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# SIMULATION OF AN INDUSTRIAL COMPLEX FCCU PART I: BUILIDING THE MODEL AND VALIDATION

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**ABSTRACT.** The Fluid Catalytic Cracking process is a proven state-of-the-art technology for the conversion of gasoils and resids to lighter, higher-value products. A mathematical model for this process has been developed. The model describes not only the most phases of chemical engineering fundamentals, such as fluidization, heat/mass transfer, and distillation, but also incorporates the process kinetics, based on a lumping strategy which lumps molecules and reactions according by their boiling point and treated as pseudo-components. Based on the experimental data it was analyzed the process variables behavior in the presence of disturbances.

## 1. INTRODUCTION

A petroleum modern refinery is composed of processing units that convert crude oil into usable products such as gasoline, diesel, jet fuel, heating oil, fuel oil, propane, butane, and chemical feedstocks that are very useful in producing other products such as plastics, synthetic rubbers and fabrics and also cosmetics. Fluid Catalytic Cracking Unit (FCCU) is one of the most important conversion processes in a petroleum refinery. The main propose of this unit is to convert high-boiling petroleum fractions (gasoil) to high value, high octane gasoline, high cetane diesel and heating oil [1]. The three dominant reactions are cracking, isomerization, and hydrogen transfer. The catalyst acid sites have a major influence on the reaction chemistry. The introduction of zeolites into the FCC catalyst drastically improved the performance of the catalytic cracker reaction products. The zeolite catalysts are active and selective. The higher activity and selectivity translate to more profitable liquid product yields and additional cracking capacity [2].

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The process consist in the following: raw material is mixed with the regenerated catalyst in reactor riser. Here took place the cracking reactions and coke formation. The products (gasoline, disesel, slurry) are separated in fractionator and the catalyst poisoned with coke is regenerated in regenerator (Figure1).

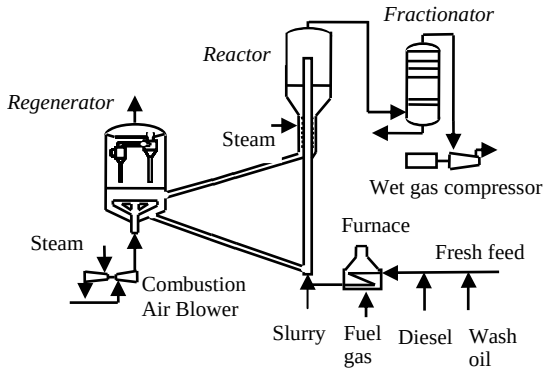


**Figure 1**. Fluid Catalytic Cracking Unit

## 2. PROCESS MATHEMATICAL MODELING

Mathematical modeling in the chemical engineering field has multidisciplinary character, dealing with different processes which must be described. A mathematical model is a system of equations that defines the intrinsic interdependencies of a system. Analytical mathematical models are based on conservation equations (mass, energy, momentum), laws of the physical and chemical processes that are taking place in the system and are able to describe proper the process [3].

Numerous studies are concerned with the modeling of this unit, which are very useful in elucidating of the main characteristics of this unit The FCCU dynamic model has been developed on the basis of reference construction and operation data from an industrial unit and consists of detailed models of: the feed and preheat system, reactor stripper, riser, regenerator, air blower, wet gas compressor, catalyst circulation lines and main fractionator. The FCCU model has been developed on the basis of reference construction and operation data from an industrial unit: ROMPETROL Refinery, Romania. The

resulted global model of the FCCU is described by a complex system of partial-differential-equations, which was solved by discretizing the kinetic models in the riser and regenerator on a fixed grid along the height of the units, using finite differences. The resulted model is a very high order DAE, with 933 ODEs (133 from material and energy balances and 800 resulted from the discretization of the kinetic models). The model captures the major dynamic effects that can occur in an actual FCCU system. It is multivariable, strongly interacting and highly nonlinear.

A model to predict the yields of valuable products is included: the five lump kinetic model for the riser reactor, which can describe the composition of the major product:gasoline and the raw material conversion [4,5]. The following assumptions have been made: approximately 10% of the HCO was uncrackable; effectively no gasoline overcracking takes place; diesel only cracks to gas and is not converted into gasoline. The kinetic model is schematically presented in Figure 2.

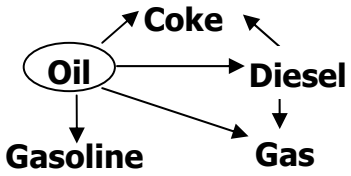


**Figure 2.** Five lump model for the catalytic cracking

This model is described by the following set of differential equations:

$$\frac{\partial y_{slurry}}{\partial t} = ((-(k_1 + k_2 + k_3)(y_{slurry} - x_{slurry}))\psi_{conv} - (k_5(y_{slurry} - x_{slurry})CTO \quad (1)$$

$$\frac{\partial y_{diesel}}{\partial t} = ((k_1(y_{slurry} - x_{slurry}) - k_4 y_{diesel})\psi_{conv} - (k_6 y_{diesel})\psi_{coke})CTO \quad (2)$$

$$\frac{\partial y_{gasoline}}{\partial t} = ((k_2(y_{slurry} - x_{slurry}))\psi_{conv} CTO \quad (3)$$

$$\frac{\partial y_{gas}}{\partial t} = ((k_3(y_{slurry} - x_{slurry}) + k_4 y_{diesel})\psi_{conv} CTO \quad (4)$$

$$\frac{\partial y_{coke}}{\partial t} = ((k_5(y_{slurry} - x_{slurry}) + k_6 y_{diesel})\psi_{coke} CTO \quad (5)$$

The activity function of coke formation is described by the following equation:

$$\frac{\partial \psi_{coke}}{\partial t} = -\alpha \psi_{coke} \quad (6)$$

The activity function of conversion is assumed to be the same for all the reactions:

$$\frac{\partial \psi_{conv}}{\partial c_c} = -k_d \psi_{conv} \tag{7}$$

## 3. MODELING RESULTS

The five lump kinetic model for the riser section leads to a set of partial differential equation who can give a good prediction of the cracabiliy of the aromatic gas oil. For the riser section, described by the five-lump kinetic model, a sensitivity analysis at different catalyst-raw material-ratio (which is an important disturbance in a real process) for the raw material conversion has been made and it was observed that the CTO has a small influence on the raw-material conversion; the increase of the CTO leads to an approximate the same value of conversion (~ 80%), as Figure 3 shows:

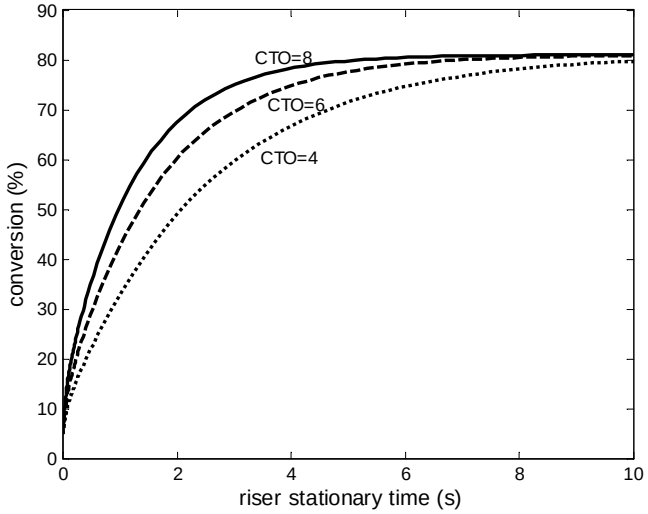


**Figure 3**. Raw-material conversion at different catalyst-raw material-ratio (CTO)

Comparison between modeling results and industrial operating data form ROMPETROL Refinery has been performed for sets of data, confirming the main trends of the dynamic process behavior. Simulated variables are situated in a range corresponding to industrial unit behavior as can be shown in Table 1, Figure 4 and Figure 5.

**Table 1**

Typical operating conditions and values obtained with the simulator

| Process variable | Measure unit | Data Plant | | Value in simulator |
|---|---|---|---|---|
| | | Minimum value | Maximum value | |
| Catalyst-to-Oil Ratio | - | 6.5 | 8.5 | 7.4 |
| Reactor pressure | bar | 1.5 | 2.2 | 1.51 |
| Regenerator pressure | bar | 1.7 | 2.4 | 1.7 |
| Main fractionator pressure | bar | 0.9 | 1.5 | 1.3 |
| Regenerator temperature | $^0$C | 682 | 735 | 709.6 |
| Reactor temperature | $^0$C | 505 | 535 | 524.5 |
| Raw material temperature | $^0$C | 190 | 320 | 303.5 |
| $CO_2$ concentration in flue gas | % | 16 | 19 | 16.07 |
| $O_2$ concentration in flue gas | % | 0.8 | 2.5 | 1.02 |
| Reactor Catalyst Inventory | tons | 35 | 50 | 39.7 |
| Total Catalyst Inventory | tons | 175 | 195 | 191 |

Next figures present the open-loop dynamic simulation results together with the industrial data form ROMPETROL Refinery. It is presented the the reactor and regenerator pressure behavior when the raw material flow disturbance appears. For the first set of experiments the fresh feed flow decreases with 5.5 $m^3/h$ at t=80 min. The simulation results are presented comparatively with the experimental data from the plant in Figure 4. In the second set of experiments, fresh feed flow decrease with 1.2 $m^3/h$ at t=10 min then it decrease with another 13.8 $m^3/h$ at t=70 min. The simulation results are presented comparatively with the experimental data from the industrial plant in Figure 5.

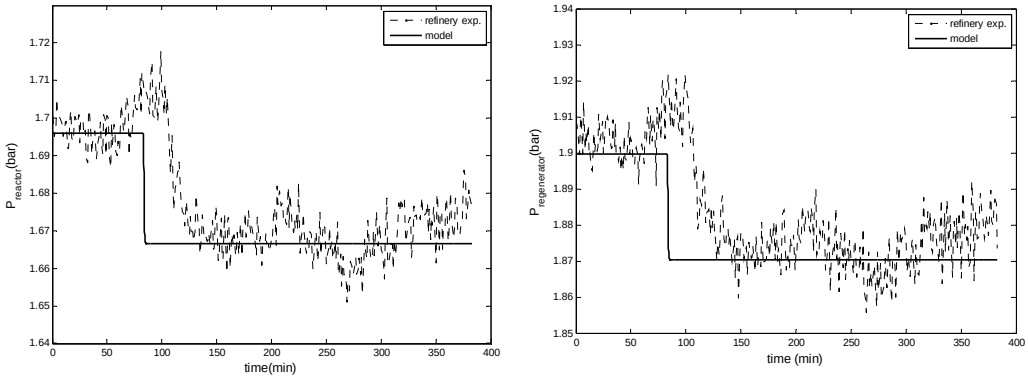


**Figure 4.** Open-loop simulation of FCCU dynamic behavior- comparison with industrial data (first set of experiments)

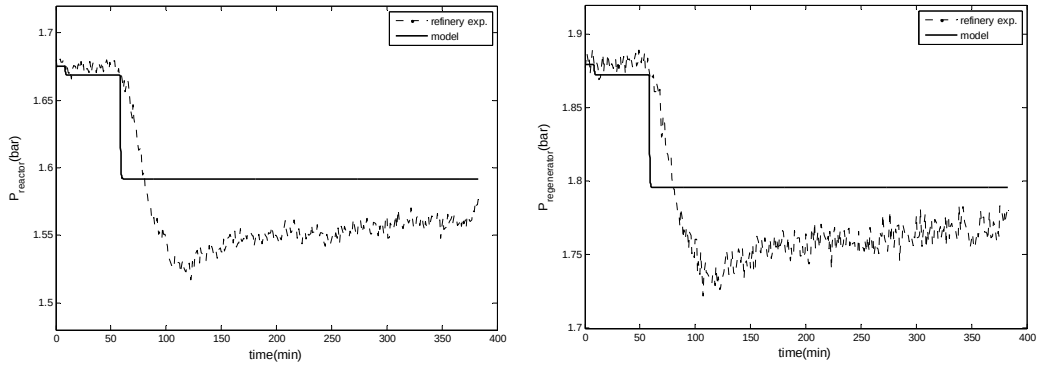


**Figure 5.** Open-loop simulation of FCCU dynamic behavior- comparison with industrial data (second set of experiments)

## 4. CONCLUSIONS

A five lump kinetic model (namely: gas-oil, gasoline, diesel, gases and coke) capable to predict raw material conversion was introduced in the FCC process global model. Based on the experimental data, comparisons between the output values in simulator and industrial data, in the presence of disturbances where made. Results obtained by the simulations present a good fit with industrial operating data. With this new model, the FCCU complex behavior in the presence of disturbances can be studied in order to improve the productivity and profitability of the modern process.

## ANNEX

$k_I$ = reaction rate constant (gfeed · gcat · $s^{-1}$)
$kd$ = deactivation constant for conversion (wt%)
$\alpha$ = deactivation constant for coke formation ($s^{-1}$)
$\alpha$ = deactivation constant for coke formation ($s^{-1}$)
$c_c$ = coke content on catalyst (wt %)
$CTO$ = catalyst-to-oil ratio (gcat/gfeed)
$\phi_{\text{coke}}$ = activity function for coke formation
$\phi_{conv}$ = activity function for conversion
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