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SOLVING THE PROBLEM OF MULTI-CRITERIA OPTIMIZATION OF THE SYNTHESIS REACTION OF BENZYLALKYL ESTERS BY THE METHOD OF «IDEAL» POINT AND LEXICOGRAPHIC ORDERING*

K.F. Koledina[1], A.A. Alexandrova[2]

[1] Institute of Petrochemistry and Catalysis of RAS, Ufa, Russian Federation
[2] Ufa State Petroleum Technological University, Ufa, Russian Federation

✉ nastena1425@gmail.com, koledinakamila@mail.ru

The result obtained in the course of solving optimization problems is relevant for use in industrial and laboratory processes. Multi-criteria optimization involves optimizing two or more conflicting objective functions.

Materials and methods. On the basis of the kinetic model of the catalytic reaction of the synthesis of benzylalkyl esters, the task of multi-criteria optimization is set taking into account the variable parameters: temperature, molar ratio of reagents and the time of carrying out, which have limitations. The use of the methods of «ideal» point and lexicographic ordering is justified.

Results. An algorithm for solving the multi-criteria optimization problem has been developed. Using the kinetic model of the synthesis of benzylalkyl esters, the problem of MKO of the conditions of conducting was solved and optimal values of the variable parameters of the system were obtained, at which the output of the target product was maximized and the by-products of the chemical process were minimized.

Discussion and conclusions. Multi-criteria optimization of this process will make it possible to give technological recommendations for the industrial implementation of the process with maximum output of target products and minimum content of by-products. The paper presents two methods for solving the problem, since in order to apply the results obtained in practice, the recommendations of the decision-maker must be taken into account.

Keywords: multi-criteria optimization, nonlinear programming problem, Pareto front, kinetic model, molar ratios of initial reagents, «ideal» point method, lexicographic ordering.

Introduction. Real optimization tasks include several target criteria that conflict with each other. When researching chemical production, problems arise with maximizing the output of the target product, minimizing the output of the by-product and increasing productivity or profit. The mathematical formulation of such a problem defines the task of multi-criteria optimization (MCO).

To solve the problem of multi-criteria optimization, it is necessary to determine the parameters according to which the optimal value of the variable parameters of the reaction will be found. It is necessary to understand that the final result of process optimization depends on the choice of the method of solving the MCO problem and the importance of the objective functions that are maximized (minimized) during the process.

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The object of the study is the catalytic reaction of the synthesis of benzylalkyl esters, namely benzylbutyl ether. The catalytic reaction of the synthesis of benzylalkyl esters occurs by intermolecular dehydration of benzyl and n-butyl alcohols with the formation of three esters: target benzylbutyl and side dibenzyl, dibutyl. The kinetic model of the catalytic reaction of the synthesis of benzylalkyl esters is presented in [1]. The model represents a system of differential equations. The initial conditions are determined, as well as the permissible range of changes in the optimal values of temperature, reaction time and molar ratio of reagents. These data do not allow for a strong change in the values of the optimality criteria. For the MKO problem, the methods of solution are selected and justified, and the analysis of the results obtained is carried out.

2. Materials and methods. The result of solving optimization problems is the search for the extremum (minimum or maximum) of the objective function. The objective function is a real and integer function of several variables characterizing certain parameters (price, weight, efficiency, profit, etc.) under certain constraints.

Let the continuous function $f(x)$ be the objective function, $h_1(x) \dots h_m(x)$ define constraints in the form of equalities, and $g_{m+1}(x) \dots g_p(x)$ are constraints in the form of inequalities, where $x = [x_1, \dots, x_n]^T$ is a column vector of components $x_1, \dots, x_n$ n n-dimensional Euclidean space.

Based on this, the formulation of the nonlinear programming problem looks like this [2-5]:

Minimize $f(x)$,

$$x \in E^n, \tag{1}$$

for m linear or nonlinear constraints in the form of equalities

$$h_j(x) = 0, j = 1, \dots, m \tag{2}$$

and $(p - m)$ linear or nonlinear constraints in the form of inequalities

$$g_j(x) \geq 0, j = m + 1, \dots, p \tag{3}$$

The general problem of nonlinear programming can be reduced to solving particular problems of linear and quadratic programming. If both the function (1), the equations (2), and the constraints (3) are linear, then we have a linear programming problem. If the objective function (1) is quadratic and the constraints are linear, this is the task of quadratic programming:

to minimize

$$f(x) = a_0 + c^T x + x^T Q x \tag{4}$$

under restrictions

$$a^T x \geq b \quad , \tag{5}$$

$$x \geq 0, \tag{6}$$

where Q is a positive definite or non–negative definite quadratic symmetric matrix, and a and b are coefficient matrices.

3. Multi-criteria optimization in the form of Pareto dominance. If the vector of variable parameters $X = (x_1, x_2, \dots, x_n)$ is defined in the domain Dx, and the target vector is the function $F(x) = (f_1(X), f_2(X), \dots, f_m(X))$. Then the multi-criteria optimization problem in the form of Pareto dominance has the form [6-8]:

$$\max F(X) = F(X^*)F^* \tag{7}$$

$$X \in Dx \tag{8}$$

where X^* is the set of unimproved solutions in the field of variable parameters – the Pareto set (the desired solution in the field of variable parameters), $F^*$is the set of unimproved solutions in the field of objective functions – the Pareto front (the desired solution in the field of objective functions).

The kinetic model of the catalytic reaction of the synthesis of benzylalkyl esters is as follows [1]:

$$\frac{dy_i}{dt} = \sum_{j=1}^{J} v_{ij} k_j^0 \exp\left(-\frac{E_j}{RT}\right) \prod_{i=1}^{I} y_i^{|a_{ij}|}, i = 1, \dots, I \quad (9)$$

With initial conditions $t = 0, y_i(0) = y_i^0, t \in [0,\ t^*]$.

Here y_i is the concentration of substances involved in the reaction, mol/l; t is the time, min; J is the number of stages; I is the number of reagents; v_{ij} are coefficients of the stoichiometric matrix; k_j^0 are preexponential multipliers of the constants of the stages, 1/min; a_{ij} are negative elements of the matrix k_j^0; E_j are activation energies of the stages, kcal/mol; R is the gas constant, 2 kal/(mol·K); T is the temperature, K.

Optimality criteria for the multi-criteria optimization problem:

$$f_1(X) = y_{PhCH_2OBu(Y_6)}(t^*, T, N) \to \max \quad (10)$$

$$f_2(X) = y_{PhCH_2OCH_2Ph(Y_9)}(t^*, T, N) \to \min \quad (11)$$

$$f_3(X) = y_{BuOBu(Y_{12})}(t^*, T, N) \to \min \quad (12)$$

4. The «ideal» point method. The ideal point method consists of two stages. At the first stage, n problems of the following type are solved [9, 10]:

$$u_i^0 = \max u_i(x), x \in X \quad (13)$$

Thus, there is an «ideal» point in all parameters. In a real problem with constraints, this point is not included in the definition area, so at the second stage, the point closest to the ideal is searched:

$$R(u(x), u^0) \to min, x \in X, \quad (14)$$

where R is the distance metric, the distance from $u(x)$ to u^0.

As R we can take the Minkowski distance:

$$\left(\sum_{i=1}^{M} (u_i^0 - u_i(x))^l\right)^{\frac{1}{l}} \quad (15)$$

The Minkowski distance is a metric in a normalized vector space, which makes it possible to maintain the induced norm metric–homogeneous and translational [4].

5. Lexicographic ordering method. The use of the lexicographic ordering method is due to the fact that when optimizing the process of benzylalkyl esters, it is important to take into account the opinion of the decision maker (DM). The essence of this method lies in the fact that according to the DM survey, the criteria are ranked by importance, then an alternative is selected with the maximum score according to the most important criterion, if there is one such alternative, then it is declared optimal. At the last stage, alternatives are selected with the maximum score according to the second criterion of importance, and so on, depending on the number of optimized criteria [11-15].

6. Results of optimization application. The solution of the MCO problem was carried out using the Python programming language.

At the first stage, the solution of a system of differential equations was implemented, a set of solutions satisfying the constraints of the system and the Paretto front were visualized:

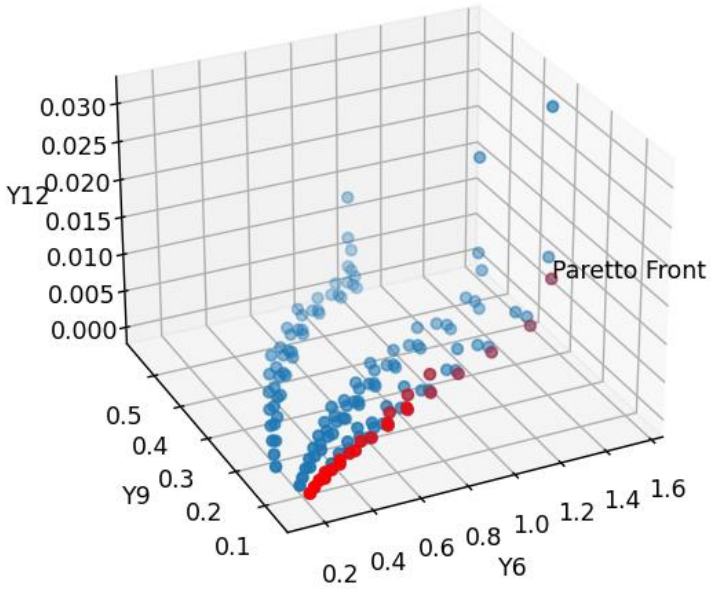

Fig. 1. Visualization of the set of SDE solutions and the Paretto front

During the application of the «ideal» point method and the lexicographic ordering method, the following results were obtained.

```
Y6 =  1.5482192182653352
Y9 =  0.06131423890663392
Y12 =  1.3505019474538902e-06
0.008590254845065589
```

Fig. 2. The «ideal» point according to all criteria

```
Y_ 1 :  1.5482192182653352
Y_ 2 :  0.2951130855534961
Y_ 3 :  0.008590254845065589
NN:  3
TT:  170
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Fig. 3. Results of using the «ideal» point method

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X_ 1 :  0.18469145110089547
X_ 2 :  0.06131423890663392
X_ 3 :  4.995994381727574e-06
NN:  3
TT:  140
```

Fig. 4. Results of using the lexicographic ordering method

When applying the lexicographic ordering method, the criteria were ranked in importance as follows: the output of the target benzylbutyl ether is maximized first, and then the output of the side dibenzyl and dibutyl esters is minimized.

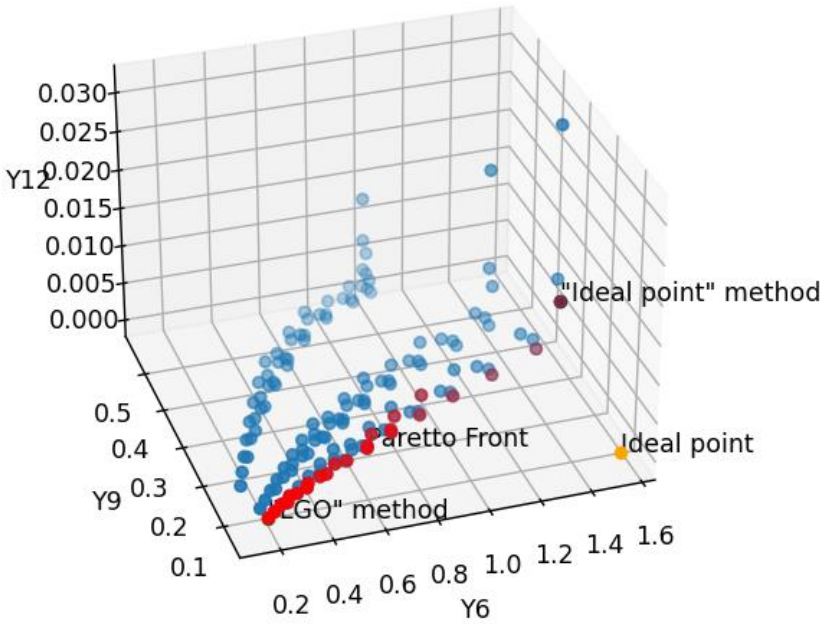

Fig. 5. Visualization of the results

As expected, the results turned out to be different from each other due to the difference in methods. When using the «ideal» point method, the result is a variant of the reaction that is close to the ideal outcome. In the case of lexicographic ordering, there is the possibility of choosing which should be optimized first – the output of the target product or reduce the output of by-products.

Conclusion. The result obtained in the course of solving the problem of optimizing the synthesis reaction of benzylalkyl esters is relevant for use in industrial and laboratory processes for the selection of optimal parameters of the chemical process. It is important to understand that the choice of the method used directly depends on the intended result of the reaction.

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Authors:

Kamila F. Koledina, Doct.Sci. (Phys.-Math.), associate professor, researcher, associate professor of the Mathematics Department, Institute of Petrochemistry and Catalysis of RAS, Ufa State Petroleum Technological University (Kosmonavtov St., Ufa, Russian Federation), koledinakamila @mail.ru

Anastasiya A. Alexandrova, student, Ufa State Petroleum Technological University (Kosmonavtov St., Ufa, Russian Federation), nastena1425@gmail.com

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РЕШЕНИЕ ЗАДАЧИ МНОГОКРИТЕРИАЛЬНОЙ ОПТИМИЗАЦИИ РЕАКЦИИ СИНТЕЗА БЕНЗИЛАЛКИЛОВЫХ ЭФИРОВ МЕТОДОМ «ИДЕАЛЬНОЙ» ТОЧКИ И ЛЕКСИКОГРАФИЧЕСКОГО УПОРЯДОЧИВАНИЯ *

К.Ф. Коледина[1], А. А. Александрова[2]

[1]Институт нефтехимии и катализа УФИЦ РАН, г. Уфа, Российская Федерация
[2]Уфимский государственный нефтяной технический университет, г. Уфа, Российская Федерация

✉ nastena1425@gmail.com, koledinakamila@mail.ru

Результат, получаемый в ходе решения задач оптимизации актуален для применения в промышленных и лабораторных процессах. Многокритериальная оптимизация подразумевает оптимизацию двух или более конфликтующих целевых функций.
Материалы и методы. На основе кинетической модели каталитической реакции синтеза бензилалкиловых эфиров поставлена задача многокритериальной оптимизации с учетом изменяемых параметров: температуры, мольного соотношения реагентов и времени проведения, имеющих ограничения. Обосновано использование методов «идеальной» точки и лексикографического упорядочивания.
Результаты. Разработан алгоритм решения задачи многокритериальной оптимизации. Используя кинетическую модель синтеза бензилалкиловых эфиров, решена задача МКО условий проведения и получены оптимальные значения изменяемых параметров системы, при которых достигается максимизация выхода целевого продукта и минимизация побочных продуктов химического процесса.
Обсуждение и заключения. Многокритериальная оптимизация данного процесса позволит дать технологические рекомендации по промышленной реализации процесса с максимальным выходом целевых продуктов и минимальным содержанием побочных. В работе представлено два метода решения задачи, так как для применения полученных результатов на практике должны учитываться рекомендации лица, принимающего решения.

Ключевые слова: многокритериальная оптимизация, задача нелинейного программирования, фронт Парето, кинетическая модель, мольные соотношения исходных реагентов, метод «идеальной» точки, лексикографическое упорядочивание.

Авторы:

Камила Коледина, доктор физико-математических наук, доцент кафедры математики Уфимского государственного нефтяного технологического университета (ул. Космонавтов, 1, Уфа, Российская Федерация)

Анастасия Александрова, студентка Уфимского государственного нефтяного технологического университета (ул. Космонавтов, 1, Уфа, Российская Федерация)

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