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OPTIMAL CONTROL OF THE ALKYLATION PROCESS REACTORS

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Abstract: *Recent studies show that one of the most important issues of static optimization of structurally complex non-stationary technological processes is the development of appropriate methods for problem decomposition. The issue of optimization of non-stationary alkylation processes and ways to solve the problems arising in this regard has been investigated in this paper. It is known that there are several ways to increase economic efficiency of control systems for petrochemical technological processes. It includes checking of instruments and regulators, identify improvements in the control and monitor of performance, etc. One of the main ways to increase the efficiency of control systems for technological processes which depend on current conditions is to develop models and algorithms that allowing control these processes in more optimal modes compared to current ones. In this regard, the presented article is relevant as it is dedicated to the development of optimal control algorithms for multistage petrochemical technological processes consisting of series-connected non-stationary technological devices.*

Keywords*: optimal control, alkylation process, optimization problem, constraint.*

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1. Introduction

Most of the catalytic processes in the chemical, petrochemical and oil refining industries refer to the number of non-stationary complex and multi-stage processes. The decomposition approach is mainly used for optimal management of non-stationary processes, taking into account the size of the problem (Dolganova et al., 2012; Ivanchina et al., 2021). On the other hand, the requirement to satisfy the conditions of convexity imposed on the objective function and on the limiting conditions for solving the problem leads to a number of difficulties. The need to take into account the specifics of the processes of reaction and rectification in decomposition approaches is also associated with a number of difficulties (Dolganova et al., 2014; Dolganova et al., 2012).

The optimization is a way to find the best of possible solutions. Generally, optimization is the task of finding the extremum (minimum or maximum) of the objective function in bounded interval limited by a set of linear and/or non-linear equalities and/or inequalities.

Set of refinery and petrochemical processes are carried out in the presence of ideal mixing or stationary catalyst. A distinctive feature of catalytic processes of this class from other processes is that the activity of the catalyst used in the reaction process decreases as a result of the action of the mixtures formed during the reaction. In addition, since the main factor influencing the course of catalytic processes is the activity of the catalyst, it is necessary to control the process of reducing its activity during the technological process. Models and algorithms for solving optimization problem in reactor-regenerator, which is considered one of the main technological devices of modern petrochemical industry, were developed in (Frantsina et al., 2014; Ivanchina et al., 2016).

In recent years, scientific works have been carried out on the optimal design of technological processes in various industries in the absence of sufficient initial information. These studies show that when using classical approaches in designing optimal schemes of technological processes, it is not always possible to obtain effective results for some parameters, such as the absence of sensors capable of measuring the reaction rate, heat transfer and other parameters. Taking into account these features, methods and algorithms for solving optimal design problems were developed in (Pronzato, Wynn, & Zhigljavsky, 2009).

In general, when designing control systems for technological processes in the petrochemical industry, special attention should be paid to the development of optimal control algorithms (Hale et al., 2016). At present, L.S. Pontryagin's principle of maximization and R. Bellman's dynamic programming methods, which are considered to be the mathematical basis of optimal control theory, are used in the design of control systems of non-stationary petrochemical technological processes, as well as in technical systems (Pereira & Sousa, 2009). In recent years, very interesting scientific results have been obtained in both scientific and applied areas of optimal management of non-stationary technological processes (Boscain & Piccoli, 2005; Boscain, Sigalotti, & Sugny, 2021; Lawrence, 2010).

Therefore, one of the main ways to improve the control of complex non-stationary technological processes is the effective development of control algorithms. In addition, optimal control of complex process systems requires a holistic approach to the system in order to establish coordination between its various objects. These conditions allow to determine the formulation of this problem and the properties of the corresponding optimal control algorithms.

Taking all this into account, in order to solve the problems of optimal control in technological system of multi-stage process of obtaining alkyl gasoline by sulfuric acid alkylation an algorithm based on L.S.Pontryagin's modified principle of maximization independently from the above shortcomings has been developed. In this paper we propose an approach that, unlike previous works, allows us to overcome the above difficulties without additional complications of Pontryagin's principle of maximization, including the modified Hamilton function to the problem. Thus, by introducing special additives (Boscain & Piccoli, 2005; Boscain et al., 2021; Hale et al., 2016) it is possible to reduce the problem of convex programming.

A comparative assessment of the proposed decompositional approach and the direct method show that in the first case, the time to solve this problem is reduced almost twice. In addition, this approach makes it possible to take into account all necessary specific features of reaction and rectification apparatuses. By introducing special additives, the solution of the problem can lead to a convex programming problem, which significantly simplifies the solution of the optimal control problem for continuous multistage systems.

2. Materials and Methods

2.1. Description of the investigated technological process

To solve the problem of controlling the alkylation process, it was studied as the research object.

The reaction block of sulfuric acid alkylation is intended for the production of a high-octane component of gasoline. The raw material for the reactors is butane - butylene fraction of *BBF*. Sulfuric acid is also fed into the reactor as a catalyst. When BBF interacts with concentrated sulfuric acid, aviation alkylates, motorized alkylate and process reaction gases are obtained, which, in a single stream through acid and alkaline sedimentation tanks, enter the distillation compartment for separation.

The initial concentration of sulfuric acid fed into the alkylation reactor is typically 98%. After 2-3 days, the concentration of sulfuric acid decreases to 83% due to its dilution with water and organic impurities released during the reaction, dissolved in acid.

When the catalyst activity decreases to 83%, it is not fed into the reaction zone. The rate of decrease in the activity of the catalyst depends on the regime parameters of the reaction process. In particular, an increase in the temperature in the reactor creates conditions for the formation of acid-soluble compounds, which causes a decrease in the activity and selectivity of the catalyst.

The main purpose of the research is to develop mathematical models and control algorithms that provide optimal control of non-stationary technological processes for the production of alkyl gasoline by sulfuric acid alkylation.

2.2. Formatting of Mathematical Components

The process of reactor optimization will be considered on the time interval, where in general case *T* is variable, and in some cases, it is a given fixed moment of final stage of the control process. In this case, the control functions are limited

$$u_q(t)\in U,\ q=\overline{1,m},\ 0<t<T \tag{1}$$

where u_q is a control vector of the object *q*, *U* is a given closed bounded area in m - dimensional space. To maximize objective function the control $u_q \in U$ should be selected for all time in the range of $t \in [0, T]$.. Objective function can be expressed as follows:

$$J_1=\int_0^T x_1(u, x_0, f_\gamma)dt, \tag{2}$$

Satisfying functional constraints:

$$J_i=\int_0^T x_1(u, x_0, f_\gamma)dt, \leq A\ t/h\ (i=2,3,\ldots,l) \tag{3}$$

here *J* is the yield of the target product for the time interval *T*; J_i is the output of the *i*-th by-product *(i=2,3, ...)*; $X_0(T)$- are the catalyst activities at the end of the process *T.* In other cases, final condition $X_0(T)=X_0T$ can be more stringent and have the form

$$g[x_0(T)]=0, \tag{4}$$

where *T* is a fixed moment in time; g is an unknown function.

2.3. Solving Optimization Problem

Suppose that the mathematical model has the form [11]:

$$\frac{dx_0^I}{dt}=f^I(u_q^I, x_s^I, X_0, \xi^I, t), \tag{5}$$

$$f_i^I(u_q^I, x_s^I, X_0, \xi^I)=0,\ q=\overline{1,m};\ s=\overline{1,l};\ i=\overline{1,n} \tag{6}$$

$$f_i^{II}(x_s^{II}, u_q^{II}, \xi^{II})=0,\quad i=\overline{1,n} \tag{7}$$

$$f_i^{III}(x_s^{III}, u_q^{III}, \xi^{III})=0,\quad i=\overline{1,n} \tag{8}$$

$$f_i^k(x_s^k, u_q^k, \xi^k)=0,\quad i=\overline{1,n} \tag{9}$$

here, the differential equations describe the state of the reactors, and the final equations describe the quantitative relationship between the output and mode variables of the stages (upper indices are the stage numbers).

To solve the problem (1) - (4) the principle of maximization is applied. Pontryagin's principle of maximization is used in optimal control theory to find the best possible control for taking a dynamical system from one state to another, especially in the presence of constraints for the state or input controls.

To solve the problem numerically, the following conversion simplifications were introduced.

The mathematical model of the reactor, describing the quantitative relationship between the outputs and the regime parameters, is in the form of:

$$x_1=-21{,}5607+0{,}5485U_1+0{,}1456U_2+0{,}742U_3+0{,}2388X_0(t)$$
$$-0{,}242\gamma-0{,}0024U_1^2-0{,}00159U_2X_0(t)-$$
$$-0{,}00844U_3X_0(t)+0{,}0157\gamma^2 \tag{10}$$
$$x_2=-11{,}6827-0{,}2576U_1+0{,}000256U_2+0{,}0336U_3-0{,}2174X_0(t)$$
$$-0{,}0972\gamma+0{,}0028U_1X_0(t)-$$

$-0,0045U_3\gamma+0,00094X_0^2(t)+0,002028X_0(t)$

where x_1, x_2 are the outputs of alkyl benzene and motoalkylate, respectively; U_2 is the flow rate of *BBF* (raw materials) into the reactor; γ is the qualitative indicator of *BBF* (the ratio of the amount of isobutane to the amount of unsaturated hydrocarbons); X_0 is the activity of sulfuric acid.

$$dx_0/dt= -[0,392-0,0132U_1+0,00074U_2-0,0108U_3+0,0152\mu +0,00059U_1U_2+0,00086U_1U_3+0,0004U_1\mu+ +0,0000628U_2U_3-0,000744U_2\mu+0,0173U_3\mu-0,00132U_1^2- 0,000109U_2^2-0,000648U_3^2-0,0011\mu^2]\, X_0^2(t)/X_0(0)Q. \quad (11)$$

The development of optimal control of the considered process consists in determining such equations and from the range:

$$5\ m/h \le u_1(t) \le 15\ m/h;\quad 30\ m/h \le u_2(t) \le 65\ m/h;\quad 10°C \le u_3(t) \le 19°C \quad (12)$$

and the completion time of the process *T,* which satisfies the maximum to the functional:

$$J_1=\int_0^T x_1(t)dt \quad (13)$$

and the constraint $x_2 \le 0,45$ m/hour for solving equations (10), (11). In this case, $x_0(0)=98\%$, $x_0(T)=83\%$. It is required to find the control $u_q^1(t)$ ⍰ U^1 $(0 \le t \le T)$ from (12), which should satisfy the maximum to the functional (13) and the solution of equation (11).

Differential equation (11) is transformed into the form [12]:

$$dx_0/dt=a_1u_1^2x_0^2+a_2u_2^2x_0^2+a_3u_3^2x_0^2-a_4u_1^2x_0^2+a_5u_1u_3x_0^2-a_6u_1u_3x_0^2- a_7u_1x_0^2+a_8u_2x_0^2-a_9u_3x_0^2+a_{10}x_0^2 \quad (14)$$

$a_1=\alpha_6\times r$; $a_7=(\alpha_2+\alpha_9\gamma)r$; $a_2=\alpha_{10}\times r$; $a_8=(\alpha_3-\alpha_{12}\gamma)r$;
$a_{13}=\alpha_{13}\times r_1$; $a_9=(\alpha_4-\alpha_{14}\gamma)r$; $a_4=\alpha_7\times r$; $a_{10}=(\alpha_1-\alpha_5\gamma+\alpha_{12})r$;
$a_4=\alpha_7\times r$; $a_5=\alpha_8\times r$; $r=1/X_0(0)\times Q$; $Q=100T$; $a_4=\alpha_7\times r$,

where $\alpha_1, \alpha_2,..., \alpha_{15}$ are the corresponding coefficients of the differential equation;

(13) the functionality is presented as
$x_1(x_0, u, f\gamma)=b_1u_1^2-b_2u_1+b_3u_2+b_4u_3+b_5$
$b_1=\beta_1$; $b_2=\beta_2$; $b_3=\beta_5x_0-\beta_3$; $b_4=\beta_6x_0-\beta_4$; (15)
$b_5=-\beta_7x_0-\beta_8\gamma^2+\beta_9\gamma+\beta_{10}$,
the restriction to the functionality is written as
$x_2(t) \le d_1u_1-d_2u_2+d_3u_3+d_4 \le 0,45$ T/hour,
$d_1=\beta_1$; $d_2=\delta_3$; $d_1=\delta_7x_0-\delta_2$; $d_3=\delta_4-\delta_8\gamma$, (16)
$d_4=\delta_9x_0^2+\delta_{10}\gamma x_0-\delta_8x_0+\delta_6\gamma+\delta_{10}$.

Substituting (14) and (10) into (16), we get modified Hamiltonian function [12]:

$$H\big(x_0, u, f_\gamma, t=c_1u_1^2+c_2u_2^2+c_3u_3^2-c_4u_1u_2+c_5u_1u_3x_0^2-c_6u_2u_3-c_7u_1+c_8u_2+c_9u_3+c_{10}\big)$$

where
$c_1=a_1x_0^2\psi_1+b_1\psi_0$ $c_6=-a_6x_0^2\psi_1$
$c_2=a_2x_0^2\psi_1$ $c_7=a_1x_0^2\psi_1-b_2\psi_0$
$c_3=a_3x_0^2\psi_1$ $c_8=a_8x_0^2\psi_1+b_1\psi_0$ (17)

$c_4=-a_4x_0^2\psi_1$ $\quad\quad$ $c_9=-a_9x_0^2\psi_1+b_4\psi_0$

$c_5=a_5x_0^2\psi_1$ $\quad\quad$ $c_{10}=a_{10}x_0^2\psi_1+b_5\psi_0$

Based on the proposed algorithm, optimal values of *u1(t), u2(t), u3(t)* from the permissible range (12) were found for various values of disturbances satisfying a maximum (14). Thus, by introducing special additives (17), problem (1)-(4) can be reduced to a convex programming problem, which greatly simplifies the solution of the optimal control problem for continuous multistage systems.

It is proposed to solve the optimization problem in two ways:

a) fixed point in time *T*
b) with changing times (see table 1)

Figure 1 illustrates the trajectories of optimal controls for a fixed time point of completion of the process T=72 hours. Figure illustrates the changing trajectories *U1*, *U2*, *U3* under normal control.

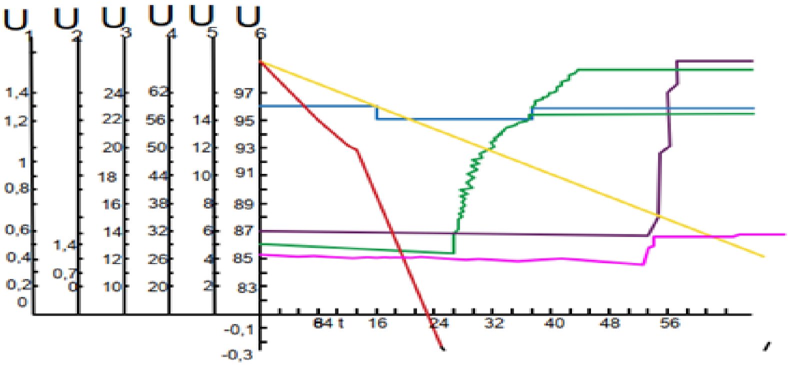

Figure 1. Trajectories of optimal controls at a fixed moment of completion of the alkylation process

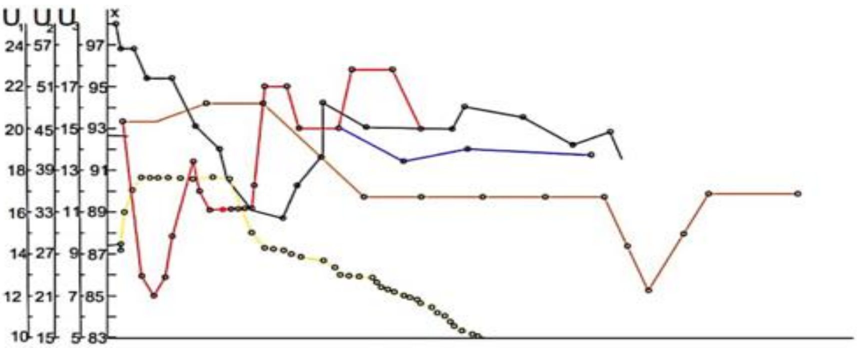

Figure 2. Trajectories of change $u_1(t)$, $u_2(t)$, $u_3(t)$ under normal control (Source: compiled by the authors)

3. Results

Table 1 shows the construction results of optimal control of the reaction process of sulfuric acid alkylation production at different values of the raw material composition.

On the basis of the proposed algorithm, at different values of disturbance $-X_0(T)$ (catalyst activities), optimal values *of* $U_1(t)$ (consumption of raw material), $U_2(t)$ (consumption of catalyst), $U_3(t)$ (temperature in the reactor) from the permissible range (12) were found satisfying a maximum (2). In the table the activity of the catalyst and the output of alkyl benzene at different values of the composition of the raw material during one cycle- T are presented.

Table 1. Results of optimal control of the reaction process of sulfuric acid alkylation production at different values of the raw material composition

	With free right end			With a fixed right end		
The ratio isobutane to unsaturated hydrocarb	Cycle Duration *T* (hour)	Activity catalyst at the end cycle *(X/T)*, %	The yield of alkyl benzene during one cycle,	Cycle Duration *T* (hour)	Activity catalyst at the end of Cycle *(X/T)*, %	The output of alkyl benzene during
4	72	85.4	188	92	83	243
5	72	85	281	90.5	83	249
6	72	84	175	89.5	83	254
7	72	84.7	172	87.5	83	213
8	72	84.6	172	86	83	208
9	72	84	172	85	83	200
10	72	85.3	172	86	83	215
11	72	84.2	183	83	83	215

(Source: compiled by the authors)

4. Discussion and Conclusion

4.1 Discussion

In the presented paper, mathematical formalization and solution of a physically based optimal control problem are considered, taking into account the real dynamics of external material flows of a technological facility that carries out the alkylation process. External material flow in technological processes refers to the dynamics of changes in raw materials and their quality indicators. The obtained about the operating parameters of technological processes is always somewhat different from its real value. The main reason for this is errors in the transmitter of primary information, the converter, communication channels and, finally, in the algorithms for processing information in the measuring circuit. This shows that, due to the above reasons, mathematical models of any class, built on the basis of primary information, will always have certain errors. On the other hand, since the parameters specific to the input flows in the facility have a wide range of variation, mathematical models and algorithms that can take this feature into account should be developed in order to conduct the reaction process in the reactor in optimal modes in each current situation.

As a result of the research of this apparatus, it was found that it operates under the influence of internal and external disturbances, quantitative and qualitative indicators of raw materials, changing in a wide range, which directly affect the work of the technological process. The practical significance of this study is the solution of the problem in the condition that is mentioned above. As a result, the solution of the problem, indicators are obtained that provide the required quality of the alkylation process.

The above mathematical statement of optimal control problem of technological systems in which devices are connected in series and the current state of methods for solving the optimization problem give us reason to express several considerations on this matter. As it is known, even with a smaller dimension of the original problem and sufficiently large N stages, the solution of the mathematical programming problem makes it an extremely difficult circumstance so that when solving the optimal control problem based on the discrete maximum principle, at each step it becomes necessary to solve the multiextremal problem. The above difficulties are exacerbated by the fact that with an increase in the number of stages, the number of local extrema also increases (Dolganova et al., 2012; Ivanchina et al., 2021).

The possibility of using the non-linear programming methods to solve only large-scale problems was studied by a number of authors (Dolganova et al., 2014). The conclusion reached by these authors is that using the method makes it possible to decompose large mathematical problems into small-sized problems that are easy to solve, but the results of solving these problems, that are not mathematically complex, do not allow determining the optimal mode of the system operation as a whole. Hence, we can conclude that the best indicator of the used methods is the mathematical size of the optimization problem being solved (Lawrence, 2010; Pronzato et al., 2009). The problem of mathematical size in the optimization problems to be solved creates problems in terms of the operability of the solution even on modern computers.

4.2 Implications

The experience of operating the optimal control systems of alkylation technological processes showed that the lack of information on the course of processes in many cases reduces their efficiency and productivity. On the other hand, the change in a wide range of quality indicators and consumption of raw materials for processing makes their efficiency even more unsatisfactory . In some cases, this is due to the nonlinear and non-stationary dynamic characteristics of these systems.

İn order to solve the problem of optimal control of reactors of the alkylation process, taking into account the specific features and characteristics of the process. is used the modified method of the maximum principle. The solving the optimization problems proposed in two ways:

a) fixed point in time T

b) with changing times (see table 1)

Based on the proposed algorithm, optimal values of $u_1(t)$, $u_2(t)$, $u_3(t)$ from the permissible range were found for various values of disturbances satisfying a maximum a yield of alkyl-benzene .

Figure 1. shows the trajectories of optimal controls at a fixed time point for the completion of the alkylation process T = 72 hours. Figure 2. shows the trajectories of $u_1(t)$, $u_2(t)$, $u_3(t)$ under normal control. A comparative analysis of the optimal and conventional controls shows that in the first case the yield of the target product - alkyl-benzene can be increased by 2.5% and the consumption of sulfuric acid can be reduced by 5%, also the time for solving this problem is almost halved.

In the second variant of solving the reactor optimization problem, $u_{1opt}(t)$, $u_{2opt}(t)$,

$u_{3opt}(t)$ and T were also determined, which at $x_0(T)=83\%$ are satisfied by max J_1.

4.3 Conclusion

On the basis of the modified method of the maximum principle at different values of the composition of raw material, the activity of the catalyst, optimal values of the output of alkyl benzene have been determined, which are shown in table 1. As a result of a comparative analysis, it was determined that the successful solution of the optimization problem makes it possible to increase the amount of target product - alkyl gasoline by 2.5% and reduce the consumption of sulfuric acid by 5%. A comparative assessment of the proposed decomposition approach to this problem shows that the time for solving this problem is almost halved. In addition, this approach makes it possible to take into account all necessary specific features of reaction and distillation apparatus.

The results obtained in the paper allow us to design an optimal control system to ensure the production of output coordinates with minimal energy costs during the control of technological devices of this class. This type of control algorithms can be useful for flexible control systems.

4.4 Limitation and Future Research Recommendation

There are some limitations to this study. It can be considered more appropriate to use the control algorithms proposed in this research work in multistage petrochemical, oil refining technological processes consisting of non-stationary technological devices connected in series. The features of such technological processes are that the series-connected technological apparatuses operate in modes that differ from each other in the degree of regulation and in the absence of information about the intermediate states of the system.

Based on this, the methods and algorithms applied in the research work can be used in the development of optimal control systems of multi-stage, non-stationary technological complexes with a complex structure, more precisely, in solving the issue of optimization at the upper level of this system. The obtained optimal parameters can be used as set-point for control systems of these processes.

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