UDC 66:65.015.13

MODELING AND OPTIMIZATION OF CHEMICAL-TECHNOLOGICAL COMPLEX FOR CRACKING AND PYROLYSIS GASES PROCESSING

A.R.Safarov

Acad. M.Nagiyev Institute of Catalysis and Inorganic Chemistry H.Javid Ave., 113, Baku AZ 1143, Azerbaijani Republic; e-mail: agil s@mail.ru

The paper deals with the results of the stage-by-stage method of optimal designing of chemical-technological complex for processing of cracking and pyrolysis gases. A scheme of chemical-technological complex has been worked out to designate all its input and output streams and establish inter-regional links between material recycling streams. On the basis of overall mathematical models involved in the process and balance equation, an economic-mathematical model of the complex has been developed and its optimization to thus identify optimal regimes of process accomplishment has been suggested.

Keywords: method, modeling, optimization, cracking, pyrolysis, profit rate.

At present, the volumes of production of hydrocarbon gases significantly exceed their share in the qualified use due to irrational use of hydrocarbon gases accompanied by their flaring; irretrievably lost valuable chemical raw materials; ever worsening environmental conditions in the areas of mining and processing of oil and gas. This situation is unacceptable, since the cracking gases contain significant amounts of olefins from which it is possible to produce valuable products, such as monomers, aldehydes, ketones, acids and esters, etc. widely applied in industry. These gases include almost all unsaturated hydrocarbons; however, percentage content of each of them is low, i.e. for petro-chemistry cracking gases valuable raw materials, true, with potential. Therefore, to meet needs in olefins petrochemical enterprises, gases of pyrolysis produced at EP-300 Sumgait plant "Ethylene-Polyethylene" (Azerbaijan) are applied. From the above it becomes clear that there is need in creating a large-scale production plant for joint processing of cracking and pyrolysis gases, because it is the complex production plants only that allow to fuller use various kinds of raw materials with lesser investments required for the establishment of high-capacity industry for production of a wide range of projected synthetic products. In this connection, it was suggested build new chemicalto a

technological complex (CTC) for joint processing of cracking and pyrolysis gases. The complex of this type would make it possible to fuller use cracking gases, burning of which is fraught with high economic and environmental losses and, even worse, additional use of pyrolysis gases to achieve a required capacity of the complex production of projected products in our Republic. The challenge may be formulated as follows: to develop a CTC for processing of cracking and pyrolysis gases which provides for required release of products for our Republic with minimum costs. To attain the goal, we have developed a method of designing such a complex based on successive steps as follows:

- 1. Statistical processing of industrial data in order to determine average component volumes of complex-forming cracking and pyrolysis gases.
- 2. Analysis and synthesis of the designed complex for processing of cracking and pyrolysis gases. A scheme of the complex, including new and existing processes for obtaining required projected products in our Republic, has been worked out of the basis of this elaboration.
- 3. Development of the overall kinetic models of all the processes in the complex formation and selection of

optimal types of reactors, the calculation of preliminary distribution of material recycling flows between reactors on their basis, as well as preliminary material balance of all the processes.

- Creation of mathematical model of the entire complex based solely on overall kinetic models of its reactor elements.
- 5. Identification of optimally coordinated material flows of the complex, provision of maximum performance on all projected products to comply with criteria of optimal local subsystems on the basis of the mathematical model.
- 6. Making of overall mathematical models of each process on the basis of preliminary results of the complex optimization.
- 7. Use of overall mathematical models of all subsystems and economic optimality criterion to ensure optimization of the whole complex and determine precise distribution of material and heat flows between reactor elements.

Note that the compliance with all the items of the proposed methodology would lead eventually to the optimally coordinated operation of the entire complex.

To resolve the problem of the complex synthesis, it is essential, first of all, to get informed about the total volume of gas in the complex, and for this purpose – to identify an average composition of appropriate gas multiply it into values component, production capacity of plants and thus establish the mass flow input into the complex. A statistical analysis of a great number of refinery data on gasoline pyrolysis from furnaces of Sumgait plant "Ethylene-Polyethylene" and on cracked gases from a combined catalytic cracking unit G-43-107M of the Heydar Aliyev Baku Oil Refinery has been carried out in order to identify an average component. Average component volumes of cracking and pyrolysis gases have been identified on the basis of an updated technique of statistical processing and a program designed to eliminate abnormal items of the

analysis [1,2]. Total volume of cracking and pyrolysis gases in the complex have been calculated to comply with the data above. That was the end of the first stage.

Priority-oriented products have been selected on the basis of market studies in the Republic, as well as the analysis of the input mass flow of overall cracking and pyrolysis gases. New and current processes have been mirrored in the scheme to produce these products (total 22). Practically, all the new processes involved in the complex have been developed at the M.F.Nagiyev Institute of Catalysis and Inorganic Chemistry at the laboratory "Catalysis on zeolites" based on high activity of ecologically pure zeolite catalysts. They have been developed in softer conditions (atmospheric pressure, low temperatures) with high conversion and selectivity conformably to a specific product in contrast to currently identical processes, often using aggressive catalytic substances at high pressures and temperatures.

According to the method of optimal designing (second stage), preliminary material balance of the complex has been calculated and the production capacity of the reactor elements identified for specific products in order to reaffirm correct direction for chemical synthesis of the projected products [3].

preliminary or stoichiometric calculation of mass balance, no awareness of kinetic characteristics is required, just values of conversions. At this stage of designing of the complex, types of raw materials and resources are to be identified. It is essential to estimate possible volumes of specific products and degrees of utilization of raw materials. Also, total material balance allows finding out if there is an excess of various chemical components in the complex which is available either as impurities in the final products, or form byproducts after their separation. Results of the analysis show the feasibility of further continuation of the development of this embodiment of the projected complex, or the necessity to move to a new one.

Calculation of chemical complex by the suggested method is based on integrative, deterministic approach, where the rate of everyone involved in the process has been

expressed to comply with basic laws of chemical kinetics. Therefore, well-proven kinetic models for all 22 processes as known from the literature have been selected. It has to be kept in mind that kinetic models have been developed at the M. F. Nagiyev Institute of Catalysis and Inorganic Chemistry to be used in the new processes. At this stage, an optimal type of reactors designed in structural dimensions has been selected for new processes on the basis of their kinetic equations. Also, theoretical optimization has been provided at this stage of each process to identify optimum technological regimes as follows:

$$\max_{k} \{T, v, C_0, \theta, \tau\}_k,$$
 (1)

where Q_k – performance of k-th reactor; T – temperature; V – volume speed; C_0 – initial concentration of the reactant; θ – molar ratio of the initial reactants entering into the reactor; τ – contact time. Naturally, specific limitations are imposed on control parameters in view of each process.

Some of CTC-involved processes occur in the reactor and regenerator system. When adjusted for mutual influence of the reactor and regenerator components, the reactor-regenerator unit has to be considered as simple system in these processes when designing the mathematical model.

In optimizing these mathematical model-based processes, authors suggested the following criteria of optimization:

$$\max \overline{\overline{Q}} = \left\{ T_{G,0}^{(1)}, G_{CC}, \tau, t_R, \nu, B, \overline{C}_i, T_R \right\}, (2)$$

where B – fuel gas consumption in the regenerator; \overline{Q} – capacity of the reactor for a specific product per unit time in the cycle; $T_{G.0}^{(1)}$ – temperature of gas and catalyst in the reactor; T_R – temperature in the regenerator; t_R – regeneration time; G_{cc} – amount of circulating catalyst.

Having determined optimal conditions for process implementation and their appropriate maximum performance for projected products, researchers recalculated its industrial input quantities of reagents. Thus, proceeding from theoretical optimization of kinetic models of the processes considered

individually, researchers established an input and output amounts of the reactants and products of each element of the reactor. That was the end of the third stage.

Calculations presented at the third stage of the theoretical optimization have been performed for individual reactor elements which are not dependent upon each other and their interaction is taken into no account. It is transfer of projected products and issues related to byproducts that remain to be within the chemical-technological system. One of the main objectives in the design of the complex was to create a closed, non-waste technology that takes system principles into consideration. Thus, the method suggested at the fourth stage embraced the development of a mathematical model of CTC on the basis of kinetic equations of the processes that considered into account the constraint equations between all elements of the reactor.

Mathematical model of CTC consists of three parts: 1) a set of mathematical models of individual reactor elements (at this stage. just kinetic models); 2) the system of equations on the structure of technological links of CTC – functional constraints (equations and inequalities); 3) the system of restrictions on the values of certain parameters and variables elements of CTC – positional restrictions.

The mathematical model of each k-th element of CTC can be written as follows:

$$\begin{split} \overline{Y}^{(k)} &= \overline{F}^{(k)} \big(\overline{X}^{(k)}, U^{(k)} \big); \quad k = \overline{1, N}. \quad (3) \\ \text{where} \quad \overline{Y}^{(k)} &= \big(y_1^{(k)}, ..., y_m^{(k)} \big); \quad \overline{X}^{(k)} &= \big(x_1^{(k)}, ..., x_n^{(k)} \big); \\ \overline{U}^{(k)} &= \big(u_1^{(k)}, ..., u_r^{(k)} \big); \quad n \big(m \big) \quad - \text{ the dimension of the input (output) variables; } r \quad - \text{ the dimension of the vector of control variables; } N \quad - \text{ number of elements of the CTC.} \end{split}$$

Vectors of variables $\overline{Y}^{(k)}$ and $\overline{X}^{(k)}$ are in line with parameters of the input and output vectors of the technological streams of the k-th element, and the vector of control variables. Note that $\overline{U}^{(k)}$ includes structural and technological parameters of CTC's elements, changes of which may affect the functioning of the k-th element. In this regard, it is necessary to have mathematical models of all reactor elements provided by its scheme to create a mathematical model of the entire

CTC. Hence, building of mathematical model plays a large role in the whole complex of works on optimization of CTC.

To describe CTC, it is essential to specify functions of the branches (constraint equations between elements) of the complex, which are designed to characterize changes in individual parameters during the transition from one reactor element to another:

$$\overline{X}_{k} = A\overline{Y}_{k-1} \tag{4}$$

Limits imposed on CTC's parameters can be presented as boundary conditions for functioning of each process unit of CTC, i.e. in the form of inequality constraints imposed on the parameters of terms of feasibility and production safety. These limits indicate the range of the input, output and control parameters for each reactor element of CTC and are specified as:

$$X_{k,min} \le X_k \le X_{k,max}$$

$$U_{k,min} \le U_k \le U_{k,max}$$

$$Y_{k,min} \le Y_k \le Y_{k,max}$$
(5)

Issues related to transforming byproducts into appropriate processes have been resolved at this stage (fourth stage) with the purpose of determining the constraint equations and creating the closed technology. So, through sending byproducts to suitable areas, we have been successful in developing a closed technological structure of CTC (Fig. 1).

As a result, a mathematical model of the CTC has been elaborated on the basis of all kinetic models of the involved processes and balance equations of the material flows for their further optimization.

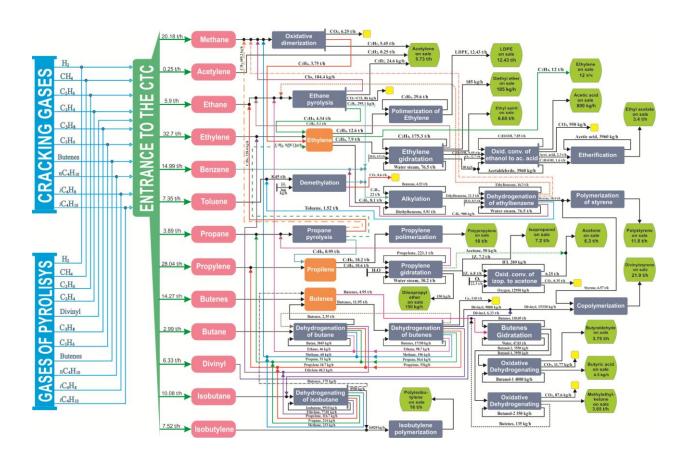


Fig. 1. Scheme of CTC.

Thereafter, its optimization is made at the fifth stage. This stage is characterized by optimization of the complex on the basis of a mathematical model of CTC using overall kinetic models of processes. The goal of optimization is to choose operating modes of processes that could provide maximum productivity of all reactor elements of CTC:

$$\sum_{k=1}^{22} Q_k \to \max \tag{6}$$

Data obtained from theoretical optimization at the stage (3) are to be used as initial values for identification of optimal modes on the mathematical model (3) with due regard for restrictions (5) and optimization criterion (6). Note that the use of the method of multivariate analysis of Rosenbroke [4] made it possible to identify optimum modes of processes to ensure the maximum performance

of all reactor elements.

Naturally, the data obtained at the fifth stage can not be accepted as definitive because appropriate calculations were carried out for isothermal conditions. As is known, temperature gradients and pressure differences are typical for processes in industrial reactors. The factors mentioned above essentially affect the rates of reactions and thus predetermine operations of reactor elements. Therefore, overall mathematical models have been developed at the sixth stage for each reactor element of CTC and on their basis an overall mathematical model of the complex has been created.

Below-cited are mathematical models of the main types of processes involved in the CTC. Thus, a model for reactors with fixed bed catalyst in general is as follows:

$$D_{E}\left(\frac{\partial^{2}C_{i}}{\partial R^{2}} + \frac{1}{R}\frac{\partial C_{i}}{\partial R}\right) - q\frac{\partial g_{i}}{\partial l} + \sum_{j=1}^{m} v_{ij}r_{j}(\bar{c}_{i}, T) = 0$$

$$\alpha_{E}\left(\frac{\partial^{2}T}{\partial R^{2}} + \frac{1}{R}\frac{\partial T}{\partial R}\right) - qC_{p}\frac{\partial T}{\partial l} + \sum_{j=1}^{m} Q_{j}r_{j}(\bar{c}_{i}, T) = 0$$
(7)

where D_E – coefficient of effective diffusion; R – radial coordinate; g – mass concentration; v_{ij} – stoichiometric coefficient of i-th substance in j-th reaction; q – rate of mass flow; r_j – rate of j-th reaction; α_E – effective thermal conductivity of the layer; Q_j – the thermal effect of j-th reaction.

As for processes taking place in the reactor-regenerator unit with fluidized catalyst circulating between them, authors used a cell model. During a model projecting, it was supposed that the reactor consists of a separate

two-zone cell (pseudo section) connected in parallel together with overall mixing of the gas in the zone of dense phase and the piston flow in the zone of bubbles. In addition, each cell is noted for gas exchange between the bubble and dense phases. It is assumed that no particles or least of them are found in the bubbles, so chemical conversion mainly occurs in the dense phase.

The equations describing the process in the n-th reactor cell at a distance z from the grating for i-th component of the bubble phase can be formulated as follows:

$$Q(1-q)\frac{dC_{_{B}}^{^{i}}}{dz} = -\frac{Q_{_{M}}^{^{i}}}{H}(C_{_{B}}^{^{i}} - C_{_{H,n}}^{^{i}}), \tag{8}$$

material balance for the dense phase

$$Qq(C_{H,(n-1)}^{i} - C_{H,n}^{i}) = Q_{M}\Delta H_{n}C_{H,n}^{i} - Q_{M}\Delta H_{n}\frac{1}{H_{n} - H_{n-1}}\int_{(n-1)H}^{nH} (z)dz + \frac{G_{k}^{(1)}}{N}\sum(r_{\infty})_{j}^{i}$$
(9)

total concentration of the i-th component in the output from the n-th cell

$$C_n^i = (1 - q)C_{B.D.} + qC_{H.D.},$$
 (10)

heat balance equation

$$C_{P.K} \cdot G_{IIK} \left(T_{k,n+1}^{(1)} - T_{k,n}^{(1)} \right) = N_0 C_{P.F} \left(T_{k,n}^{(1)} - T_{k,n-1}^{(1)} \right) + \sum_{i=1}^k N_{0,i} \left(\alpha_n^i - \alpha_{n-1}^i \right)_j Q_{P,j} + Q_{nor} \Delta H_i$$
(11)

$$C_{P.K} \cdot G_{IJK} \left(T_{k,n+1}^{(1)} - T_{k,n}^{(1)} \right) = a \hbar \left(T_{k,n}^{(1)} - T_{\Gamma,n}^{(1)} \right), \tag{12}$$

with boundary conditions:

$$C_{H,0}^{i} = C_{B}^{i} = C_{0}^{i}; T_{k0}^{(1)} = T_{km}^{(2)}$$
 (13)

Here Q – volume rate; q – share of gas passing through a continuous phase; Q_M^i – rate of interphase exchange; C_B^i μ C_n^i – concentration of i-th component in the bubble and dense phase; H – height of the fluidized bed; N – number of cells; $C_{P.K}$ μ $C_{P.\Gamma}$ – heat capacity of catalyst and gas; $Q_{P,j}$ – heat effect of j-th reaction; α^i – conversion of i-th component; $T_k^{(i)}$ μ $T_\Gamma^{(i)}$ – gas and catalyst temperature in reactor; N_0 – mole rate of initial raw material; \hbar – coefficient of heat transfer; a – surface of interphase per unit volume.

Similarly, equations describing the process in m-th cell of regenerator have been worked out.

It should also be noted that no economic estimates have been taken into account when optimizing the fifth stage. So the rated optimal conditions of the processes and, hence, consumption of energy resources for obtaining maximum benefits from the complex may result in essential growth of costs for final products. Therefore, there has been developed an economic and mathematical model of the complex at the seventh final stage, and an economic criterion adopted with due regard for the profit rate, which meant the profit ratio received from sales of finished products to overall costs of their production:

$$H_{n} = \frac{\sum_{i \in I_{np}^{k}} c_{i} g_{i}^{k} - \sum_{k=1}^{22} \left(\sum_{i \in I_{k}^{k}} c_{i} g_{i0} + S \right)}{\sum_{k=1}^{22} \left(\sum_{i \in I_{k}^{k}} c_{i} g_{i0} + S \right)} \cdot 100\%$$
 (14)

 $\sum_{i \in I_{np}^{\kappa}} c_i g_i^{\kappa} \ - \ revenues \ from \ sales \ of \ finished$

products; $\sum_{i \in I_i^*} c_i g_{i0} - \text{raw material-related costs}$;

S – overall production costs for the entire complex.

The task of global optimal design of CTC could be stated as follows: on the basis of the method to determine such optimal matching between the reactor elements as material, heat and recycled streams with due regard for products of adverse reactions (in order to create a closed technological scheme), which would correspond to the optimum value of economic criteria.

To solve a problem of global optimization, there has been used a method of dynamic programming [5]. As a whole, the basic principle of dynamic programming for k-th reactor element can be expressed by following equation:

$$f_k(C_{k+1}) = [P_k + f_{k-1}(C_k)]_{max},$$
 (15)

where $f_k(C_{k+1})$ – maximum value of criterion function in the inlet of reactors sequence; P_k – increment of selected criterion function as a result of k-th reactor element effect; $f_{k-1}(C_k)$ – maximum value of criterion function for the (k-1)-th reactor element sequence depending on the state of vector stream in the output from the k-th reactor.

Table 1 shows the results of the global optimization of CTC – optimal operating modes per each process of the suggested CTC, performance values (Q_i) for projected products and their heat powers (Q_i) .

Table 1. Results of global optimization of CTC based on economic criteria

1	Oxidative	$T^{I}=815^{\circ}C$, $T^{II}=710^{\circ}C$. Volume rate -19000 h^{-1} . Conversion -69.9 . Yield
	dimerization of methane.	of acetylene – 23.5%, ethylene – 17.5%, carbon monoxide – 2.1%, carbon dioxide – 26.8%. Q_1 =8.5 t/h. Q_1 =68728 kW.
2	Pyrolysis of ethane.	Temperature in the reaction zone – 845°C, inlet pressure – 0.5 MPa, the weight ratio of water steam: ethane – 1.5:1. Conversion of ethane – 40.12%. Yield of ethylene – 32%, methane – 1.3% acetylene – 0.15%, propane – 0.45%, propylene – 0.8%, divinyl – 0.9%, butane – 0.5%, butene – 0.3%, benzole – 2.35%, carbon monoxide – 0.25%, carbon dioxide – 0.32%, hydrogen – 0.8%. Q ₂ =3.8 t/h. Q ₂ =5160 kW.
3	Polymerization of ethylene.	Total conversion of ethylene – 95%; volume concentration of oxygen – 0.003%; pressure – 230 MPa; temperature – 320°C. Q ₃ =12 t/h. Q ₃ =12976 kW.
4	Direct hydration of ethylene.	Temperature -300° C, total pressure -8.3 MPa. Molar ratio water steam: ethylene $-0.9:1$; conversion of ethylene -4.395% . Yield of ethanol -4.1% , diethyl ether -0.15% , acetaldehyde -0.06% , ethane -0.045% , polymers -0.04% . $Q_4=11.5$ t/h. $Q_4=3166$ kW.
5	Oxidative conversion of ethanol to acetic acid.	Temperature -225^{0} C, pressure $-$ atmospheric, molar ratio of oxygen to ethyl alcohol -2.7 . Conversion of ethyl alcohol -26.5% ; $A_{\text{CH}_3\text{COOH}} = 13\%$; $A_{\text{CH}_3\text{CHO}} = 10\%$; $A_{\text{CH}_3\text{COOC}_2\text{H}_5} = 0.3\%$; $A_{\text{CO}_2} = 3.2\%$. $Q_5 = 3.05$ t/h. $Q_5 = 21661$ kW.
6	Esterification of acetic acid with ethyl alcohol.	Temperature – 190^{0} C; molar ratio of acetic acid to ethyl alcohol – 2.6. Conversion of acetic acid – 38%. Yield of ethyl acetate – 43%. Q ₆ =3.3 t/h. Q ₆ =42 kW.
7	Hydrodemethyla- tion of toluene.	Volume rate – 2200 h ⁻¹ ; temperature – 840 K; molar ratio toluene: water steam – 1:5. Conversion of toluene – 49.6%. Yield of benzene – 39%, by carbon monoxide and carbon dioxide – 6.4%, methane – 1.4%, xylols – 3.8%. Q ₇ =5.01 t/h. Q ₇ =756 kW.
8	Alkylation of benzol with ethylene.	Temperature – 120°C; pressure – 0.6 MPa; molar ratio benzol to ethylene – 2:1; space velocity – 2200 h ⁻¹ ; conversion of ethylene – 94%; conversion of benzene to ethylbenzene – 24%, in diethylbenzene – 4.01%. Q ₈ =19 t/h. Q ₈ =5278 kW.
9	Dehydrogenation of ethylbenzene.	Temperature – 740°C; pressure – 0.05 MPa; weight ratio of water steam: ethylbenzene – 2.5:1. Conversion of ethylbenzene – 42.45%. Yield of styrene – 35.6%, toluene – 3.5%, benzene – 2.7%, methane – 0.3%, ethane – 0.35%. Q ₉ =16.02 t/h. Q ₉ =5006 kW.
10	Polymerization of styrene.	Temperature – 100° C. Conversion – 93%. Ratio of monomer: water – 1:1.3. Q_{10} =11.1 t/h. Q_{10} =2208 kW.
11	Dehydrogenation of propane.	Temperature – 900 K, pressure (P_0) – 0.5 MPa. Ratio of water steam:raw – 1.5:1. Overall conversion of propylene and ethylene – 66.52%. Yield of propylene – 21%; ethylene – 29%, methane – 10.02%, ethane – 3.9%, butylenes – 1.65%, hydrogen – 0.95%. Q_{11} =1.01 t/h. Q_{11} =835 kW.
12	Polymerization of propylene.	Pressure – 13 atm; temperature – 85°C. Volume ratio propylene:solvent – 2:1. Conversion – 96%. Q ₁₂ =17.5 t/h. Q ₁₂ =9794 kW.

13	Direct hydration of propylene.	Pressure -37 atm; temperature -200° C. Volume rate -1800 h^{-1} . Propylene conversion per pass -4.429% at the optimum mole aspect ratio $H_2O:C_3H_6=0.3:1$. Yield of isopropyl alcohol -5.4% , disopropyl ether -0.34% , polymer -0.03% , acetone -0.006% , propane -0.003% . $Q_{13}=13.8 \text{ t/h}$. $Q_{13}=4691 \text{ kW}$.
14	Oxidative conversion of isopropyl alcohol to acetone.	Volume rate – 2100 h ⁻¹ ; temperature – 185 ^o C. Conversion of alcohol – 87.2%. Yield of acetone – 83%; carbon dioxide – 4.2%. Q ₁₄ =6.1 t/h. Q ₁₄ =5373.1 kW.
15	Dehydrogenation of butane to butylene.	Temperature -585° C. Conversion of butane -41.08% . Yield of butylene -34.5% ; butadiene -3.3% ; methane -0.75% ; ethane -0.55% ; ethylene -0.5% ; propane -0.47% ; propylene -0.76% ; carbon -0.25% . $Q_{15}=2.1$ t/h. $Q_{15}=1364.6$ kW.
16	Dehydrogenation of butene to divinyl.	Temperature -640° C. Ratio of water steam:raw $-16:1$. Conversion -40.45% . Yield of divinyl -31% , butane -3.1% , isobutane -2.1% , carbon dioxide -1.8% , isobutylene -1.3% , methane -0.45% , ethane -0.3% , propane -0.3% , propylene -0.1% . $Q_{16}=8.7$ t/h. $Q_{16}=5325.6$ kW.
17	Copolymerization of styrene and butadiene.	Copolymerization temperature – 8°C; pressure – 4·10 ⁵ Pa; mass ratio butadiene: styrene – 7:3. Conversion of monomers in the copolymer – 96%. Q ₁₇ =20.5 t/h. Q ₁₇ =2523 kW.
18	Hydration of butenes to 1- butanol and 2- butanol.	Temperature -180° C. Pressure -42 atm. Molar ratio water steam:raw $-0.4:1$; volume speed -1950 h ⁻¹ . Conversion of butene -3.9% . Yield of butanol-1 and butanol-2 -3.8% , butyl ether -0.1% ; butanal output -0.05% ; butane -0.015% ; polymers -0.025% . $Q_{18}=7.2$ t/h. $Q_{18}=1550$ kW.
19	Oxidative conversion of 1-butanol in butyraldehyde.	Temperature – 215°C. Volume rate – 1800 h ⁻¹ . Conversion – 46.24%. Yield of aldehyde yield – 46%, oleic acid – 0.065%, carbon dioxide – 0.18%. Q ₁₉ =3.5 t/h. Q ₁₉ =2320 kW.
20	Oxidative conversion of 2-butanol to methylethylketone.	Temperature -300° C. Volume rate -2200 h^{-1} . Conversion -85.2% . Yield of methylethylketone -82.5% , butylenes -1.6% , carbon dioxide -1.1% . $Q_{20}=3.4 \text{ t/h}$. $Q_{20}=2455 \text{ kW}$.
21	The dehydrogenation of isobutane to isobutylene.	Temperature -600° C. Volume rate -270 h^{-1} . Conversion -39.75% . Yield of isobutylene -36% , methane -1.05 , propane -1.15 , propylene -0.45 , ethylene -0.35 , butylenes -0.75 . Q_{21} =8.1 t/h. Q_{21} =4821.4 kW.
22	Polymerization of isobutylene.	In liquid ethylene at -105°C. Yield of polyisobutylene – 97%. Mass ratio of isobutylene:ethylene – 1:1.15. Q ₂₂ =15.8 t/h. Q ₂₂ =3276 kW.

Rate of profit for all projected products was 21.71%.

REFERENCES

- 1. Aliyev A.M., Safarov A.R., I.I.Osmanova, Aliyev F.V. Method of statistical processing of the oil-refinery data. *Azerb. Himich. Jurnal Azerbaijan Chemical Journal*. 2013 no 2, pp.44-54.
- 2. Aliyev A.M., Safarov A.R., Aliyev F.V., Aliyeva X.A. //Method of obtaining an average values of the component-wise composition of cracking-gas. *Azerb. Himich. Jurnal. Azerbaijan Chemical Journal.* 2013, no.3, pp.9-15.

- 3. Aliyev A.M., Safarov A.R., Guseynova A.M. Calculation of preliminary material balance of chemical-technological complex for processing of cracking and pyrolysis gases. *Himicheskaya promishlennoct segodnya Chemical Industry today*. Moscow, 2016, no. 3, p. 16–28. (In Russian).
- 4. Panteleyev A.V., Letova T.A.

 Metodi optimizasiyi v primerax i
 zadachax. Uchebnoye posobiye. M.
 Lan Publ., 2015, 512 p. (In
 Russian).
- 5. Lew A., Mauch H. Dynamic Programming. A Computational Tool. Springer, 2007, 378 p.

KREKİNQ VƏ PİROLİZ QAZLARININ EMALININ KİMYA-TEXNOLOJİ KOMPLEKSİNİN MODELLƏŞDİRİLMƏSİ VƏ OPTİMALLAŞDIRILMASI

A.R.Səfərov

Akademik M.F.Nağıyev adına Kataliz və Qeyri Üzvi Kimya İnstitutu AZ 1143, Bakı, H.Cavid pr., 113; e-mail: agil_s@mail.ru

Məqalədə krekinq və piroliz qazlarının emalının kimya-texnoloji komleksinin optimal layihələşdirilməsi metodunun yerinə yetirilmiş mərhələlərinin nəticələri göstərilib. Kimya-texnoloji komleksin bütöv giriş və çıxış axınlarını və həmçinin regionlar arasında material və resirkulyasiya axınlarını göstərməklə onun texnoloji sxemi tərtib edilib. Kompleksə daxil olan proseslərin tam riyazi modelləri və material axınlarının balans tənlikləri əsasında riyazi-iqtisadi modeli yaradılıb və onun qlobal optimallaşdırılması aparılıb. Bunun nəticəsində proseslərin optimal iş rejimləri təyin olunub.

Açar sözlər: metod, modelləşdirmə, optimallaşdırma, krekinq, piroliz, mənfəət dərəcəsi.

МОДЕЛИРОВАНИЕ И ОПТИМИЗАЦИЯ ХИМИКО-ТЕХНОЛОГИЧЕСКОГО КОМПЛЕКСА ПО ПЕРЕРАБОТКЕ ГАЗОВ КРЕКИНГА И ПИРОЛИЗА

А.Р.Сафаров

Институт Катализа и Неорганической Химии им. акад. М.Нагиева AZ 1143 Баку, пр.Г.Джавида, 113; e-mail: agil_s@mail.ru

В статье приведены результаты выполненных этапов метода оптимального проектирования химико-технологического комплекса по переработке газов крекинга и пиролиза. Разработана схема химико-технологического комплекса с обозначением всех его входных и выходных потоков, а также с установлением связей материальных и рециркуляционных потоков между регионами. На основе полных математических моделей участвующих процессов и балансовых уравнений материальных потоков разработана экономико-математическая модель предлагаемого комплекса и проведена её оптимизация, в результате которой определены оптимальные режимы ведения процессов.

Ключевые слова: метод, моделирование, оптимизация, крекинг, пиролиз, норма прибыли.

Поступила в редакцию 05.10.2016.