Optimization of group oil refineries on the example of production of alkyl gasoline regarding technological process of sulphuric acid alkylation

R A Khakimov and N S Shcherbo

Department of Magistracy and Elite Education, Omsk state technical university, 11, Mira avenue, 11, Omsk, Russia

E-mail: scherbonsch88omsk@gmail.com

Abstract. The article describes the task of optimizing the process of sulfuric acid alkylation as part of a group of plants for the production of alkyl benzine. The main methods and approaches to solving this problem from the point of view of real-time optimization (RTO) are presented. A modified method is proposed in the form of a multi-model approach and decomposition of the original optimization problem into local ones with a sequential solution. To test the method, an analytical model of the sulfuric acid alkylation process was used, its evaluation was carried out and the problem of maximizing alkyl benzine was solved using the Hook – Jeeves algorithm in Matlab. The results of the solution were compared with the real historical data of the process and confirmed the operability of the solution.

1. Introduction

In case of the difficult technological productions multiple by quantity and quality of raw materials, intermediate products, final products, global optimization of technological processes of group of the installations entering production chains can bring considerable economic effect. Each installation has the technological modes characteristic with maximum efficiency, however, can differ from the required planned modes. Therefore, when calculating loadings of units and optimum selections it is necessary to distribute streams so that each installation worked with the minimum deviation from the planned mode and considered efficiency of the technological mode. It is a problem of optimization of technological processes of a production chain in real time. In practice there are various definitions for this task: refinery-wide optimization [1], multi-unit optimization [2] and also real-time optimization [3]. In this article for the solution of problems of optimization of the technological regime of group of installations the term Real-time optimization (RTO) will be used.

The majority of algorithms and approaches were created in the 60-70th years of last century. So, for example, in work [4] optimization methods (the classical analysis, calculus of variations, the principle of a maximum, dynamic, linear and nonlinear programming) in the plane of their applicability to objects of chemical technology are stated. In addition, authors formulate the basic provisions concerning the choice of criteria by optimization of chemical and technological processes and also give the mathematical models describing the main technological processes (the reactor of ideal mixture, ideal replacement, mass-exchanged processes). In recent years actively the direction of dynamic optimization of the technological modes of chains of installations or DRTO (Dynamic RTO) allowing to solve a problem of optimization not only in steady state but also for transition processes develops. The
complexity and labor input of work with the bulky DRTO models received as a result of parametrization induced some researchers to look for options of use of nonlinear kinetic models of the reactor with linear dynamic communications. These models are used in MRS controllers for connection of the MPC and RTO levels in a whole [5]. In turn DRTO can be divided into the following types: OL-DRTO (Open-Loop DRTO), approach in which only the trajectory of management is calculated on the basis of DRTO, without transfer of restrictions and target settings on execution on the lower level, and CL-DRTO (Closed-Loop DRTO) in which transition from OL-RTO to full feedback control is carried out. Let's consider optimization of group of oil refineries on the example of production of alkylgasoline.

2. Problem definition

Main objective of work is the solution of a problem of optimization group of installations on the example of production on release of a component of commodity gasoline – alkylgasoline. Alkylgasoline has high octane number (96 by a research method), does not contain benzene, is not toxic, is the final product of installation of sulphuric acid alkylation and an important component of a compounding of commodity gasolines. Production of alkylgasoline covers group of installations (figure 1): catalytic cracking, alkylation, gasfractionation.

From the mathematical point of view of RTO is a multidimensional problem of nonlinear programming taking into account restrictions in the form of linear and nonlinear equalities and inequalities.

Criterion function for optimization in real time usually represents economic model of process which is usually limited to the influencing variables, and does not consider constant expenses, such as labor, overhead costs, etc.

Typical criterion function looks as follows:

$$F = P - Q_c - Q_p + C$$

where $F$ – criterion function; $P$ – products cost; $Q_c$ – costs of raw materials; $Q_p$ – costs of installation service; $C$ – other variables of economic effect.

Input parameters for the solution of a task of RTO are: plan for development of products, restrictions on quality, technological restrictions and restrictions on amount of raw materials, economic restrictions (domestic prices of model of optimizing planning). Results of the solution of a task of RTO are: the optimum technological modes (loadings of installations, selections, a technological framework on process and quality products) for separate installations. RTO usually represents a system which cornerstone the nonlinear model of production which allows to calculate optimum target tasks,
restrictions for parameters of separate installations is. As a target task of RTO usually serves the function minimizing the cost of production or maximizing profit taking into account the technological restrictions following from the steady material and power balances of processes, physical restrictions of the equipment.

For achievement of a goal of optimization of group of units for production of alkylgasoline it is necessary to solve the following number of problems:

- Definition of methods of the solution of a problem of optimization of group of installations.
- The choice of restrictions and the influencing factors.
- Modeling of technological process of alkylation.
- Assessment of adequacy of model.
- The solution of a problem of optimization on the example of maximizing alkylgasoline regarding technological process of alkylation.
- Assessment of results of the decision.

3. Theory
The general principles and also specific practical objectives are formulated in work [6]. In this work the fundamental moments of the theory of RTO are considered and examples according to the solution of the simplest practical tasks for petrochemical industries by means of RTO technology are given.

On the basis of the analysis of sources [7-12] the following methods of the solution of a task of RTO were allocated.

*Classical method on the basis of strict models, RTO generation 1.* The classical way of solving the task of RTO, surely includes the following elements: the analysis algorithms of steady state of process, algorithms of filtration and data processing, algorithms of assessment of parameters of model, stationary mathematical model of technological process describing everything technological blocks (columns, the reactor, etc.), and algorithms of optimization of criterion function arrived (figure 3). Pluses of this method is that the developed decision is already approved, the principles and approaches mostly are studied and presented in the majority of scientific works, also at the market ready decisions are presented in the software form. In addition, authors noted that the solution of problems of optimization can be reached for considerable periods or at all be absent because of use of strict models on the basis of the static modes.

*Method with use of technology MPC, RTO generation 2.* Pluses of this method are that for the account MPC application, at the solution of a problem of optimization is considered dynamics of an object and the non-stationary modes and also robustness of a system due to updating of the forecast at each stage of calculation is provided what the fact of existence of scientific works and the description of the received practical results testifies to. However, when using this approach, it is necessary to work carefully the strategy of management, to carry out a set of step-by-step tests for creation of models and periodically to calibrate them. The main minus which can will come to light during operation of a system, the fact that it does not describe all possible borders of the technological modes is

*Data-driven method, RTO generation 3.* A positive aspect of this method is that all minuses of strict analytical models are leveled, but it is also minus of the method as the accuracy of models directly depends on quality and the number of statistical data. Also there is a risk of loss of adequacy in a question of work of model and, as a result, reproduction only of those situations which participated during creation of a system.

As an optimization method within this work it is offered to use classical approach, but to modify it due to multimodel approach (in a classical method one global model describing all technological processes is used) decomposition of an initial global problem of optimization and the iterative consecutive decision.

We will consider the scheme of interrelation between separate stages of process of sulphuric acid alkylation (figure 2) in more detail.
**Figure 2.** The scheme of interrelation between separate stages of process of alkylation.

In table 1 the description of technological process of alkylation is given (with the indication of subprocesses).

| Table 1. Alkylation process stages |
|-----------------------------------|
| **Subprocess Stage** | **Input stream** | **Output stream** |
| Block reactor | Butane-butylene fraction, isobutane recycling, freshisobutane | Alkylate, isobutane recycling, acid, alkylsulfates |
| Cooling block | Isobutane, propane, N-butane | Isobutane, propane, N-butane |
| The block of acid cleaning | Alkylate, i-butane recycling, acid | Alkylate, isobutanerecycling, acid |
| The block of alkaline cleaning | Alkylate, i-butane recycling, acid traces, alkali, water | Alkylate, isobutanerecycling, acid |
| Block of division of products of reaction | Alkylate, replenishing isobutane | Alkylate, isobutane recycling, N-butane |

For process of sulphuric acid alkylation factors and restrictions are:

- Raw materials dilution by isobutane fraction. On alkylation installation a ratio isobutane: an olefin it is equal to the relation of total volume of isobutane in the integrated raw materials from a coagulator of raw materials circulating coolant from a flash drum to the volume of olefins in the integrated raw materials from a raw materials coagulator. As a rule, higher ratios isobutane: the olefin is provided by higher quality of alkylate and lower consumption of acid. Minimum volume ratio isobutane: the olefin is 7.5: 1. This number will allow to avoid an overload of plates, the reboiler and a condenser of a column-deisobutanizer.

- Volume speed of reaction. Volume feed rate of olefins is defined as the relation of volume of the olefins loaded in the reactor in an hour to the volume of the sulfuric acid which is in reactors. At a consumption of the total olefin raw materials arriving on installation of alkylation at the level of 80.8 m3/h the volume feed rate of olefins makes 0.371 Parts-1 that allows to carry out norms on alkylate.

- Temperature in a reaction zone. Temperature of reaction has to be from 4 °C to 13 °C. If temperature of reaction falls below plus 4 °C, then upholding of acid and hydrocarbons happens worse,
leading to the fact that hydrocarbons at the exit from the reactor entrain acid. At a temperature plus is lower 2 °C sulfuric acid stiffens that causes increase in power consumption at its hashing and interferes with formation of an emulsion of necessary quality.

Concentration of sulfuric acid. For alkylation of fractions of C4 hydrocarbons usually use the sulfuric acid containing (90 ÷ 98) % of monohydrate. At increase in concentration of sulfuric acid the alkylate octane number (anti-detonation characteristics) increases.

Mix saturation in the reactor. Saturation of hydrocarbon mix in contactors is defined by a difference between raw materials pressure in the reactor and forcing of blades of the mixer. Differential pressure is in limits (0.5 ÷ 0.8) kgs/cm² (0.05 ÷ 0.078 MPa).

4. Results of an experiment
In figure 3 the dependence of an exit of alkylgasoline on a BBF raw materials consumption on installation is presented. Increase in a consumption of raw materials appears positive influence on an alkyl gasoline consumption.

![Figure 3. Dependence of an exit of alkylate on BBF.](image)

In figure 4 the dependence of an exit of alkylgasoline on a BBF raw materials consumption and also replenishment isobutane is presented to the reactor block. Considering the factors presented earlier increase in alkylgasoline is also influenced by increase in a consumption of recirculating isobutane, however strengthening coefficient at the same time is lower than at a BBF raw materials consumption.

![Figure 4. Dependence of an exit of alkyl gasoline on an expense BBF and Circus. isobutane on installation.](image)
As the mathematical model describing technological process of alkylation the results presented in work [13] were used.

Modeling of process of alkylation which proved adequacy of model is carried out. At increase in a consumption of coolant there is an increase in an exit of alkylate (figure 6). It is caused by the fact that the frequency rate isobutane increases: olefins temperature in the reactor also decreases that reduces course of collateral reactions of polymerization.

![Graph showing dependence of alkylate on combined raw materials consumption.](image)

**Figure 5.** Dependence of a consumption of alkylate on a consumption of the combined raw materials.

Comparison of exits (not displaced assessment) with real technological data was made for assessment of accuracy of model, the schedule is presented in figure 7.

![Graphs comparing model and real data for MON, RON, and alkylate.]  

**Figure 6.** Schedule of comparison of exits of model and these technological processes.
For assessment of quality of model, it is used statistical metrics, namely:

- RMSE.
- Correlation coefficient.
- The given mistake.

Assessment of accuracy of model is presented in table 2. The model has high precision in comparison with real to data (coefficient of correlation higher than 85% at low the given mistake) that allows to use it for the solution of a problem of optimization.

| Parameter                      | Mistake | Correlation Coefficient | The Given Mistake |
|--------------------------------|---------|-------------------------|-------------------|
| RON Alkylate prepack           | 0.56    | 0.87                    | 1%                |
| MON Alkylate prepack           | 0.56    | 0.89                    | 1%                |
| Consumption of alkylate        | 2.95    | 0.92                    | 4%                |

Let's consider results of the solution of a problem of maximizing alkyl gasoline with application of a method of Hooke-Jeeves in the environment of Matlab. As basic data and restrictions the following parameters presented in table 3 were used. Also results of calculation are presented in the table 3.

| Parameter                              | Unit of measurement | Lower bound | Upper bound | Optimum value |
|----------------------------------------|---------------------|-------------|-------------|---------------|
| RON Alkylate prepack                   | item                | 95          | -           | 95.78         |
| MON Alkylate prepack                   | item                | 92          | -           | 92.29         |
| Consumption of alkylate                | Tn/h                | -           | 12          | 47.59         |
| Temperature in a zone of reaction      | °C                  | -5          | 12          | 1.58          |
| A consumption of the circulating isobutane | m³/h              | 115         | 125         | 121           |
| Consumption of isobutane of coolant    | m³/h                | 20          | 30          | 25            |
| Consumption of BBF raw materials      | Tn/h                | 40          | 40          | 40            |
| Pressure in reactionary zone           | MPa                 | 0.434       | 0.434       | 0.434         |
| Consumption of replenishment isobutane | Tn/h                | 0           | 10          | 8             |
| Main tenance of olefins               | %                   | 30          | 50          | 50            |

Calculation results were checked with the similar periods of operation of the process unit which confirmed adequacy of calculations. In addition, calculations for optimum conducting technological process in real time which increase an alkyl gasoline exit at increase in make-up isobutane and the maintenance of olefins in raw materials were carried out. Further an investigation phase is the analysis of a possibility of realization of these actions on installations of catalytic cracking and gas fractionation by means of creation of mathematical models and the subsequent iterative solution of an algorithm of optimization.
5. Conclusions

The solution of a task of RTO generally consists in the solution of a problem of finding of a minimum/maximum of criterion function at observance of all restrictions in the form of inequalities (definition of area in which search of the decision is run) and equalities (the material, power balances, etc.). The basis of criterion function is made by models of the objects entering RTO task perimeter.

Within work methods for the solution of a problem of optimization of group of units for production of alkylgasoline regarding process of sulphuric acid alkylation are analyzed. The modified method in the form of multimodel approach and decomposition of an initial problem of optimization on local with the consecutive decision was chosen. Various approaches will allow to define optimality of methods in terms of the accuracy of models and the field of their application. Application of various approaches will allow to use diverse models of columns depending on requirements to time and an error of calculations of the solution of problems of optimization.

For process of sulphuric acid alkylation the influencing factors and restrictions are shown, the mathematical model which has high precision (coefficient of correlation higher than 85% at low the given mistake) is made. Model tests confirmed adequacy of model in terms of fundamental knowledge of process.

Calculations of an optimizing task of obtaining the maximum quantity of alkyl gasoline with application of a method of Hooke-Jeeves in the environment of Matlab are carried out. Results of the decision were compared to real static data of technological process of alkylation and confirmed the adequacy.

As a result of a research objectives were reached. Further an investigation phase is creations of mathematical models of catalytic cracking and gas fractionation for the subsequent iterative solution of an algorithm of optimization.

References

[1] Hao Z, Yiping F, Xiaoyang D and Gang R 2014 Integration Optimization of Production and Utility System for Refinery-wide Planning IFAC Proceedings Volumes 47(3) 9599-604
[2] Woodward L, Perrier M and Srinivasan B 2009 Improved performance in the multi-unit optimization method with non-identical units Journal of Process Control 19(2) 205-15
[3] Kadam, J, Schlegel M, Marquardt W, Bosgra O, Dunnebier A, Tiagounov A and Brouwer P 2003 Towards integrated dynamic real-time optimization and control of industrial processes In Proc
[4] Boyarinov A and Kafarov V 1969 Optimization methods in chemical technology Chemistry 564
[5] Darby M 2011 RTO: An overview and assessment of current practice J Process Control 21 874-84
[6] Sigurd S 2008 Chemical and Energy Process Engineering *CRC Press Taylor & Francis* 395-413
[7] Qin S and Badgwell A 2003 A survey of industrial model predictive control technology *Control EngPract* **11** 733-64
[8] Kadam J and Marquardt W 2007 Integration of economical optimization and control for intentionally transient process operation *Lecture Notes in Control and Information Sciences* 419-34
[9] Engel S 2007 Feedback control for optimal process operation. *J Process Control* **17**(3) 203-19
[10] Ying C and Joseph B 1999 Performance and stability analysis of LP-MPC and QP-MPC cascade control systems *AIChE Journal* **45**(7) 1521-34
[11] Goldberg D 1989 Genetic Algorithms in Search. Optimization and Machine Learning *Addison-Wesley*
[12] Ivashkina E, Ivanchina E, Nurmakanova A, Boychenko S, Ushakov A and Dolganova I 2016 Mathematical Modeling Sulfuric Acid Catalyzed Alkylation of Isobutane with Olefins *Procedia Engineering* **152** 81-6