfer coefficient [s⁻¹], H_{be} is the heat transfer coefficient [kJ/(m³.K.s)], T_{ar} is the air temperature to the regenerator [K], c_{pe} is the emulsion specific heat [kJ/(kg.K)], and u_b is the gas velocity in the bubble phase [m/s].

The other phases mass balances are:

$$\frac{dC_{i,e}}{dt} = \frac{u_e}{h_e} (C_{i,0} - C_{i,e}) + \frac{K_{be} \delta}{\epsilon_{mf} (1-\delta)} (\bar{C}_{i,b} - C_{i,e}) - \frac{R_{i,e}}{\epsilon_{mf}} \quad (\text{emulsion phase}) \quad (8)$$

$$\frac{dC_{i,d}}{dt} = \frac{u_e (1-\delta) \epsilon_{mf} C_{i,e} + u_b \delta C_{i,b}(h_e)}{\epsilon_d h_d} - \frac{u_d C_{i,d}}{h_d} - \frac{R_{i,d}}{\epsilon_d} \quad (\text{diluted phase}) \quad (9)$$

$$\frac{dC_{i,g}}{dt} = \frac{u_d C_{i,d} - u_g C_{i,g}}{h_g} - \frac{R_{i,g}}{\epsilon_d} \quad (\text{flue gas phase}) \quad (10)$$

where the subscripts e , d , and g means emulsion, diluted, and gas phases, respectively, u is the gas velocity in phase i [m/s], h is the height of phase i [m], δ is the bubbles fraction in the fluidized bed, ϵ is the minimum fluidizing voidage, ϵ_d is the void fraction in the diluted and gas phases, $\bar{C}_{i,b}$ is the average molar concentration of component i in the bubble phase [(kmol of i)/(m³ of gas)], R_j is the formation rate of component i in the phase j [kmol/s].

The regenerator pressure, P_{rg} [bar], is evaluated by an overall mass balance for the disengagement, assuming the gas behaves as an ideal gas:

$$\frac{dP_{rg}}{dt} = \frac{(F_g - F_{out})}{(V_d + V_g)} R T_g + \frac{P_{rg}}{T_g} \frac{dT_g}{dt} \quad (11)$$

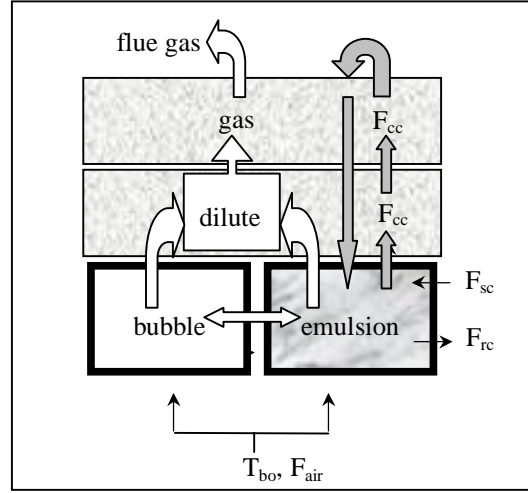


Figure 3 - Regenerator phases.

where F_g is the flue gas flow rate [kmol/s], F_u is the total flue gas flow rate leaving the regenerator to the CO boiler [kmol/s], V is the volume of phase i [m³], and R is the universal constant [bar.m³/(kmol.K)].

An overall mass balance for the catalyst in the regenerator gives:

$$\frac{dM_{rg}}{dt} = F_{sc} - F_{rc} \quad (12)$$

where M_{rg} is the catalyst hold-up in regenerator emulsion phase [kg] and F is the spent catalyst flow rate [kg/s]. Considering that all the entrained catalyst returns to the emulsion phase and there is a catalyst carryover from each phase, the coke mass balance for each phase becomes:

$$M_{rg} \frac{dC_e}{dt} = F_{sc} (C_{sc} - C_e) + F_{cc} (C_g - C_e) - R_{cb,e} \quad (\text{emulsion phase}) \quad (13)$$

$$\frac{dC_d}{dt} = \frac{F_{cc} (C_e - C_d) - R_{cb,d}}{\rho_c V_d (1 - \varepsilon_d)} \quad (\text{diluted phase}) \quad (14)$$

$$\frac{dC_g}{dt} = \frac{F_{cc} (C_d - C_g) - R_{cb,g}}{\rho_c V_g (1 - \varepsilon_d)} \quad (\text{flue gas phase}) \quad (15)$$

where C_i , C_e are the coke on catalyst of phase i and on spent catalyst [(kg of coke)/(kg of catalyst)], respectively, and $R_{cb,i}$ is the coke rate burned in phase i [kg/s]. All the reaction rates are described in Neumann et al. (1999).

The energy balance for the emulsion, diluted, and gas phases can be written as follow.

$$Cp_{me} \frac{dT_e}{dt} = \frac{\varepsilon_{mf} u_e \rho_{ar}}{h_e} \Delta h_{ar} + \frac{F_{sc} cp_c (T_{sc} - T_e)}{V_e (1 - \delta)} + \frac{F_{cc} cp_c (T_g - T_e)}{V_e (1 - \delta)} + \frac{\delta}{(1 - \delta)} K_{be} (\bar{C}_{O_2,b} - C_{O_2,e}) \Delta h_{O_2} + \frac{\delta}{(1 - \delta)} H_{be} (\bar{T}_b - T_e) + \sum (-\Delta H_i) r_{i,e} - \frac{4h_w (T_e - T_w)}{D_{rg} (1 - \delta)} \quad (16)$$

$$Cp_{md} \frac{dT_d}{dt} = \frac{(1 - \delta) \varepsilon_{mf} u_e \rho_e}{h_d} \Delta h_e + \frac{\delta u_b \rho_{bf}}{h_d} \Delta h_b + \frac{F_{cc} cp_c (T_e - T_d)}{V_d} + \sum (-\Delta H_i) r_{i,d} - \frac{4h_w (T_d - T_w)}{D_{rg}} \quad (17)$$

$$Cp_{mg} \frac{dT_g}{dt} = \frac{u_d \rho_d}{h_g} \Delta h_d + \frac{F_{cc} cp_c (T_d - T_g)}{V_g} + \sum (-\Delta H_i) r_{i,g} - \frac{4h_w (T_g - T_w)}{D_{rg}} \quad (18)$$

where $\Delta h_{ar} = \int_{T_{ar}}^{T_e} cp_g dT$, $\Delta h_{O_2} = \int_{\bar{T}_b}^{T_e} cp_g dT$ and $Cp_{me} = \rho_e \varepsilon_{mf} cp_e + \rho_c (1 - \varepsilon_{mf}) cp_c$ and the others specific heat capacities [kJ/(m³.K)] and enthalpies [kJ/kg] are obtained in the same way (Santos, 2000), ρ , ρ_{ar} , ρ_b are the gas density in phase i , air stream, and exit of bubble phase [kg/m³], respectively, cp is the catalyst specific heat [kJ/(kg.K)], T_i , T_s , T_w are the phase i , stripper, and wall temperatures [K], \bar{T}_b is the average bubble temperature [K], ΔH is heat of combustion of i -th reaction [kJ/kg], h_w is the overall heat transfer coefficient [kJ/(m².K.s)], r_j is the combustion rate of i -th reaction in phase j [kmol/(m³.s)], and D_{rg} is the regenerator diameter [m].

The minimum fluidizing voidage, ε , is given by Broadhurst and Becker (1975), and the void fraction in the regenerator diluted and flue gas phases are considered to be the same, ε_d , and estimated by

$$\varepsilon_{mf} = 0.586\phi_p^{-0.72} \left(\frac{\mu^2}{\rho_e g (\rho_c - \rho_e) d_p^3} \right)^{0.029} \left(\frac{\rho_e}{\rho_c} \right)^{0.021} \quad \text{and} \quad \varepsilon_d = \frac{F_{ar} + F_{sc} C_{sc}}{F_{cc} \frac{\rho_g}{\rho_c} + F_{ar} + F_{sc} C_{sc}} \quad (19)$$

and the minimum fluidizing Reynolds number, Re , is evaluated by the following equation (Kunii and Levenspiel, 1969):

$$\frac{1.75 Re_m^2}{\varepsilon_{mf}^3} + \frac{150(1-\varepsilon_{mf}) Re_m}{\varepsilon_{mf}^3} - \frac{\rho_g g (\rho_c - \rho_g) d_p^3}{\mu^2} = 0 \quad (20)$$

where ϕ_p is the particle sphericity, μ is the gas viscosity [kg/(m.s)], g is the gravity acceleration [m/s^2], d_p is the particle diameter [m], and F_{ar} is the air flow rate [kg/s].

The bubble and emulsion velocities below, and the mass and heat transfer coefficients in bubbling beds are taken from Kunii and Levenspiel (1969).

$$u_b = u_0 - u_{mf} + 0.711\sqrt{g \cdot d_B} \quad \text{and} \quad u_e = \frac{u_{mf}}{\varepsilon_{mf}(1-\delta)} \quad (21)$$

where $u_{mf} = \frac{Re_m \mu}{\rho_g d_p}$ is the minimal fluidizing velocity [m/s], $\delta = \frac{u_0 - u_{mf}}{u_b}$, u_0 is the superficial bed velocity at inlet condition [m/s], and d_B is the bubble diameter [m] given by Errazu et al. (1979), for a nozzle with N holes over the distributor:

$$d_B = 0.667 \left(\frac{F_{ar}}{\rho_{ar} N} \right)^{0.375} \quad (22)$$

4. RESULTS AND DISCUSSION

Since the FCC units began processing heavier feeds, the regeneration conditions are changing. Emulsion phase temperature turned to be higher than diluted and gas phases temperatures. It happens because there are more coke to burn, and there is not enough air to burn the CO to CO₂. This kind of operation is called behind burn. To represent this kind of operation, Neumann et al. (1999) modeled the regenerator dense phase as a continuous stirred tank reactor (CSTR). This model did not represent well the coke partial burning. The regenerator temperatures were unsatisfactory, as shown in Figs. 4 and 5. This could be due to the fact the oxygen, in the real plant, is not homogeneously available at each phase mainly in dense phase. Then the authors introduced a heat transfer efficiency factor between the solid and gas phase (METT), which improved the regenerator temperatures, but the system turned to be unstable for large changes in manipulated variables. The bubble-emulsion model (b-e) has good agreement with the plant data for partial burning and temperatures, presenting similar dynamics to the real plant.

The Riser model also has a good agreement with the plant data (gasoline, conversion and coke yields, and temperature profiles) as shown in Fig. 6. It was only necessary to adjust (increase) the catalyst activity, A_a , and the relative catalyst coke rate, z_a . This increasing is reasonable, because the new zeolite catalysts are much more active than the catalyst used by

Jacob et al. (1976) to estimate the rate constants. The Riser model was discretized by finite differences with the mesh points distributed according to the following generating function:

$$z_i = \exp(\log(h_{ris}) i/M) \quad (23)$$

where h_r is the riser height [m], M is the mesh size, and $i = 1, 2, \dots, M$. A mesh size of 20 points showed to be satisfactory. The resulting model, represented by a non-linear system of differential-algebraic equations, was written in language C and implemented in MATLAB / SIMULINK.

The effect on the products for increasing 2.5% the feed is shown in Fig. 6. The tendency is to decrease the severity and, consequently, the conversion also decreases. The converter dynamic model, using bubble-emulsion and ten lumps approaches, was able to reproduce the plant main characteristics as shown in Fig. 6.

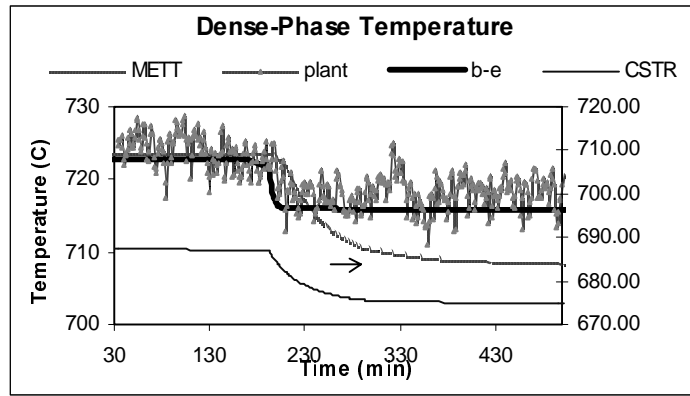


Figure 4. Dense-phase regenerator temperatures.

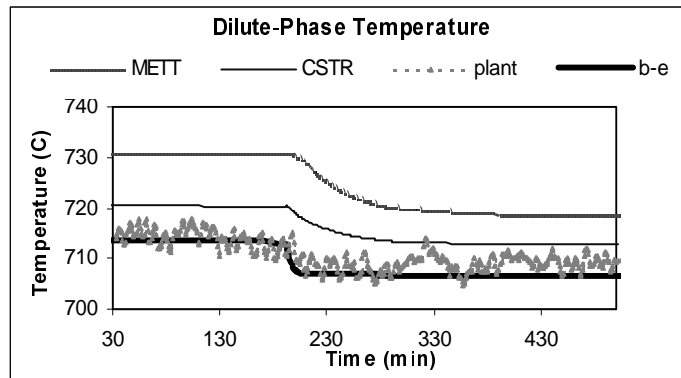


Figure 5. Dilute-phase regenerator temperatures.

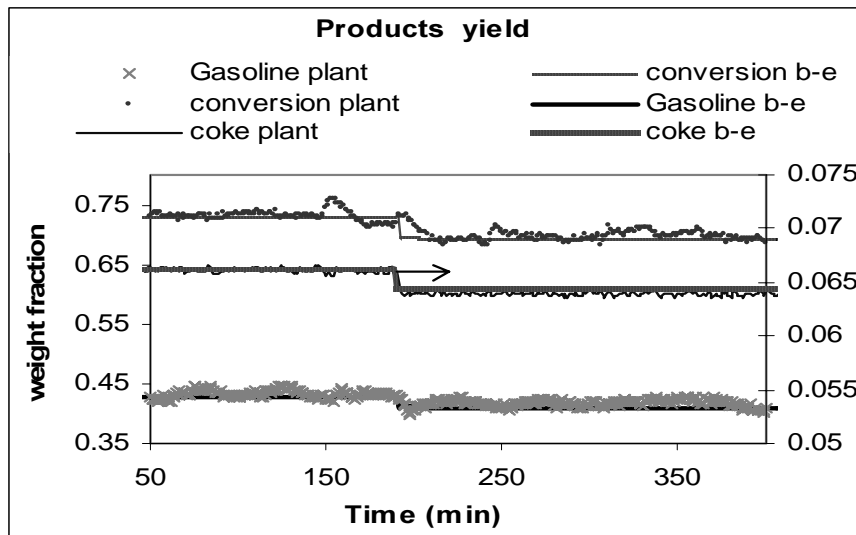


Figure 6. Riser products yield

Figure 7 shows the riser temperature, gasoline, and coke profiles given by the model at the new steady-state condition after the feed step change. It is possible to observe that along the first 30% of the reactor length prevail the catalytic cracking reaction, which are highly endothermic, making the riser temperature drop quickly, and presenting a high conversion rate of coke and gasoline. In the rest of the reactor length, the overcracking reactions are

relevant. These reactions are less endothermic, reducing the temperature drop and conversion rate.

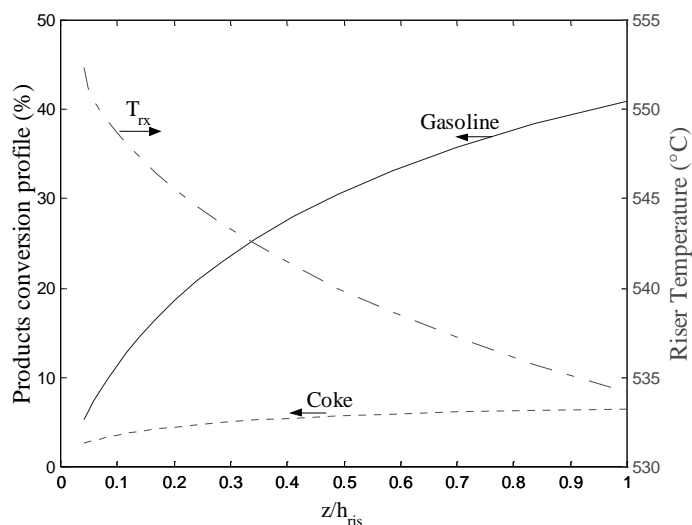


Figure 7 - Riser temperature and conversion profiles.

5. CONCLUSION

A theoretical dynamic regenerator-riser model for FCC was presented in this work. The most important fact is the model was validated with data obtained in commercial fluidized-bed catalytic cracking unit. The model predicts operating variables and describes satisfactorily all major dynamics effects that occur in the system. The regenerator was modeled as bubble and emulsion phases that better describes partial CO combustion and behind burn conditions operations.

The literature assumption of homogeneous temperature between solids and gas phases in the dense phase are very stringent. In order to represent after burn, traditional operation, and behind burn conditions, the very high gas velocity and its inefficient heat transfer with the catalyst particles have to be considered. The bubble-emulsion model described in this work is a reasonable alternative to take the non-homogeneity into account, without compromising the computational load. A more complex and expensive model would treat the whole regenerator as a distributed model, not suitable for control purposes.

The ten lumps model allows to adjust the control production based on the market demand. It has good results to conversion, gasoline and coke yields. New control strategy will be developed to maximize the desired products from the FCC, in future work. The system is multivariable, strongly interacting, nonlinear, and highly constrained. However, the computational overhead is not prohibitive to use as a reference model in control analysis, optimization, and design.

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