FCC DYNAMIC MODELING: FIRST PRINCIPLES OR SYSTEM IDENTIFICATION?

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Resumo—Um modelo dinâmico integrado para o reator UOP de craqueamento catalítico em leito fluidizado (FCC) da refinaria Alberto Pasqualini (REFAP) da PETROBRAS é apresentado. O modelo é suficientemente complexo para capturar os principais efeitos dinâmicos que ocorrem no sistema. O modelo, representado por um sistema não linear de equações algébrico-diferenciais, foi escrito em linguagem C e implementado no MATLAB / SIMULINK, dentro de uma estrutura para o desenvolvimento de estratégias de controle. Os resultados são comparados com dados obtidos da planta industrial da REFAP e com um modelo identificado a partir de várias perturbações do tipo degrau realizadas na planta real.

Abstract—An integrated dynamic model for the UOP Stacked Fluidized-bed Catalytic Cracking (FCC) of the PETROBRAS' Alberto Pasqualini Refinery (REFAP) is presented. The model is sufficiently complex to capture the major dynamic effects that occur in this system. The model, represented by a non-linear system of differential-algebraic equations, was written in language C and implemented in MATLAB / SIMULINK within a framework to develop control strategies. The results are compared with the data obtained in the REFAP's industrial plant and with an identified model based on several step disturbances in the real plant.

Keywords—Fluidized-bed catalytic cracking, dynamic model, ten lumps kinetic model, system identification.

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 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. Most of these works is based on model with a high degree of empiricism, and makes use of pseudo-components corresponding to different groups of species, usually called lumps. Among the cracking kinetic models, it is pointed out the 3 lumps 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, was not satisfactory to describe the heat transfer between gas and solid. As already pointed out by Elnashaie and Elshishini (1993), an important limitation in most of these models is the fact that they ignore the complex two-phase nature of the fluidized beds in the regenerator. In Secchi et al. (2001) the regenerator was modeled as an emulsion-bubble bed, and the whole phenomenological model presented satisfactory results when compared with plant data.

The objective of this work is to present the framework developed to use the FCC model of Secchi et al. (2001) to design control strategies for the FCC unit. A comparison between this model and an identified model, based on plant data, is also presented.

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. The system riser-regenerator is called converter. Figure 1 shows a schematic representation of a 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 catalyst particles are separated from the vapor products by cyclones (b). 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 a 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 maintains the converter pressure at its desired value.

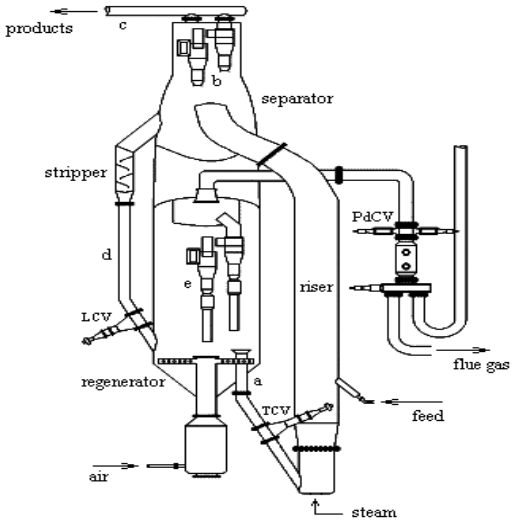

Fig. 1. FCC converter.

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 First Principles Modeling

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 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 takes the catalyst circulation into account. The dynamics of the gas phase and the riser are also considered by the model. The nomenclature used in the model is the same used in Secchi et al. (2001), and was omitted due to lack of space.

3.1 The Riser

The Riser is modeled as an adiabatic plug flow reactor, with the kinetics described by the ten lumps model of Jacob et al. (1976), and 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 with 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:

$$\frac{\partial w_n}{\partial t} = -\frac{F_{tf}}{\varepsilon_{ris} A_{ris} \rho_{ov}} \frac{\partial w_n}{\partial z} + R_n \qquad (1)$$

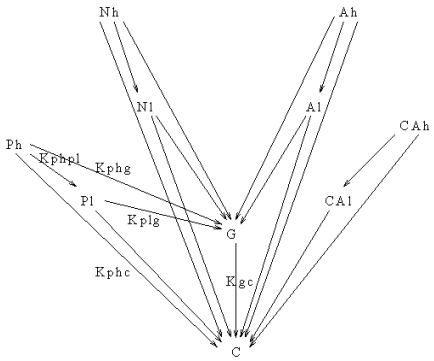

Fig. 2. Ten lumps kinetic model.

The lump rate formation, using the kinetic model showed in Figure 2, is given by (Arbel et al., 1995):

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

The coking rate ($n = ck$) is given by the overall rate equation, based on the Voorhies relation (Krambeck, 1991):

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

where ϕ is the catalyst deactivation function given by Krambeck (1991), which is also function of the Ramsbottom carbon residue (*RCR*, the coke content in the feed), and φ is the feed coking tendency function of Gross et al. (1976).

The energy balance is written as:

$$\frac{\partial T_{rx}}{\partial t} = -\frac{F_{tf}}{\varepsilon_{ris} A_{ris} \rho_{ov}} \frac{\partial T_{rx}}{\partial z} - \frac{F_{tf}}{(F_{rc}+F_{tf}) cp_m} \sum_{n=1}^{10} R_n \Delta H_n \qquad (4)$$

3.2 The Separator

The separator is assumed to be a continuous stirred tank, where catalyst and vapor products are separated. The catalyst and coke mass balance are given by:

$$\frac{dM_{ra}}{dt} = F_{rc} - F_{sc} \quad (5)$$

$$M_{ra}\frac{d\,C_{sc}}{dt} = F_{rc}(C_e - C_{sc}) + F_{tf}\left(f_{ck}RCR + w_{ck}\big|_{z=h_{ris}}\right) \quad (6)$$

The energy balance for the separator is written as:

$$(M_{ra}\,cp_c + M_v cp_v)\frac{dT_{ra}}{dt} = (F_{rc}\,cp_c + F_{oc}\,cp_v)(T_{rx}\big|_{z=h_{ris}} - T_{ra}) \quad (7)$$

3.3 The Wet Gas Compressor

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. A mass balance around the compressor is given by assumed dynamics:

$$\tau_{P_{suc}}\frac{dP_{suc}}{dt} = Y_{wg}F_{tf} - W_{comp} + W_{rec} \quad (8)$$

3.4 The Regenerator

The regenerator, a fluidized bed reactor, 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 Figure 3.

The kinetic model was built with the following assumptions. The coke and CO 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:

$$C + \frac{1}{2}O_2 \xrightarrow{k_1} CO$$

$$C + O_2 \xrightarrow{k_2} CO_2$$

$$CO + \frac{1}{2}O_2 \xrightarrow{k_{3c}} CO_2 \quad \text{(heterogeneous)}$$

$$CO + \frac{1}{2}O_2 \xrightarrow{k_{3h}} CO_2 \quad \text{(homogeneous)}$$

$$H_2 + \frac{1}{2}O_2 \xrightarrow{k_4} H_2O$$

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

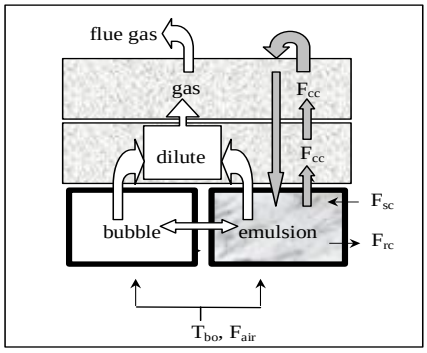

Fig. 3. Regenerator phases.

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

$$C_{i,b}(z) = C_{i,e} + \left(C_{i,0} - C_{i,e}\right).\exp\left(-\frac{K_{be}}{u_b}z\right) \quad (9)$$

$$T_b(z) = \frac{T_e\,T_{ar}}{T_{ar} + (T_e - T_{ar})\exp\left(-\dfrac{H_{be}}{\rho_e\,u_b\,cp_e}z\right)} \quad (10)$$

where z is the height coordinate; i = O_2, CO, CO_2, H_2O; *b:* bubble phase*; e*: emulsion phase*;* 0: income conditions, $C_{CO,0} = C_{CO2,0} = C_{H2O,0} = 0$.

Mass balance for emulsion phase:

$$\frac{dC_{i,e}}{dt} = \frac{u_e}{h_e}\left(C_{i,0} - C_{i,e}\right) + \frac{K_{be}\,\delta}{\varepsilon_{mf}(1-\delta)}\left(\overline{C}_{i,b} - C_{i,e}\right) - \frac{R_{i,e}}{\varepsilon_{mf}} \quad (11)$$

Mass balance for dilute phase:

$$\frac{dC_{i,d}}{dt} = \frac{u_e(1-\delta)\varepsilon_{mf}C_{i,e} + u_b\,\delta\,C_{i,b}(h_e)}{\varepsilon_d h_d} - \frac{u_d\,C_{i,d}}{h_d} - \frac{R_{i,d}}{\varepsilon_d} \quad (12)$$

Mass balance for flue gas phase:

$$\frac{dC_{i,g}}{dt} = \frac{u_d\,C_{i,d} - u_g\,C_{i,g}}{h_g} - \frac{R_{i,g}}{\varepsilon_d} \quad (13)$$

The regenerator pressure is evaluated from an overall mass balance for the disengagement, assuming the gas behaves as an ideal gas:

$$\frac{dP_{rg}}{dt} = \frac{(F_g - F_{out})}{(V_d + V_g)}RT_g + \frac{P_{rg}}{T_g}\frac{dT_g}{dt} \quad (14)$$

Overall mass balance for catalyst:

$$\frac{dM_{rg}}{dt} = F_{sc} - F_{rc} \quad (15)$$

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 (emulsion, diluted, and flue gas phase, respectively):

$$M_{rg}\frac{dC_e}{dt} = F_{sc}(C_{sc} - C_e) + F_{cc}(C_g - C_e) - R_{cb,e} \quad (16)$$

$$\frac{dC_d}{dt} = \frac{F_{cc}(C_e - C_d) - R_{cb,d}}{\rho_c V_d(1-\varepsilon_d)} \quad (17)$$

$$\frac{dC_g}{dt} = \frac{F_{cc}(C_d - C_g) - R_{cb,g}}{\rho_c V_g (1-\varepsilon_d)} \quad (18)$$

All the reaction rates are described in Neumann et al. (1999). The energy balance for each phase can be written as below. Emulsion phase:

$$Cp_{me}\frac{dT_e}{dt} = \frac{\varepsilon_{mf} u_e \rho_{ar}}{h_e}\Delta h_{ar} + \frac{F_{sc}\, cp_c (T_{sc} - T_e)}{V_e(1-\delta)} + \\ + \frac{F_{cc} cp_c (T_g - T_e)}{V_e(1-\delta)} + \frac{\delta}{(1-\delta)} K_{be}(\overline{C}_{O_2,b} - C_{O_2,e})\Delta h_{O_2} + \\ + \frac{\delta}{(1-\delta)} H_{be}(\overline{T}_b - T_e) + \Sigma(-\Delta H_i) r_{i,e} - \frac{4h_w (T_e - T_w)}{D_{rg}(1-\delta)} \quad (19)$$

Dilute and flue gas phases:

$$Cp_{md}\frac{dT_d}{dt} = \frac{(1-\delta)\varepsilon_{mf} u_e \rho_e}{h_d}\Delta h_e + \frac{\delta\, u_b\, \rho_{bf}}{h_d}\Delta h_b + \\ + \frac{F_{cc}\, cp_c (T_e - T_d)}{V_d} + \Sigma(-\Delta H_i) r_{i,d} - \frac{4h_w}{D_{rg}}(T_d - T_w) \quad (20)$$

$$Cp_{mg}\frac{dT_g}{dt} = \frac{u_d\, \rho_d}{h_g}\Delta h_d + \frac{F_{cc}\, cp_c (T_d - T_g)}{V_g} + \\ + \Sigma(-\Delta H_i) r_{i,g} - \frac{4h_w}{D_{rg}}(T_g - T_w) \quad (21)$$

where the specific heat capacities and enthalpies can be found in Santos (2000).

The minimum fluidizing voidage is obtained from Broadhurst and Becker (1975), and the minimum fluidizing Reynolds number, Re_m, is evaluated from the following equation (Kunii and Levenspiel, 1969):

$$\frac{1.75 Re_m^{\,2}}{\varepsilon_{mf}^3} + \frac{150(1-\varepsilon_{mf}) Re_m}{\varepsilon_{mf}^3} - \frac{\rho_g\, g (\rho_c - \rho_g) d_p^3}{\mu^2} = 0 \quad (22)$$

The bubble diameter, for a nozzle with *N* holes over the distributor, is given by Errazu et al. (1979):

$$d_B = 0.667\left(\frac{F_{ar}}{\rho_{ar} N}\right)^{0.375} \quad (23)$$

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

4 Control Framework

The model, represented by a non-linear system of differential-algebraic equations, was written in language C and implemented in MATLAB / SIMULINK within a framework to develop control strategies. The Riser model was discretized by finite differences with the mesh points distributed according to the following generating function:

$$z_i = \exp(\log(h_{ris})\, {}^{i}\!/_{M}) \quad (24)$$

where M is the mesh size, and i = 1,2,...,M. A mesh size of 20 points showed to be satisfactory.

The graphical user interface to simulate the FCC unit and to test different alternatives to control the unit is presented in Figure 4. Within this framework, the user may build graphically any control structure, and simulate any possible modeled disturbance and set-point changes.

In the example shown in Figure 4, a multi-siso control structure with three PID controllers was designed, and two step disturbances were planed to simulate the controlled FCC unit. The simulation results can be visualized directly into the framework by selecting the variables in the diagram and plot them using the right bottom of the mouse.

5 Comparative Results

In this section a comparative analysis is carried out among two models previoulsy developed by the authors, the proposed model, an identified parametric linear model, and plant data.

Since the FCC units began processing heavier feeds the regeneration conditions are changing. Emulsion phase temperature turned to be higher than dilute and gas phases temperatures. It happens because there is 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 to carbon monoxide, where almost all CO burned to CO2, see Figure 5.

The regenerator temperatures were also unsatisfactory, as shown in Figure 6. This could be due to the fact that 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 phases (CSTR f), which improved the regenerator temperatures, but the CO2 / CO ratio become worse, and the system turned to be unstable for large changes in some manipulated variables. The bubble-emulsion model 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 Figure 6. It was only necessary to adjust (increase) the catalyst activity, Acat, and the relative catalyst coke rate, zcat. 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 effect on the products for increasing 2.5% the feed is shown in Figure 6. The tendency is decrease the severity and consequently the conversion decreases too.

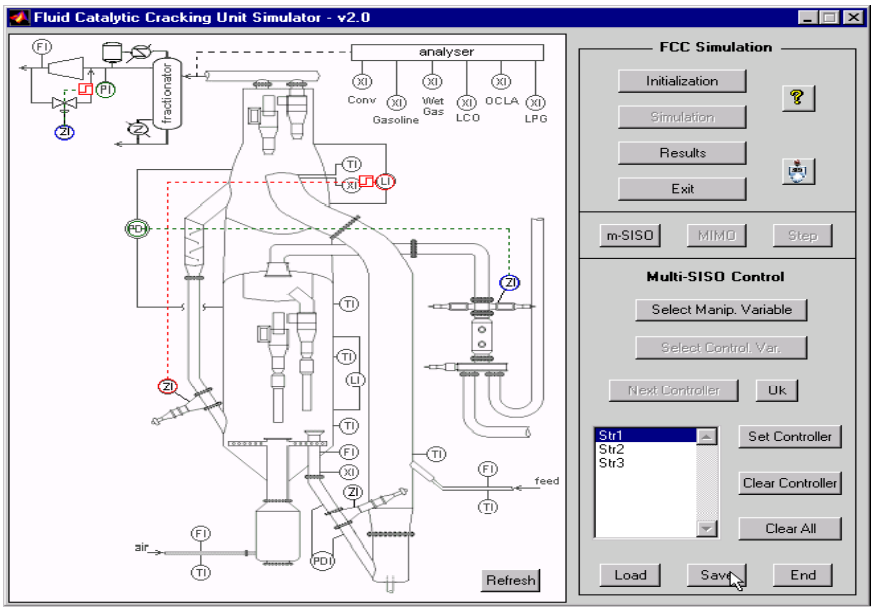

Fig. 4. Framework to analyze control structures.

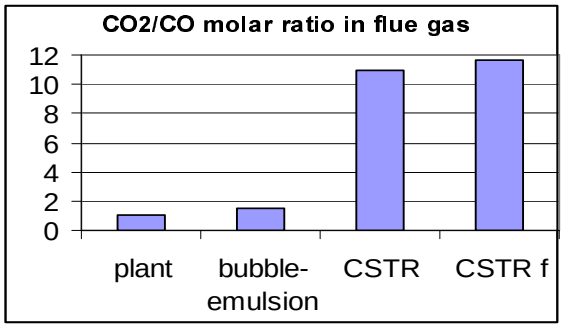

Fig. 5. CO2/CO for plant data and models.

The regenerator temperature decreases because the coke at regenerated catalyst increases and the coke yield decreases due to the lower severity. The converter dynamic model, using bubble-emulsion and tem lumps approaches, was able to reproduce the plant main characteristics.

Despite its good predictive capability, the main drawback of the non-linear model is the spent effort to its development. In order to quantify this effort, a non-theoretical parametric model was obtained based on the data of a set of step disturbances in the real plant. Although the disturbances could not be large enough to characterize the high non-linearities, due to safety reasons, the comparative results showed in Figures 7 and 8 present, at least, three situations: (1) both models may have similar results in terms of static gain (Figure 7); (2) the parametric model may have better agreement with the plant time constants (Figure 8a); (3) the parametric model may present poor long term prediction (Figure 8b). By the other side, the main drawback of the parametric model is its validity region, which depends on the non-linearities of the operating region where the model was identified. Also, the non-linear model could be significantly improved if the data used to identify the parametric model were used to re-estimate some parameters of the non-linear model.

6 Conclusion

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

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.

A linear parametric model, based on real plant data, was also developed to design multivariable linear predictive controllers. This model presented reasonable local agreement with plant data. The comparisons among the non-linear model, the

parametric model, and the plant data show the necessity to know the main limitations of each model in order to use them carefully, getting their benefits and avoiding their troubles.

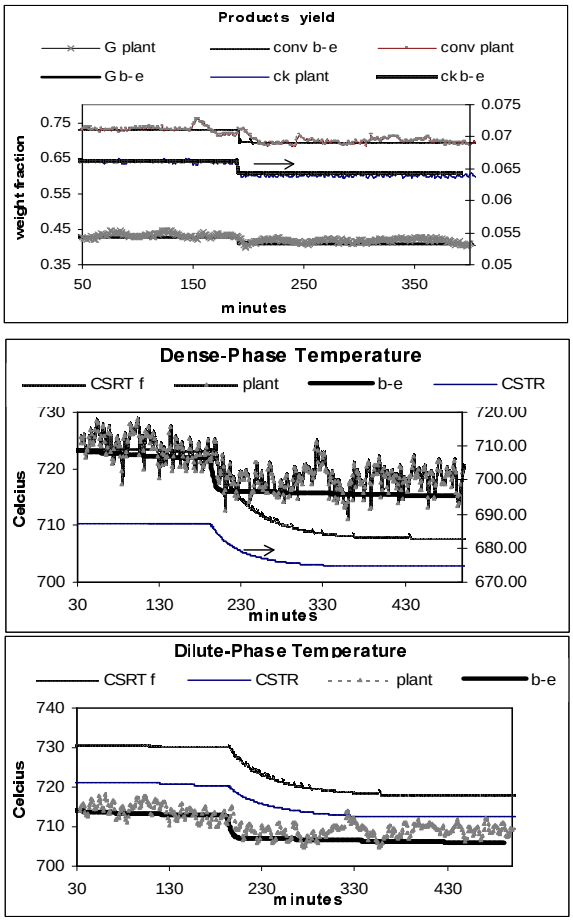

Fig. 6. Comparison among plant data and models.

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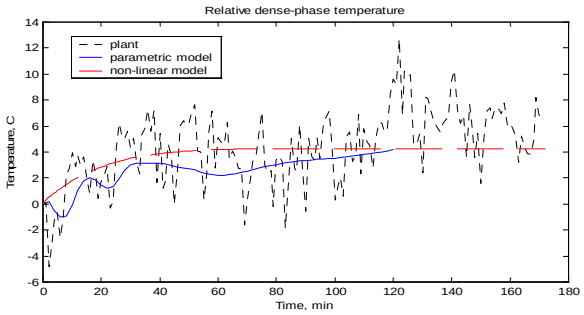

Fig. 7. Step response for 1% air flow rate disturbance.

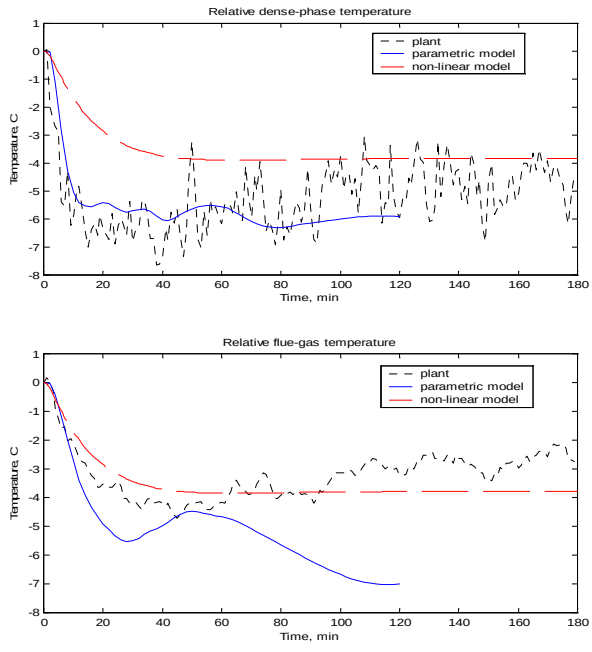

Fig. 8. Step response for 2% TCV disturbance.