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First principle modeling of an industrial Fluid Catalytic Cracking – the adaptation of the model

Roman Raluca[a], Zoltán K. Nagy[b], Paul Ş. Agachi

[a]*Department of Chemical Engineering, Babes-Bolyai University, Arany Janos Str., Cluj-Napoca 400028, Romania, romanr@chem.ubbcluj.ro, sagachi@chem.ubbcluj.ro*
[b]*Department of Chemical Engineering, Loughborough University, Loughborough, LE11 3TU, United Kingdom, Z.K.Nagy@lboro.ac.uk*

Abstract

A complex dynamic model of the reactor-regenerator-fractionator system of an industrial FCCU is developed. The novelty of the model consists on the complex dynamics of the reactor-regenerator system and it also includes the dynamic model of the fractionator, as well as a new five lumped kinetic model for the riser, and hence it is able to predict the final production rate of the main products (gasoline and diesel). Based on the experimental data comparisons between the simulated output values and industrial data have been done, for certain disturbance scenarios.

Keywords: catalytic cracking, dynamic simulator, five lump kinetic modeling

1. Introduction

The Fluid Catalytic Cracking (FCC) process is a proven state-of-the-art technology for the conversion of gasoils and resids to lighter, higher-value products. Since its beginning in the late 1960s, the FCC process has been continually upgraded to meet the most current challenges facing refineries. Modern FCC units can take a wide variety of feedstocks and can adjust operating conditions to maximize production of gasoline, diesel or light olefins to meet different market demands [3, 5].

2. Description of the process

The schematic diagram of the FCCU, for which the mathematical model was developed, is presented on Fig. 1.

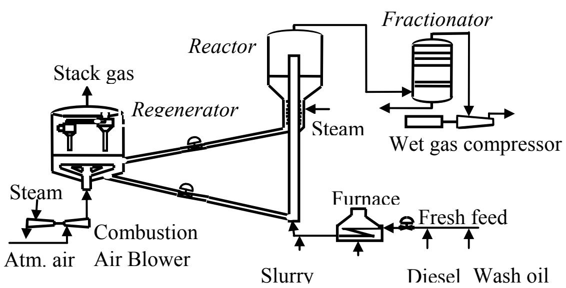

Fig 1. FCCU plant

Pre-heated feed is mixed with the hot slurry recycle (from the bottom of the main fractionator) and injected into the reactor riser, where it mixes with hot regenerated catalyst and totally vaporizes. As a result of the cracking reactions, a carbonaceous material (coke) is deposited on the surface of the catalyst. The spent catalyst separated by the riser-reactor cyclones is degassed of most of the reaction vapor as it is discharged via diplegs into the catalyst stripper-reactor. In the upper part of reactor, hydrocarbons are effectively removed from the catalyst by efficient contacting with steam. Reactor products (gases, gasoline, diesel, slurry) are passed to the main fractionator for further separation. Since coke poisons the catalyst, continuous regeneration is required. The carbon-rich portion of the coke deposits is burned off in the turbulent dense phase of the regenerator. Regeneration flue gases are first routed through cyclones to minimize catalyst losses and then sent to energy recovery and environmental treatment before being ejected from the stack. The regeneration system restores catalytic activity of the coke-laden spent catalyst by combustion with air. It also provides heat of reaction and heat of feed vaporization by returning hot, freshly regenerated catalyst back to the reaction system [1, 2]

3. FCCU dynamic modeling

The FCCU model has been developed on the basis of reference construction and operation data from a Romanian industrial unit. The developed dynamic simulator 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[2,3]. The developed model is sufficiently complex to capture the major dynamic effects that occur in an actual FCCU system; it is multivariable, strongly interacting and highly nonlinear. Based on the assumption given in [4], a *five lump kinetic model* (schematically shown on Fig. 2) that predicts the yields of valuable products is included in the simulator. Since the catalyst deactivation is the most important phenomena in the Fluid Catalytic Cracking process, for the coke formation was used an advanced activity function expressed as follows:

$$\frac{d\varphi_{coke}}{dt} = -\alpha\varphi_{coke}$$

In this equation, φ_{coke} is the activity function of coke conversion, t is the riser residence time and α is the deactivation constant for coke formation.

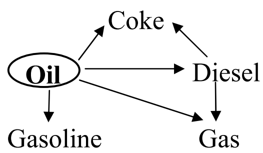

Fig .2. Five lump model for the catalytic cracking

The FCCU main fractionator was modeled as a continuous *distillation column* with 38 stages including a reboiler and a total condenser. The feed flow enters into the column at the stage 6 (counted from the bottom) and is considered as the main source of disturbance, together with the feed flow composition. The 114 order main fractionator model describes the composition of gasoline and diesel and also the liquid hodups in each stage. 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 2133 ODEs (133 from material and energy balances and 2000 resulted from the discretization of the kinetic models). The model was implemented in C programming language for efficient solution and was used to study the dynamics of the process.

The introduction of the five lump kinetic model can give a good prediction of the cracability of the aromatic gas oil (Fig.3): especially during the first 0.4 seconds, a rapid decrease in the rate of conversion of raw material is found, due to the coke formation. After 4 seconds, no net diesel is formed, but only disappears. During the first 5 seconds, gas is predominantly formed from gas oil, but is taken over by diesel afterwards. Fig. 3 also presents the unconverted gas oil fraction.

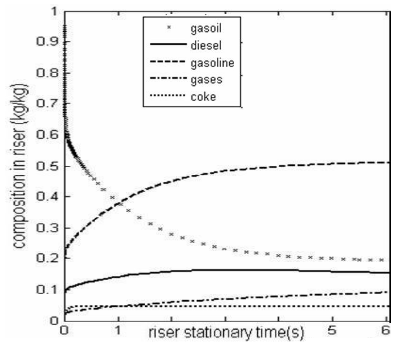

Fig. 3. Feed and products distribution along the riser

The introduction of kinetic model for the riser section can give the possibility to study the dynamic response of main products composition (gasoline and diesel) the fractionator. Fig. 4, for example, illustrates the simulation results in the case of three typical disturbances. The influence of these disturbances for the gasoline and diesel composition is below 1% for the coke factor and slurry feed rate disturbance, however considering the throughput of a typical FCCU this can lead to economical consequences.

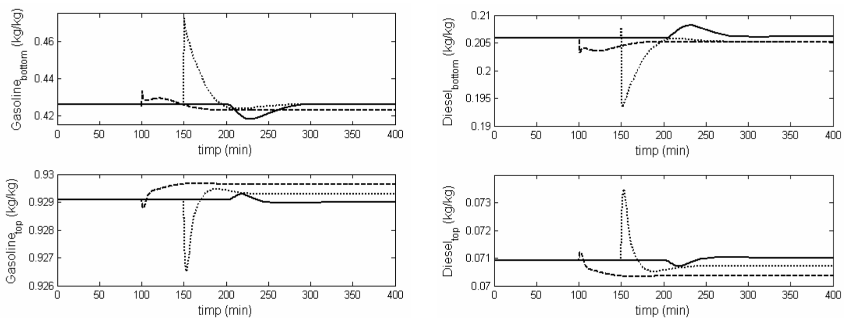

Fig. 4: Simulation of FCCU dynamic behavior in the presence of disturbances: coking rate Kc disturbance (5% increase at t=200 min - solid line); pressure drop disturbance (10% decrease at t=150min- dotted line) and slurry recycle feed rate (30% decrease at t=100 min - dashed line)

Results obtained using the developed FCCU model where compared with industrial operating data taken form a Romanian refinery. Simulated variables are situated in a range corresponding to industrial unit behaviour as can be shown in Table 1 and Fig 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
Reactor-regenerator differential pressure	bar	0.2	0.3	0.2
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 preheated 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

Fig 5 present the open-loop dynamic simulation results together with the industrial data form a Romanian refinery, taken for a period of 7 hours when the raw material flow disturbance appears (increase with 10 m3/h at t=50 min, then it increase with another 12 m3/h 300 min). The presented data (regenerator temperature, reactor pressure and regenerator pressure) where collected on May, 13, 2006, from 5 A.M to 7.12 P.M.

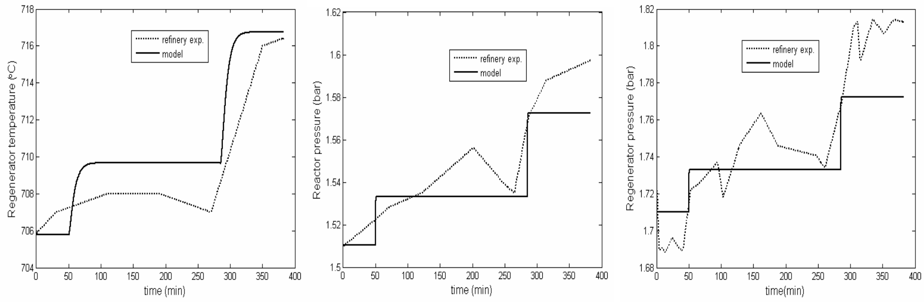

Fig. 5. Different scenarios of the simulation of FCCU dynamic behavior

4. Conclusions

The paper presents dynamic simulations for the FCCU aggregate system that includes the main fractionator and a five lump kinetic model for the riser leading to a 2133th order ODE model. The developed model simulates the dynamic behavior of the reactor-regenerator-fractionator system and also can predict the composition of the main products (gasoline and diesel). The complex model is able to capture the major effects that occur in the actual FCCU. The model was used for the study of different operating regimes induced both by design changes and by changing operation strategies and based on the experimental data where made comparisons between the simulated output values and industrial data, in the presence of disturbances. The results validate the mathematical model of the process.

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