SYNTHESIS OF OPTIMAL CONTROL OF THE OBTAINING ETHANOLAMINE PROCESS THE METHOD OF MATHEMATICAL PROGRAMMING ON THE BASIS OF REGRESSION MODELS OF THE OBJECT

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Was set and formalized the task of linear mathematical programming for optimization of the composition of the reaction mixture. The algorithm of optimization of the object. We found optimal conditions for the implementation of the production process for generating a mixture with a maximum content of the IEA in the field of admissible solutions.

Keywords: ethanolamine, synthesis, regression models

A product of production in ethanolamine synthesis joint is a reaction mixture of three components: monoethanolamine (MEA), diethanolamine (DEA), and triethanolamine (TEA) that later is exposed to division into separate components through rectification and evaporation that is linked to significant energetic costs. In fact, a part of DEA in the reaction mixture does not depend on parameters of synthesis process in the studied area of their alterations and is supported at the level of average value of a selection. Parts of MEA and TEA are controlled factors and are adequately defined by the process parameters according to basic control channels.

Target products are realized in terms of market, and their realization volume is defined by a demand for separate types of products. Depending on a demand, an objective arise – receive a reaction mixture with a maximum content of the required component in order to decrease costs at the division stage, particularly:

– receive a reaction mixture with a maximum content of MEA№

– receive a reaction mixture with a maximum content of TEA.

Therefore, optimization criterion is a content of the required component in the reaction mixture: part of MEA in the reaction mixture (Y_1) – for the first problem, and part of TEA (%) in the reaction mixture (Y_3) for the second problem. The prepared regression models describe dependences of the composition of the reaction mixture on the initial data and parameters of the production process condition:

$$\begin{gathered} Y_1 = 67,74 - 5,196 \cdot X_1 - 0,108 \cdot X_3; \\ Y_2 = 100 - Y_1 - Y_3; \\ Y_3 = 8,471 + 5,796 \cdot X_1 + 0,088 \cdot X_3 - 0,394 \cdot X_2, \end{gathered} \tag{1}$$

where Y_1 is a part of MEA in the reaction mixture at its discharge from the synthesis joint (%), Y_2 is a part of TEA (%) in the reaction mixture, X_1 is a consumption of ethylene oxide (m/hr), X_2 is a consumption of NH_3 (m^3/hr), X_3 is a temperature in the upper part of the synthesis reactor (°C).

We should consider that regression model is real only within the studied range of alteration of equation parameter X_1, X_2, and X_3 that can often limit the search for optimal solutions. Besides, we have established a highly-predictable and statistically-adequate relation between Y_1 and Y_3 (Fig. 1).

Here we can see a problem of search for an optimal solution with limitations. In this case optimization problem is solved via methods of mathematical programming, in other words, methods of solving problems of finding a function extremum at a number of final vector space that is be defined by limitations, such as equalities and (or) inequalities.

The problem of mathematical programing can be generally presented as:

$$\begin{cases} Z = f(X) \to \min; \\ F_i(X) \geq 0, \quad i = 1, 2, ..., k; \\ H_j(X) = 0, \quad j = k+1, \quad k+2, ..., m; \\ X = (x_1, x_2, ... , x_n). \end{cases} \tag{2}$$

Where Z is the optimization criterion (target function), where Z – optimization criterion (objective function), $F_i(X)$ and $H_j(X)$ are limitations, X is a vector of n-dimensional vector space of the equation parameters.

It is a standard form of putting down a problem of mathematic equation.

The number of solutions of limitation system in this case can be called acceptable multiplicity of solutions. Solving an optimization problem at a number of acceptable solutions is the multiplicity of optimal solutions.

Setting a problem in case when we need to achieve a maximum part of MEA in the reaction mixture at its discharge from the synthesis angle, looks as:

$$Z = Y_1(X) \to \max.$$

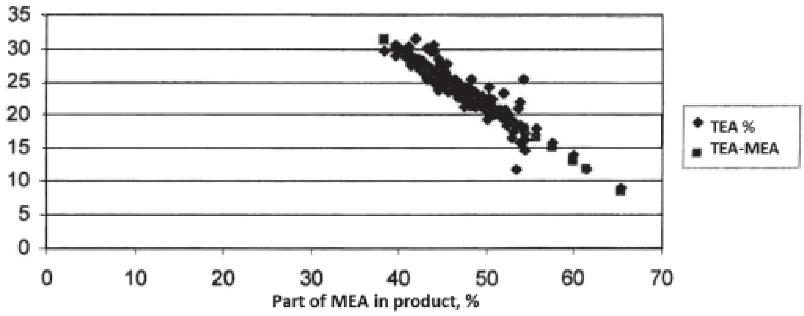

Fig. 1. Relations between parts of TEA and MEA in the product before the division. Equation of regression: $Y_3 = 63{,}847 - 0{,}8512 \cdot Y_1$; Coefficient of determination D = 0,8476; Fisher criterion F = 934,14

Limited by the following equalities:

$$Y_1 = 67{,}74 - 5{,}196 \cdot X_1 - 0{,}108 \cdot X_3;$$

$$Y_2 = 100 - Y_1 - Y_3;$$

$$Y_3 = 8{,}471 + 5{,}796 \cdot X_1 + 0{,}088 \cdot X_3 - 0{,}394 \cdot X_2;$$

$$Y_3 = 63{,}84 - 0{,}08512 \cdot Y_1.$$

Limited by the following inequalities:

$$0{,}5 \le X_1 \le 3{,}0;$$

$$6{,}0 \le X_2 \le 18{,}0;$$

$$50{,}0 \le X_3 \le 80{,}0.$$

Inequality limitations set an area, in which regression model of the process of receiving ethanolamine is adequate, and are defined by an initial statistic selection.

In a similar way we can form the second problem – search for an optimal conditions of achieving maximum part of TEA in reaction mixture before the division:

$$Z = Y_3(X) \to \max.$$

Limited by the following equalities:

$$Y_1 = 67{,}74 - 5{,}196 \cdot X_1 - 0{,}108 \cdot X_3;$$

$$Y_2 = 100 - Y_1 - Y_3;$$

$$Y_3 = 8{,}471 + 5{,}796 \cdot X_1 + 0{,}088 \cdot X_3 - 0{,}394 \cdot X_2;$$

$$Y_3 = 63{,}84 - 0{,}08512 \cdot Y_1.$$

Limited by the following inequalities:

$$0{,}5 \le X_1 \le 3{,}0;$$

$$6{,}0 \le X_2 \le 18{,}0;$$

$$50{,}0 \le X_3 \le 80{,}0.$$

Both problems are characterized by setting a target function and limitations by linear algebraic functions, in other words, these problems refer to the class of problems of linear programming. For linear problems, optimal results are usually achieved at the border of the acceptable solutions. The range of acceptable solutions is defined by solving the system of limitations, in other words, it is limited by planes in the area (X_1, X_2, X_3):

$$2{,}284 + 1{,}378 \cdot X_1 - 0{,}00323 \cdot X_3 - 0{,}394 \cdot X_2 = 0.$$

And planes:

$$X_1 = 0,5; \quad X_1 = 3,0 \text{ with a normal axis } OX_1;$$
$$X_2 = 6,0; \quad X_2 = 18,0 \text{ with a normal axis } OX_2;$$
$$X_3 = 30,0; \quad X_3 = 80,0 \text{ with a normal axis } OX_3.$$

Both problems share the same range of acceptable solutions, but their optimal solutions will differ, as there are different target functions.

Target function for the problem of optimizing the part of MEA in reaction mixture at its discharge from the synthesis joint is:

$$Y_1 = 67,74 - 5,196 \cdot X_1 - 0,108 \cdot X_3 \to \max.$$

We can see that the maximum value of Y_1 will be achieved under the smallest of all possible values of X_1 (optimal EO) and X_3 (temperature at the top of the synthesis reactor). Within the range of acceptable solutions the smallest values of $X_1 = 0,5$ and the smallest value of $X_3 = 30,0$. These limits are set by the conditions of technological process at the available equipment and are defined by the initial statistic selection. The value of factor X_2 (supply of NH_3) should be found from the condition that an optimal point is located on a limitation plane

$$2,284 + 1,378 \cdot X_1 - 0,00323 \cdot X_3 - 0,394 \cdot X_2 = 0.$$

Particularly – at its crossing with planes $X_1 = 0,5$ and the minimum value $X_3 = 30,0$

The optimum is reached at the point: supply of OX (X_1) equal 0,5 m³/hr, supply of ammonia (X_2) equal 7,3 m³/hr, and temperature of synthesis reactor (X_3) = 30 °C. The predicted composition of the reaction mixture in this case: part of MEA (Y_1) equal 61,9 %, part of DEA (Y_2) equal 27.0 %, and part of TEA (Y_3) equal 11,1 %.

For the problem of optimizing a part of TEA (Y_3) in reaction mixture before the division, the target function (optimization criterion) is:

$$Y_3 = 8,471 + 5,796 \cdot X_1 + 0,088 \cdot X_3 - 0,394 \cdot X_2 \to \max.$$

Y_3 obtains its biggest value at the line of crossing of planes that limit the range of accepted solutions from the side of the biggest values of $X_1 = 3,0$ and $X_3 = 80,0$ at the point that lies on the limiting plane

$$2,284 + 1,378 \cdot X_1 - 0,00323 \cdot X_3 - 0,394 \cdot X_2 = 0.$$

Specifically, at its crossing with planes $X_1 = 3,0$ and $X_3 = 80,0$.

The extremum takes place at the point: supply of OX (X_1) equal 3,0 m³/hr, supply of ammonia (X_2) equal 15,6 m³/hr, and temperature of synthesis reactor (X_3) = 80 °C. The predicted composition of the reaction mixture in this case: part of MEA (Y_1) equal 43,59 %, part of DEA (Y_2) equal 29,7 %, and part of TEA (Y_3) equal 26,8 %.

Other variant of extremum problems are possible within this process, for example: finding an equation that provides for receiving the minimal part of MEA (or TEA) in the reaction mixture at its discharge from the synthesis joint.

If it is necessary to find conditions of receiving a reaction mixture with the miimum part of MEA, the target function (optimization criterion) looks as

$$Z = Y_1 = 67,4 - 5,196 \cdot X_1 - 0,108 \cdot X_3 \to \min.$$

And the system of limitation remains the same. It is obvious that within the range of the accepted solutions, the minimum value of Y_1 will take place under the biggest border values of EO supply ($X_1 = 3,0$ m³/hr) and the temperature at the top of the synthesis reactor ($X_3 = 80$ °C), and supply of ammonia is defined by the point of crossing between the plane

$$2,284 + 1,378 \cdot X_1 - 0,00323 \cdot X_3 - 0,394 \cdot X_2 = 0$$

and other limiting planes. Calculations show that such point coincides with a point that provides for a maximum value of Y_3 – part of TEA in the reaction mixture.

While searching condition of receiving the reaction mixture with the minimum content of TEA, our target function is:

$$Z = Y_3 = 8,471 + 5,796 \cdot X_1 + 0,088 \cdot X_3 - 0,394 \cdot X_2 \to \min.$$

With a set range of acceptable solutions. Supply of ammonia (X_2) should be found as a point of crossing between limiting planes $X_1 = 0,5$; $X_3 = 30,0$, and

$$2,284 + 1,378 \cdot X_1 - 0,00323 \cdot X_3 - 0,394 \cdot X_2 = 0$$

Such point will coincide to the one that provides for the maximum content of MEA in the reaction mixture.

Extreme points are found in any definition of this problem on borders of the range of accepted solutions. We have found local extremums, and, in order to find global extremums, one should scan the whole surface of the accepted range of existing solutions. In case of necessity, this procedure must be realized within the process of optimal control over the object.

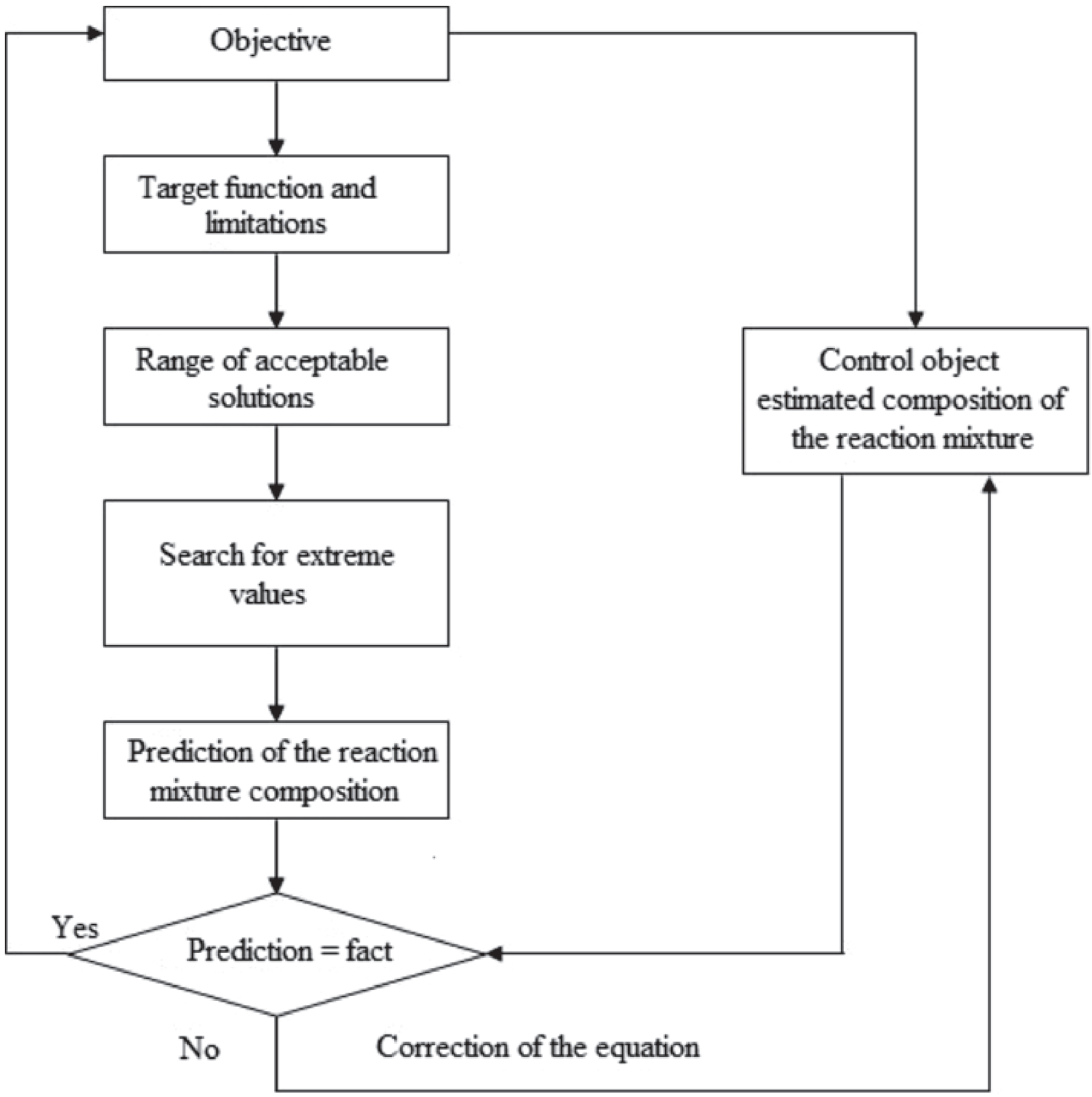

Fig. 2. Algorithm of an optimal control over the process of receiving ethanolamine

Limitations in forms of inequalities in this definition of the problem are defined by the composition of the initial statistic selection, according to which, the regression model of the control object has been received. The model is adequate within the studied area, but gives an increasing number of prediction errors as it remotes from the center of the studied area. In order to search for optimal regimes of control within a wider range of alteration in parameters of production, it is necessary to develop a determined mathematic model of the object.