New Approach in Modelling, Simulation and Hierarchical Control of the Fluid Catalytic Cracking Process

I - Process modelling

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From the economical point of view, the fluid catalytic cracking plant represents one of the most important plants on a refinery platform. Due to this reality, many researcher teams have approached partially aspects regarding this process modeling, simulation or automatic control. The authors of the present article have approached the integral problem in an original manner, starting with the process modeling and ending with the elaboration of the control hierarchical structure. The article is structured on two parts: I - Process modelling, II - Hierarchical control. In the first part there is presented the decomposition of the complex fluid catalytic cracking process into sub-processes, each sub-process being characterized by the output – input values and by dynamic characteristics. The very fast sub-processes have been modelled in a steady-state regime, and for the slow sub-processes there were elaborated dynamic models. The authors have given a special attention to the stage of adaptation of the mathematical model in a steady-state regime, the parameters of the kinetic model being adapted depending on the operation industrial data. Based on the mathematical models, the authors have elaborated a system of programs designed for the simulation in steady –state and dynamic regime of the fluid catalytic cracking process. The results obtained allowed for the validation of the mathematical model of the fluid catalytic cracking process, thus ensuring the premises of the hierarchical control approach.

Keywords: fluid catalytic cracking, steady-state model, dynamic model

The fluid catalytic cracking plant ensures the conversion of the heavy fractions into a high octane number gasoline (the main element in the commercial gasoline) and olefin –rich gases (the feed stock in the petrochemical industry).

The fluid catalytic cracking process modelling is an extremely difficult task due to the great number of variables, to the high degree of uncertainty concerning the development of some phenomena and the feedstock complexity.

Most of the papers from the special literature treat in a unitary manner the fluid catalytic cracking process modelling, the model being generally difficult and inflexible, meaning there are changes that would be hard to operate [1- 5]. Opposed to the classical versions of mathematical models, the authors propose a structural approach of the mathematical modelling of the fluid catalytic cracking process. This kind of approach grants to the mathematical model robustness and clarity and/at the same time, the possibility of testing and/or modifying independently the mathematical models corresponding to the sub-processes, without affecting their assembly. The open character of the system allows by adding new models or modifying the existing ones.

The structural approach of the mathematical model

The structural approach of the mathematical model of a complex process represents the split of the whole process into sub-processes on topological and functional points of view. This has as consequence the decomposition of the whole mathematical model of the complex system into sub-models. For the catalytic cracking process there are indentified the following types of sub-processes, figure 1[6].

The sub-process interfusion node is located at the reactor base and is designed for the instantaneous vaporization of the feedstock at direct contact with the regenerated catalyst [1]. Because the standby time of the feedstock and catalyst within the interfusion node is less than 0.1s, this sub-process may be considered a non-inertial system, the sub-process being modelled only in a steady-state regime. The input values associated to the sub-process: Q_{mp} – feedstock flow; Q_{catl} – regenerated catalyst flow; C_{cocs3} - the mass fraction of the coke residual; T_{reg} – the regenerated catalyst temperature. The output values of the sub-process are: T_{nod} - the interfusion node temperature and C_{cocsl} – the mass fraction of coke deposited on regenerated catalyst after the cracking reaction.

The sub-process riser is a plug flow tubular reactor and operated in adiabatically conditions. The standby time of the feedstock and the catalyst is of the order of 0.5s, a fact that determines the character of a non-inertial system. The riser output values are: T_r – temperature at the riser outlet, Y_A – the feedstock concentration, Y_B – the gasoline concentration, Y_C - the gas and coke concentration in the reaction environment, C_{cocs1} – the mass fraction of the coke deposited on the catalyst after the cracking reaction.

The sub-process stripper is located at the reactor top and contains a cyclones system for the separation of the feedstock and the reaction products in a gaseous phase from the catalyst particles. The sub-process was assimilated to a system with perfect mixing, the sub-process being modeled in a dynamical regime, as a system with concentrated parameters. This sub-process output values are: Q_{cqt2} - the used catalyst flow evacuated towards the regenerator, C_{cocs2} - the mass fraction of the coke deposited on the catalyst, T_s - the temperature in the stripper.

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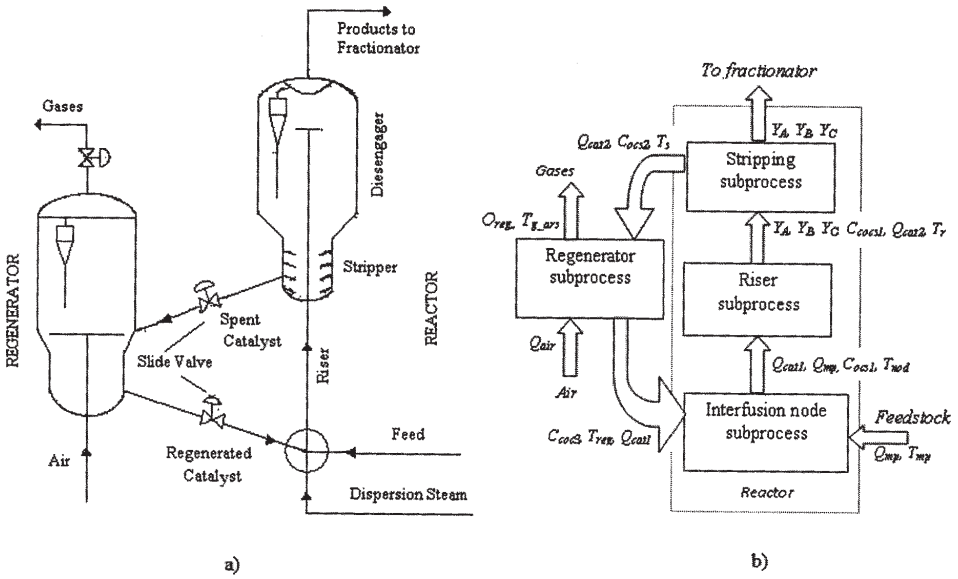

Fig.1. The cracking catalytic process: a) industrial design; b) bloc scheme

The sub-process regenerator is a complex system, assimilated to a reactor with perfect mixing (so will be treated as a system with concentrated parameters), where the catalyst regeneration takes place by the partial burning of the coke deposited on the catalyst within the catalytic cracking reactions in the riser. From the dynamic point of view, the sub-process is an inertial system. The output values are: Q_{cat1} – the regenerated catalyst flow, T_{reg} – the temperature of the regenerated catalyst, C_{cocs3}- the mass fraction of the coke residual, O_{reg} – the molar fraction of the oxygen in the regenerator, T_{g_ars} – the burned gases temperature.

The mathematical modelling in the steady-state regime

The mathematical models in steady-state regime are used in chemical engineering for the study and design of the chemical plants. In the domain control engineering of the chemical process, the mathematical models in a steady-state regime allow the determination of the statical characteristics of the chemical process for different dependencies between the output variables as compared to the input variables.

The model of the interfusion node sub-process

The model of the interfusion node sub-process is represented by a heat balance defined on the contour of the interfusion node. The considered hypotheses for the sub-process modeling are: the adiabatic regime and the instantaneous vaporization of feedstock [1]. The temperature of the interfusion node is given by the relation

$$T_{nod} = \frac{Q_{cat1} \cdot c_{p,cat} \cdot T_{reg} + Q_{mp} \cdot c_{p,mp} \cdot T_{mp} - \Delta H_{vap} \cdot Q_{mp}}{Q_{cat1} \cdot c_{p,cat} + Q_{mp} \cdot c_{p,mp}} \quad (1)$$

The model of the riser sub-process

The mathematical model of the riser sub-process contains the following components: the kinetic model, the material balance and the heat balance.

The kinetic model

In the specialized literature there are known the following model of the fluid catalytic cracking process:

-Weekman model, a kinetic model with three pseudo-components, that may be applied to any type of feedstock [7];

-Ginetto model, a model with four pseudo-components being developed to describe more exactly the kinetic behaviour corresponding to the new types of catalysts made of zeolites crystals dispersed into a silicon-aluminous matrix [8];

-the model with six pseudo-components, developed by the company Chiyoda Chemical Engineering and applied in the case of heavy feedstock [9];

-the Mobil model, a complex kinetic model, with ten pseudo-components, their defining being realized according to the criterion of the distillation limits and of the chemical composition on hydrocarbons classes [10].

Because the mathematical model of the riser will be used in a control system of the process, the authors have chosen a simple but robust model, which is the Weekman kinetic model. Within Weekman model, each pseudo-component is defined based on the distillation limits, as follows: feedstock – A, gasoline – B, gases and coke – C, figure 2. The expressions of the chemical reactions are presented in table 1.

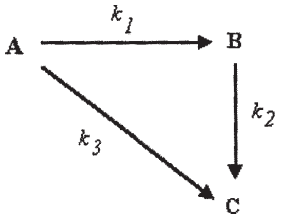

Fig. 2. Weekman kinetic scheme

Table 1
CHEMICAL REACTIONS IN WEEKMAN KINETIC MODEL

Relation number	Reaction	Reaction velocity
(2)	$A \rightarrow B$	$r_1 = -k_1 Y_A^2$
(3)	$B \rightarrow C$	$r_2 = -k_2 Y_B$
(4)	$A \rightarrow C$	$r_3 = -k_3 Y_A^2$

The constants of the reaction velocity k_1, k_2, k_3 are dependent on the feedstock nature, the temperature in the riser, the activity of the equilibrium catalyst and the operation conditions [11].

$$k_j = k_j^0 \cdot f_j(MAT) \cdot \theta_j(t_c) \cdot \gamma_j(c_{cocs}) \cdot e^{\left(\frac{E_j}{R}\right)\left(\frac{1}{T_0} - \frac{1}{T_r}\right)}, \quad j = 1,\ldots,3 \quad \left[s^{-1}\right] \quad (5)$$

In the relation (5), T_0 is the reference temperature for which the equilibrium constants were determined respectively 482°C, and the conversion reactions the feedstock into gases and coke, were merged in reactions which has index j = 0. The velocity constants k^o_j are dependent on the feedstock structure and quality, characterized by the relation between the aromatic carbon and naphtenic carbon, C_A / C_N and have the following values or expressions:

$$k_j^0 = e^{l_{0j}\cdot ln\left(\frac{C_A}{C_N}\right)+l_{1j}}, \quad j=0,1; \qquad [s^{-1}] \tag{6}$$

$$k_2^0 = 5.55\times 10^{-2}; \qquad [s^{-1}] \tag{7}$$

where l_{0j} and l_{1j} $j=0.1$ are the approximation coefficients.

For the reaction 2, there are used the next values of the velocity constant:

$$k_3^0 = k_0^0 - k_1^0. \qquad [s^{-1}] \tag{8}$$

The activity of the equilibrium catalyst, experimentally determined by MAT standard method [12], is included in the expression of the velocity constants under the form of some attenuation functions [13]:

$$f_1 = \ln\frac{MAT}{1-MAT}; \tag{9}$$

$$f_j = a_{0j} + a_{1j}\,MAT + a_{2j}\,MAT^2, \quad j=2,3. \tag{10}$$

The deactivation of the catalyst due to the coke deposits is considered by an attenuation function reported to the contacting time t_c

$$\theta_j(t_c) = e^{(-a_{dez}\,t_c)}; \tag{11}$$

$$a_{dez} = 43.5 - 7.56\,(C_A/C_N)^{-1}. \tag{12}$$

The efficiency of the catalyst regeneration is expressed by the function $\gamma_j(c_{cocs})$, the expressions of the attenuation functions being as follows:

$$\gamma_1 = 1 + 0.151\,c_{cocs}; \tag{13}$$

$$\gamma_2 = 1 - 3.125\,c_{cocs}; \tag{14}$$

$$\gamma_3 = 1/(1+3.53\,c_{cocs}). \tag{15}$$

The residual coke, c_{cocs}, is expressed depending on the temperature of the regenerator T_{reg}

$$c_{cocs} = 4.31\cdot 10^8\; e^{-(0.568+0.03195\,T_{reg})}. \qquad [kg/h] \tag{16}$$

The material and heat balance

The riser sub-process is a plug flow tubular reactor, operated adiabatically. The material balance is represented by three differential equations, each differential equation being associated to a pseudo-components present in the reaction environment. The heat balance is also described by differential equations. The simplified assumptions taken into account for the heat balances are:

-the neglection of the heat contributions of the components groups represented by gasoline and gases + coke, due to flows and their heat capacities that are very small;

-the neglection of the heat effects resulted from conversion of the gasoline into gases + coke and neglection of the thermal effect resulted by conversion of the feedstock into gases + coke due to the reduced conversion of the gasoline into gases - coke and the values of the enthalpy of this reaction.

Material and heat balance can be described by a system of differential equations with distributed parameters under the form

$$\begin{cases} \dfrac{dY_A}{dz} = -\dfrac{1}{U_v}\left(k_1 + k_3\right) Y_A^2 \\ \dfrac{dY_B}{dz} = \dfrac{1}{U_v}\left(k_1\, Y_A^2 - k_2\, Y_B\right) \\ \dfrac{dY_C}{dz} = \dfrac{1}{U_v}\left(k_2\, Y_B + k_3\, Y_A^2\right) \\ \dfrac{dT_r}{dz} = \left(-\dfrac{dY_A}{dz}\right) * \dfrac{\left(-\Delta H_{r1}\right)}{\left(Y_A c_{p,A} + R_{abur} c_{p,abur} + R_{cat} c_{p,cat}\right)} \end{cases} \tag{17}$$

In the system (17), U_v represent the vapor velocity through the riser expressed in m/s. The initial conditions used for the solving of the differential equation system (17) are

$$\begin{cases} Y_A(0) = 1 \\ Y_B(0) = 0 \\ Y_C(0) = 0 \\ T(0) = T_{nod} \end{cases}. \tag{18}$$

By solving the differential equations system (17), there is obtained the temperature profile along the riser and three pseudo-components profile of kinetic scheme along the riser.

The adaptation of the mathematical model in a steady-state regime

The authors have studied and have identified four components associated to the phase of adaptation of the mathematical models associated to the catalytic cracking process [14, 15]:

-the specification of the constructive data for the fluid catalytic cracking reactor;

-the specification of the catalyst thermodynamic properties;

-the calculation of the thermodynamic properties of the feedstock;

-the estimation of the kinetic parameters used within the kinetic model based on the industrial experimental data.

The reactor constructive data

The industrial data allowed for specification of the riser area A_r=1.32 m^2, and of its height, H_{riser}=35m [14].

The catalyst physical proprieties

The catalyst physical properties are determined experimentally or are taken up from literature [16]. The values of the catalyst physical properties are: the heat capacity, $c_{p,cat}$ = 0.28 kcal kg^{-1} grd^{-1}, the deactivation factor, MAT = 0.68. The mass ratio of dispersion steam into riser, R_{steam} = 0.0015.

The physical properties of the feedstock

The authors have investigated the relationships used to estimate the thermodynamic properties used within the kinetic model. The result of theses investigations are

Table 2
MEASURED AND ESTIMATED FEEDSTOCK PROPERTIES [15]

Type of property	Properties	Averange value	Fundamental units
Measured	Density	0.9080	-
	Sulphur	0.34	% weight
	Medium boiling point temperature	367.4	°C
Estimated	Molar boiling point temperature	358.7	°C
	Molar weight	311.5	kg kmol^{-1}
	Characterization factor	10.13	-
	Heat capacity	0.546	kcal/kg°C
	Refraction indice	1.50	-
	Aromatic carbon	23.83	%
	Naphtnic carbon	23.17	%

presented in [14, 15]. Another research direction approached by the authors was obtaining industrial data for the fluid catalytic cracking process. These industrial data allowed for the estimation of the following properties of feedstock: molar weight, molar boiling point temperature, characterization factor, refraction indices, aromatic carbon and naphtenic concentration and heat capacity. The estimated or measured medium values are presented in table 2 [14, 15].

The kinetic parameters calculus

The successful application of the mathematical model for the fluid catalytic cracking reactor depends on a large extent on the accuracy of the determination of the model kinetic constants. The authors have identified two categories of parameters specific to Weekman kinetic model:

-the values of the activation energies for each chemical reaction;

-the numerical values of the kinetic parameters used within the approximation functions (6) and (10).

The activation energy of the chemical reactions present in Weekman model was taken up from literature [16].

The second categories of kinetic parameters are estimated by minimizing an objective function, proposed by the authors, that represents the sum of the squares of the deviations. The proposed form of the functions is

$$F_{ob}=\sum_{j=1}^{m}\left[\left(T_{r,j}^{\exp}-T_{r,j}^{\mathrm{mod}}\right)^2\right], \qquad (19)$$

where $T_{r,j}^{exp}$ represents the experimental temperature for the day j; $T_{r,j}^{mod}$ - the temperature calculated based on riser model (18) corresponding to the input data on day j.

Choosing the riser outlet temperature as variable of the objective function (19) is motivated on one hand by the fact that the temperature at the riser outlet is a model variable and on the other hand by the existence of this variable into the set of available industrial data. Another argument for choosing this variable is the presence of the kinetic coefficients into the calculation relationship of the riser outlet temperature.

The mathematical model previously presented has ten kinetic parameters. These parameters represent at the same time the variable of the objective multivariable function (19). Consequently, the objective function (19) becomes a function which depends on kinetic parameters of the model and which presents the form

$$F_{ob}(a_{02},a_{12},a_{22},a_{03},a_{13},a_{23},l_{00},l_{10},l_{01},l_{11})=\sum_{j=1}^{m}\left[T_{r,j}^{\exp}-T_{rj}^{\mathrm{mod}}(a_{02},a_{12},a_{22},a_{03},a_{13},a_{23},l_{00},l_{10},l_{01},l_{11})\right]^2 \qquad (20)$$

Determination of parameters from relation (20) involves its minimization. For the minimization of the multivariable function (20) there has been used the algorithm of the cyclical exploration with optimum step [17]. The optimum solution was obtained after 162 evaluations of the objective function.

Validation of the model in a steady-state regime

A method validation is represented by comparison of industry data with results obtain from the simulations performed base on the model. Another method validation is making the adequate testing in relation to the process. The adequate of the mode is based on qualitative indicators such as the relative deviation, standard deviation and statistical test.

In the present paper, the validation method involves calculating the standard deviation for two variables of the process output that are the riser outlet temperature and gasoline yield. A comparison between the values of the model output and industrial data are presented in figures 3 and 4. Industrial data used for model validation are presented in table 3. The values of the standard deviations and the relative standard deviation calculated for the two output variables are presented in table 4.

In figure 3 there is presented the variation of the riser outlet temperature (inlet stripper) which is compared with the temperature estimated by the model. Since the real temperature of the stripper is instantaneous temperature, the temperature is taken every day at 12 o'clock and the temperature determined by the model represents a value associated to the average operating parameters, there are differences between these two values of temperatures.

In figure 4 there is presented a comparison between the evolution of the real yield of gasoline produced in the plant,

Table 3
STANDARD DEVIATION AND COEFFICIENT DEVIATION

Parameter	Standard deviation	Coefficient deviation
Riser outlet temperature T_r [^{0}C]	0.47	0.08
Gasoline yield $Q_{benzină}$ [kg/h]	776.9	1

Table 4
INDUSTRIAL DATA USED FOR THE VALIDATION OF THE MODEL

Feedstock temperature [°C]	Feedstock flow [kg/h]	Regenerator temperature [°C]	Contact ratio catalyst/feedstock	Riser outlet temperature [°C]	Gasoline flow [kg/h]
203	176292	711	4.67	531	75417
200	177083	710	4.36	531	82917
202	154333	712	4.16	530	83541
202	149042	709	4.25	530	75750
207	155667	706	4.68	530	69375
205	161083	708	4.56	530	75583
195	162292	711	4.35	531	79958
194	157792	711	4.63	531	71167
195	161750	709	4.59	531	74417
191	173583	710	4.54	530	77875
190	167083	711	4.43	531	79583
191	169542	711	4.54	532	78333
198	170375	710	4.49	531	80208
205	173167	710	4.57	531	80417
205	167333	712	4.48	531	79375

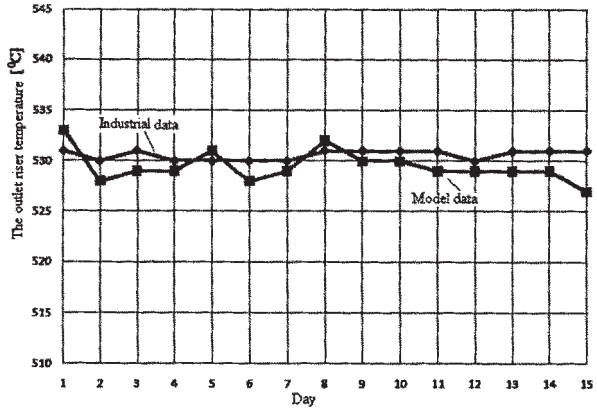

Fig. 3. Comparative evolution of the riser outlet temperature

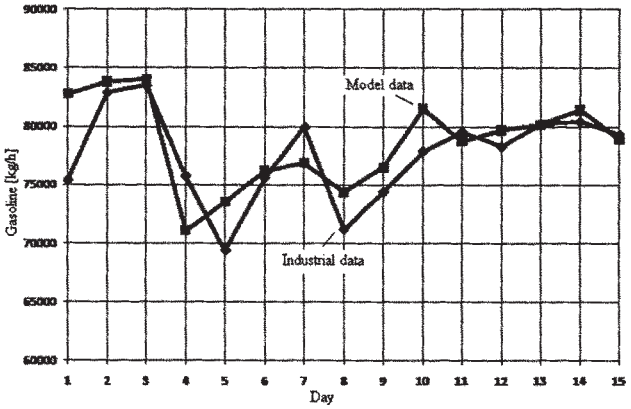

Fig . 4. Comparative evolution of the gasoline yield

with output estimated by the kinetic model. Differences between these two values of yield are limited to 1%.

Analyzing the data from table 3 and graphs 3 and 4, there is noticed that standard deviations are less than 1% of the average value of the experimental data. In this context the model elaborated for the riser sub-process can be used in the control of the process, the errors being totally insignificant.

Figures 5a and b are the results of simulations in steady state regime which evidenced a behaviour typical to the catalytic cracking process. Both the temperature along the riser and the feedstock concentration decreased exponentially in relation to the spatial coordinate associated to the riser. The concentration of gasoline, intermediate product in the kinetical scheme, achieves maximum value for $z=H_{riser}$, thus confirming optimal riser height.

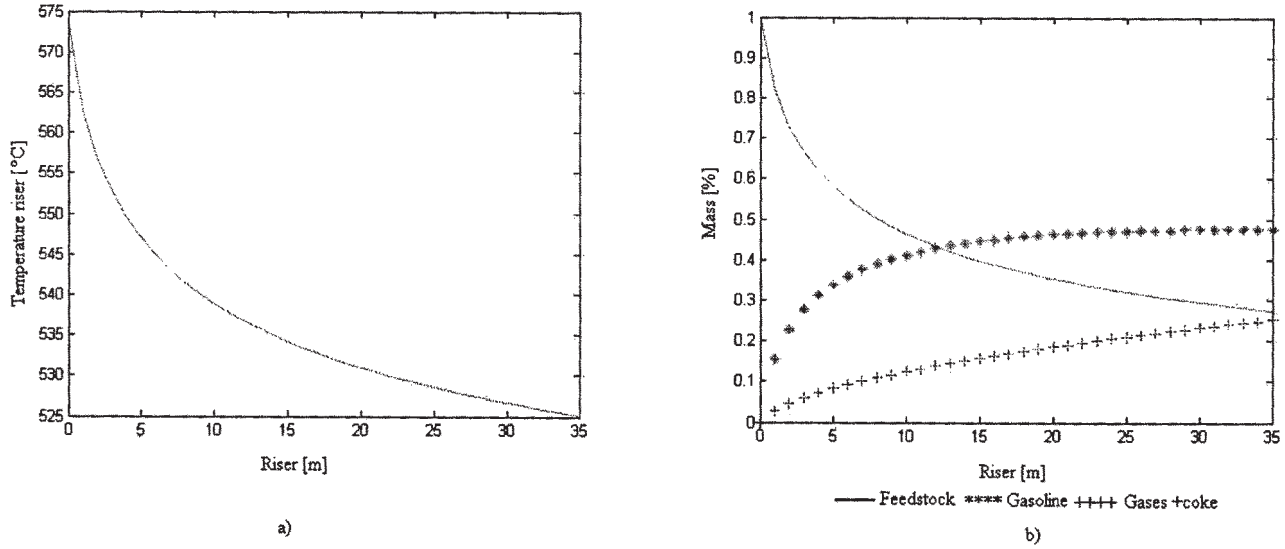

Fig. 5. Results of the riser simulation in a steady-state regime: a)temperature profile; b) profiles of the pseudo-components

From the point of view of the quantitative aspect, similar results are confirmed by the papers [16, 18,19]. Concluding there can be considered that the developed model reflects the real behaviour of the catalytic cracking process in steady state regime.

Mathematical modelling in a dynamic regime

The mathematical model in a dynamic regime of an industrial plant plays an important part in the study of the process dynamics and adjustment. The dynamic models allow for the evaluation of the performances of the adjustment algorithms of the different possible adjustment strategies, the determination of the optimum operation conditions. Nevertheless there has to be reminded that the dynamic model is used for the elaboration of dynamic simulators used for the operation staff training.

Based on the elements presented at the beginning of the article, the mathematical model in dynamic regime associated to the catalytic cracking process contains the model of the stripper sub-process and the model of the regenerator sub-process. The mathematical models of these two sub-process are based on the assumption that these sub-processes are systems with concerted parameters.

The mathematical model of the stripper sub-process

Due to the declared purpose use of the model in control, the model of the stripper sub-process, proposed by the author reflects the dynamics of the transport and propagation phenomena. The transport phenomenon refers to transport of the coke deposited on catalyst after the cracking reaction into stripper and the propagation phenomenon refers to the heat catalyst propagation from the base to the top of the stripper. It is important to underline that both phenomena are associated to transport delay.

First there is established the action frame, by formulating the simplifying hypotheses, that are used to the elaboration of the mathematical model in a dynamic regime associated to the stripper. The main simplifying assumptions used are:

-treating the stripper as a system with perfect mixing;

-the stock catalyst in the stripper is considered to be maintained constantly by a level control system;

-into the stripper there are not takeing place cracking reactions, consequently there may not take place coke deposits on the catalytic;

-the catalyst flow that enters into the stripper is equal to the catalyst flow that leaves the stripper.

Based on these assumptions, the mathematical model of the stripper sub-process consists of the associated model to the material balance of the coke deposited on the catalyst and the mathematical model associated to the heat balance.

These balances have been elaborated by the authors, using the laws of mass conservation and the law of energy conservation, that are applied on the contour around the stripper.

The law of mass conservation applied to the coke deposited on catalyst is under the form

.

$$M_s \cdot \frac{dC_{cocs2}}{dt} = Q_{cat2} C_{cocs1} - Q_{cat2} C_{cocs2} . \quad (21)$$

The law of energy conservation applied to the stripper sub-process leads to a differential equation under the form

.

$$M_s \cdot c_{p,cat} \cdot \frac{dT_s}{dt} = Q_{cat2} \cdot c_{p,cat} \cdot T_r - Q_{cat2} \cdot c_{p,cat} \cdot T_s \ . \quad (22)$$

The mathematical model of the regenerator

By hypothesis, the regenerator is considered a system with concentrated parameters, being assimilated to a vessel with perfect mixing. The chemical reaction of coke burning represents the central element of the mathematical model generating two differential equations: the material balance associated to the coke and the material balance associated to the oxygen [20]:

$$W_{cat,reg} \frac{dC_{cocs3}}{dt} = Q_{cat2} \ C_{cocs2} - Q_{cat1} \ C_{coc3} - R_{cb} ; \quad (23)$$

$$W_{aer,reg} \cdot \frac{dO_{reg}}{dt} = \frac{Q_{air}}{28.9}\left(0.2136 - O_{reg}\right) - \frac{R_{cb}\left(1+1.5\sigma\right)}{14\left(1+\sigma\right)} . \quad (24)$$

.

The heat balance associated to the catalyst dense bed is

$$W_{cat,reg} \frac{dT_{reg}}{dt} = Q_{cat2}\left(T_r + 273\right) + \left(T_{air} + 273\right) Q_{aer} \frac{c_{p,air}}{c_{p,cat}} - \quad (25)$$
$$- \left(Q_{cat1} + Q_{air} \frac{c_{p,air}}{c_{p,cat}} \right)\left(T_{reg} + 273\right) - \left(\Delta H_{CO} + \frac{\sigma}{1+\sigma} \Delta H_{CO_2} \right) \frac{R_{cb}}{14 \, c_{p,cat}} .$$

The program system for the simulation of the fluid catalytic cracking process

To properly implement the new structural approach there was necessary to use an adequate simulation environment, first allowing to describe a complex system by less complex modules, and secondly for providing the

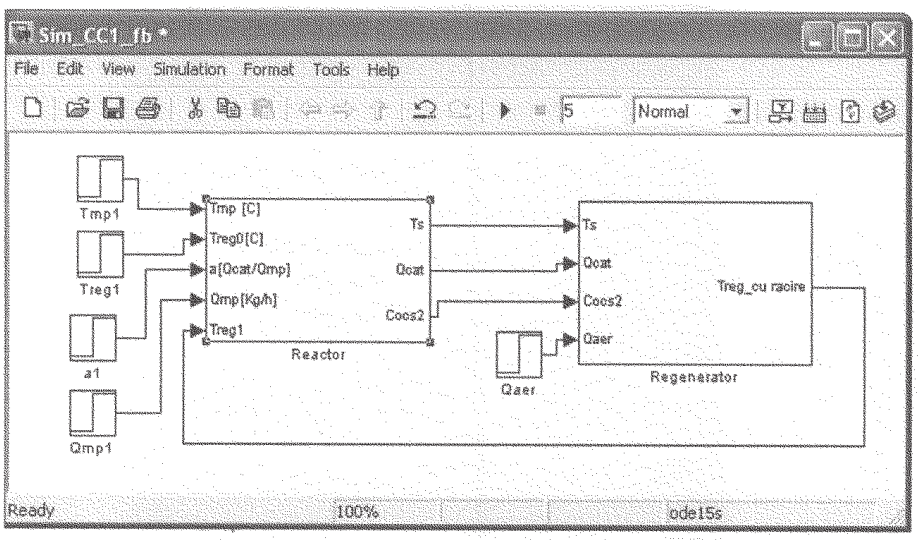

Fig. 6. The diagram of simulation of the fluid catalytic cracking process in a dynamic regime

user some numerical methods suitable for simulation. These requirements were satisfied with SIMULINK environment (the Matworks Company's product). The simulator developed by authors contains two modules associated to that reactor and regenerator, its image being presented in figure 6.

The section associated to the subsystems reactor is made up of four modules:

-*Cond_init* module, destined to the initialization of the operation static point;

-*Nod_amestec* module, a module that calculates the temperature in the interfusion node, relation (1);

-*Riser_model* module, destined to the solving of the differential equation system (17) that described the behavior of the riser sub-process. The integration of the differential system is realized with Runge-Kutta method. This allows for the display of the temperature profile in the riser and of the products yield along the riser;

-*Separator* module, a module that calculates based on the masic and the balance, the dynamic of the temperature and of the coke deposited on catalyst into the stripper.

-The regenerator module calculates based on the heat and material balance of the coke and oxygen, the regenerator temperature, the mass fraction of the residual coke and the oxygen quantity from the regenerator.

The simulator input/output variables of catalytic cracking simulator are shown in figure 7.

An example of dynamic simulator of the fluid catalytic cracking process is presented in figure 8. Raising the feedstock temperature with 20°C has as effect:

- the raise of the temperature in the interfusion node and of the temperature at the riser outlet, these two sub-processes being without inertion (fig. 8a-b);

- the raise of the temperaure at the stripper and mass fraction of the coke deposited on the catalyst in the stripper, the dynamics being of the order one, (fig. 8c-d);

- the raise of the temperature in the regenerator and the raise of the remaining coke quantity deposited on the catalyst, the dynamics being specifically to a system with inertion, (fig. 8e-f).

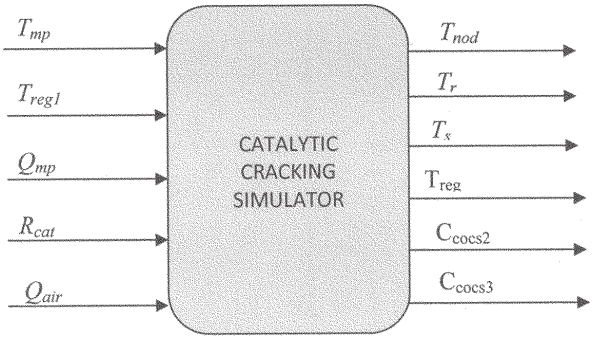

Fig. 7. The input and output of the catalytic cracking process simulator

Conclusions

In this paper there are treated aspects of modelling and simulating the fluid cracking catalytic process aiming at the elaboration of a hierarchical control structure associated to the cracking process. The main contributions brought by the authors within this paper are:

-the mathematical modelling of the fluid catalytic cracking process in a structural manner. This approach implies the decomposition of the whole process into sub-processes on topological and functional criteria;

-the structural approach attributes to the mathematical model robustness, clarity and the possibility of testing and/or modifying independently the mathematical models corresponding to sub processes, without affecting their assembly;

-the development of a simulator associated to the fluid catalytic cracking process, by using the simulation environment Simulink. This environment allowed for the elaboration of some program modules dedicated to sub-processes and the independent testing of sub-processes;

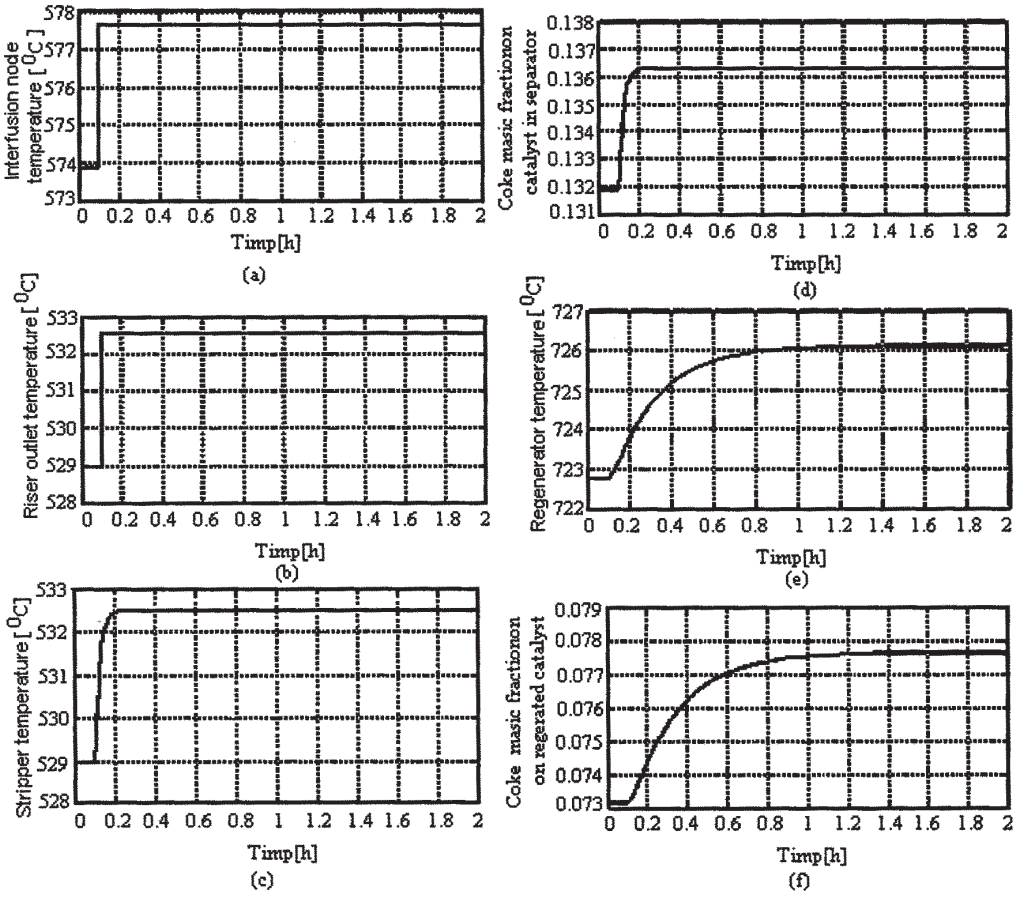

Fig. 8. Evolution in time of the output values associated to the reactor – regenerator system at the change of 10% of the feedstock temperature value: a) interfusion node temperature; b) riser outlet temperature; c) stripper temperature; d) coke quantity deposited on the catalyst after the cracking reaction; e) regenerator temperature; f) coke quantity deposited on the regenerated catalyst.

-an adaptation method of the mathematical model of the fluid catalytic cracking process has been elaborated. There has also been elaborated a multivariable objective function, used for the adaptation of the mathematical model to the plant experimental data.

-the simulation results, both in a dynamic and steady-state regime, have proved a typical behavior of the cracking process.

Nomenclature

a_{0j}, a_{1j}, a_{2j} - parameters associate to the equilibrium catalyst activity, j=2,3;
a_{dez} - the deactivation velocity constant [s^{-1}];
$c_{p,air}$ – heat capacity of the air [kcal/kg ^{0}C] ;
$c_{p,cat}$ – heat capacity of the catalyst [kcal/kg ^{0}C];
$c_{p,mp}$ – heat capacity of the feedstock especially of the component A [kcal/kg ^{0}C];
c_{cocs} – remaining coke content, [% m];
C_{cocs1} – coke masic fraction on catalyst after reaction cracking [% m];
C_{cocs2} – coke masic fraction on catalyst in separator [% m];
C_{cocs3} – coke masic fraction on regenerated catalyst [% m];
d - feedstock density [kg/m^3];
E_j - reaction activation energy [kcal/kmol];
H_{vap} - feedstock vaporization enthalpy [kcal/kg];
k_0^0, k_3^0 - reaction velocity constant associate to the reaction of transformation of the feedstock into gases and coke [s^{-1}];
k_1^0- reaction velocity constant associated to the reaction of transformation of feedstock into gasoline [s^{-1}];
k_2^0 - reaction velocity constant associated the conversion reaction of gasoline into gases and coke [s^{-1}];
l_{0j}, l_{1j}- kinetic parameters associate to velocity constant, j=0,1;
MAT - the equilibrium catalyst activity;
M_c - coke molecular fraction [kg/kmol];
M_s – holdup catalyst into striper [kg];
O_{in} – molar fraction of oxygen going into regenerator [kg/kmol];
r_1, r_2, r_3 - reaction velocity [kg_{produs}/kg_{produs} s];
R_{steam} - stripping steam ratio [kg];
R_{cat} – catalyst/feedstock contacting ratio;
R_{cb} – coke burning velocity [kg/s];
Q_{air} – air flow [kg/h];
Q_B – gasoline flow [kg/h];
Q_{cat1}- regenerated catalyst flow [kg/h];
Q_{cat2} – used catalyst flow [kg/h];
Q_{mp} – feedstock flow [kg/h];
s – sulphur concentration in feedstock;
t_c- contacting time [s];
T_0 – reference temperature for the equilibrium [^{0}C];
T_{air} – air temperature [^{o}C];
T_{nod} – temperature into the interfusion node [^{0}C];
T_{reg} –temperature of the regenerated catalyst [^{0}C];
T_r – riser outlet temperature [^{0}C];
T_{mp} feedstock temperature at inlet in the interfusion node [^{0}C];
T_{mv} – feedstock average boiling point [^{0}C];
T_s - stripper temperature [^{0}C];
U_V – riser vapors velocity [m/s];
Y – mass component concentration in the reaction [kg/kg_{vap}];
z – spatial coordinate associated to the riser [m];
$W_{cat,\ reg}$ – holdup catalyst in regenerator [kg];
$W_{cat,air}$ – air molar fraction retained in regenerator [Kmol];
σ - CO_2/CO ratio;
ΔH_{CO} – enthalpy of CO forming reactions [kcal/kg];
ΔH_{CO2} – CO_2 forming reactions enthalpy [kcal/kg];
ΔH_{r1} - reaction 1 enthalpy [kcal/kg];

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