MATHEMATICAL MODELLING AND OPTIMIZATION OF THE PROCESS OF DERIVING BORIC ACID FROM ULEXITE MINERAL

Novruz BASHIROV
1Yüzüncü Yıl University, Health Occupation High School-Van-TURKEY, novruzb@yahoo.com

Aynura Alekperova  aynurka@inbox.ru
QAFQAZ University, Azerbaijan

Jale Mustafayeva
Middle East Technical University, Graduate School of Natural Sciences, Department of Petroleum and Natural Gaz Engineering, Ankara, Turkey, jalemstfyv@gmail.com

Barati Chiyaneh
Department of Mathematics, Faculty of Art and Sciences
Yüzüncü Yıl University, Van 65080, Turkey, baratiakbar@yahoo.com

Abstract

Ulexite is a sodium calcium boron hydrate used in producing compounds. Its chemical formula is Na$_2$O2CaO5B$_2$O$_3$16H$_2$O, and it superabounds in Turkey. One of the significant boron compounds derived from boron minerals is boric acid. The aim of this study is to produce boric acid in the wake of interaction of ulexite with hydrochloric acid solution, and offering an alternative process to producing boric acid by forming the mathematical model of this processing. Full factorial design method has been used in the study. Some of the parameters used in the process have been made steady, and the others have been accepted as variable factor in formation of mathematical model. Invariant parameters are granule size, reaction time and stirring speed. Hydrochloric acid concentration has been accepted as temperature and solid to liquid ratio variable factors for the formation of mathematical model. Primarily, the mathematical model of the process and three-parameter full factorial design have been evaluated in the measureless coordinate system, then the values in the model has been assessed by Student criteria, and the validity of the originated model has been controlled by Fisher criteria. Henceforward, the current model of the process has been formed in the real coordinate system.

Thereafter, the optimization of this process was realized using the modified Hooke-Jeeves method.

Keywords: ulexite, boric acid, mathematical modeling, optimization.
1. Introduction

Boron is a crucial element used in many fields, especially strategic ones. However, boron is not directly used in numerous fields in element, it is mostly used in its compounds. Boron subsists in nature in the form of metal borates, mostly in the form of sodium, calcium, sodium-calcium and magnesium borates [12]. Those subsisting in nature prevalently are colemanite (2CaO 3B₂O₅ 5H₂O), ulexite (Na₂O 2CaO 5B₂O₃ 16H₂O) and tincal (Na₂O 2B₂O₃ 10H₂O). The products like boric acid, hydrated borax, anhydrite borax and sodium per borates are derived from these substances [5]. A lot of studies has been held on ulexite that is a sodium-calcium borate. In the studies, boric acid output has been researched by analyzing the dissolution mechanism of ulexite in different solvents [9]. Dissolution kinetics has been analyzed by using distinct parameters in the studies held. Dissolution kinetics of ulexite has been viewed in the solution saturated with CO₂ [11] and in the solution saturated with SO₂ [2]. Further there are studies on deriving boric acid and borax from ulexite [23]. The mechanism of deriving borax from ulexite has been scrutinized [8]. Some researchers have analyzed dissolution mechanism of ulexite in sulphuric acid [22]. Dissolution kinetics of ulexite has been viewed in acetic acid solutions, and found out that maximum solution ratio is in low acid concentration, and besides researchers have found that the solution ratio falls as acid concentration increases [10]. In another study dissolution of ulexite has been analyzed in ammonia solution saturated with CO₂, and researchers have found out that dissolution ratio soars with the increasement of the concentration the dissolution ratio [13]. The studies conducted are related to solution mechanism.

Boric acid is a crucial raw material for industry and trade. The abatement of difficulties that are encountered in the production of boric acid will reduce the cost. With this study, it seems that the production of boric acid by the activation of ulexite with HCl, and the production of calcium chloride as by product is possible. Calcium chloride is utilized in numerous fields from agriculture to chemical industry ([1] and [7]). Most of the studies related to ulexite are pertinent to the kinetics and mechanism of dissolution. In this conducted study, the mathematical modeling of the derivation process of production oriented boric acid has been performed. The product consisted by this modeling method may occur depending upon the reacting products. Full factorial design method has been used in numerous studies. Some researchers have utilized full factorial design method in resolving anionic red dye in aqueous solutions [6]. In another study researchers have applied full factorial design method in boron removal from aqueous solutions by adsorption [15]. Another study, researchers have employed full factorial design method in crystallizing kluyveromyces lactis β-galactosidase enzyme [17]. A researcher has observed the clearance of colorant from agricultural residue with anion exchanger by means of
full factorial design [14]. Other researchers have used cerium oxide in aqueous solutions of boron waste, and full factorial design method in the adsorption of boron waste [16]. Another study, full factorial design method was utilized for the boron removal from aqueous solutions with Al₂O₃ based adsorbents [20]. In another study was researched the optimization of the supercritical liquid extraction of Iraganox 1076, Irgafos 168 and Chimassob 81 substances with full factorial design method [18]. Erosion resistance of automotive polishers were viewed the with full factorial design method [3].

In another study, Mathematical Model of sulphometilation process of nonilphenol studied ([3] and [4]).

It is possible to remove the deficiencies that have appeared during getting the correlation in the full factorial design method and classic regression analysis used and among the coefficients of regression equations used in this study. In the study conducted, the experimental design has been determined by considering the determination of the matter and experimental results. The study consists of several phases. The results gotten after each phase help the determination of next phases of the experiment. Hence the experiment is provided to be controlled optimally. The whole differential parameters can be also changed by experimental design method, and the relations between variables can be assessed. Different from other research methods, searching the relations between variables in this method raises the productivity of experiments substantially.

2. Experimental

2.1. Dissolution studies

Dissolution operation takes place according to the following equation:

\[
\text{Na}_2\text{O} \cdot 2\text{CaO} \cdot 5\text{B}_2\text{O}_3 \cdot 16\text{H}_2\text{O} + 6\text{HCl} \rightarrow 2\text{NaCl}_{(aq)} + 2\text{CaCl}_{(aq)} \cdot 10\text{H}_3\text{BO}_3_{(aq)} + 4\text{H}_2\text{O}
\]

The ulexite used in the study conducted has been supplied from the region of Balıkesir-Bigadiç in Turkey. Boron ore has been segregated into the requested fractions by being sifted through in ASTM class after it is cleaned from the apparent contamination. The chemical analysis of ulexite ore has been given in Table 1. The hydrochloric acid used in this study is 37 % by weight, and it has been supplied from merck. In Table 2, the parameters used in the experiment has been shown.

Dissolution experiments have been held in 250 mL cylindrical glass batch reactor by using mechanical mixer. Temperature has been regulated by using a 0.1 °C sensitivity thermostate. A condenser has been used to prevent the solvent loss originating from evaporation. Initially, 100 mL hydrochloric acid has been added to the reactor, and the requested temperature has been watched over by running the mechanical mixer. Then dissolution operation has been embarked on by adding ulexite. When the time is over, the experiment has been halted, and the
substance taken from the reactor has been filtered. Henceforwards, B$_2$O$_3$, D-mannitol and volumetrik in the substance have been analyzed [23]. The transformation fraction of the solute B$_2$O$_3$ has been retained by being divided into the B$_2$O$_3$ ratio in original ore.

<table>
<thead>
<tr>
<th>Components</th>
<th>CaO</th>
<th>B$_2$O$_3$</th>
<th>H$_2$O</th>
<th>Na$_2$O</th>
<th>MgO</th>
<th>Others</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Composition</td>
<td>13.68</td>
<td>42.24</td>
<td>34.18</td>
<td>6.12</td>
<td>3.15</td>
<td>0.63</td>
</tr>
</tbody>
</table>

Table 1. The chemical analysis of the ulexite used in the study

<table>
<thead>
<tr>
<th>Variables</th>
<th>Concentration (Mol/L)</th>
<th>Solid/Liquid ratio (g/mL)</th>
<th>Temperature ($^\circ$K)</th>
<th>Fixed particle size (mm)</th>
<th>Stirring speed (rpm)</th>
<th>Reaction time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Range</td>
<td>0.5 – 2.0</td>
<td>0.02 – 0.1</td>
<td>293 – 333</td>
<td>1.205</td>
<td>400</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 2. The parameters used in the experiment

2.2. Materials and Methods

2.2.1. Mathematical Modeling

In full factorial design method, the whole combinations of variables at maximum and minimum levels are taken into consideration. The application of full factorial design method is found with the formula of the number of the experiments to be tested for $n$ slew levels of $k$ slew variables.

$$N = n^k$$

In the study conducted, there are 3 variable values that is $k=3$. If these 3 factors change at two levels consisting of maximum and minimum, the number of the experiments to be tested should be $N=2^3 = 8$.

Supposing that there are three variables consisting of $Z_1$, $Z_2$ ve $Z_3$ in the study conducted the range of these factors are as follows:

$$Z_1^{\text{min}} \leq Z_1 \leq Z_1^{\text{max}}$$

$$Z_2^{\text{min}} \leq Z_2 \leq Z_2^{\text{max}}$$

$$Z_3^{\text{min}} \leq Z_3 \leq Z_3^{\text{max}}$$

As is seen, each $Z_k$ changes between its own maximum and minimum values like $Z_k^{\text{min}}$ and $Z_k^{\text{max}}$, $Z_k \in [Z_k^{\text{min}}, Z_k^{\text{max}}]$, $k=1,2,3$. as indicated before, 8 experiments should be held in order to take mathematical model as the number of factors are 3.

Initially the following calculations are done:
\[
Z_k^0 = \frac{Z_k^{\text{max}} + Z_k^{\text{min}}}{2}, \quad k = 1, 2, 3.
\]
\[
\Delta Z_i = \frac{Z_i^{\text{max}} - Z_i^{\text{min}}}{2}, \quad k = 1, 2, 3.
\]

Here the points of \(Z_1^0, Z_2^0\) \& \(Z_3^0\) are called experimental design centre. \(\Delta Z_k\) is the changeability value of relevant variable. The values of the 8 experiment held in measureless and natural coordinate system have been shown in Table 1. Minimum values of \(Z_i\) have been displayed with \(-1\), and its maximum values with \(+1\). In compliance with this design, 8 experiments are tested and \(Y_{\text{exp}}\) basic material values derived from each experiment are added to Table 3.

Henceforward, mathematical model is formed
\[
Y = a_0 + a_1X_1 + a_2X_2 + a_3X_3 + a_{12}X_1X_2 + a_{13}X_1X_3 + a_{23}X_2X_3 + a_{123}X_1X_2X_3
\]
(4) in dimensionless coordinate system. Coefficient values of model \(a_0, a_1, a_2, a_3, a_{12}, a_{13}, a_{23}\) and \(a_{123}\)
\[
a_j = \frac{1}{N} \sum_{i=1}^{N} X_{ji} Y_i
\]
(5)
is computed with the formula above.

Table 3. The plan of full factorial design for three factors

<table>
<thead>
<tr>
<th>Experiment Number</th>
<th>(X_1)</th>
<th>(X_2)</th>
<th>(X_3)</th>
<th>(Z_1)</th>
<th>(Z_2)</th>
<th>(Z_3)</th>
<th>(Y^{\text{tec}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>(Z_1^{\text{min}})</td>
<td>(Z_2^{\text{min}})</td>
<td>(Z_3^{\text{min}})</td>
<td>(Y_1)</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>(Z_1^{\text{max}})</td>
<td>(Z_2^{\text{min}})</td>
<td>(Z_3^{\text{min}})</td>
<td>(Y_2)</td>
</tr>
<tr>
<td>3</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>(Z_1^{\text{min}})</td>
<td>(Z_2^{\text{max}})</td>
<td>(Z_3^{\text{min}})</td>
<td>(Y_3)</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>(Z_1^{\text{max}})</td>
<td>(Z_2^{\text{max}})</td>
<td>(Z_3^{\text{min}})</td>
<td>(Y_4)</td>
</tr>
<tr>
<td>5</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>(Z_1^{\text{min}})</td>
<td>(Z_2^{\text{min}})</td>
<td>(Z_3^{\text{max}})</td>
<td>(Y_5)</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>(Z_1^{\text{max}})</td>
<td>(Z_2^{\text{min}})</td>
<td>(Z_3^{\text{max}})</td>
<td>(Y_6)</td>
</tr>
<tr>
<td>7</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>(Z_1^{\text{min}})</td>
<td>(Z_2^{\text{max}})</td>
<td>(Z_3^{\text{max}})</td>
<td>(Y_7)</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>(Z_1^{\text{max}})</td>
<td>(Z_2^{\text{max}})</td>
<td>(Z_3^{\text{max}})</td>
<td>(Y_8)</td>
</tr>
</tbody>
</table>

Then in the experiment station, that is at the points of \(Z_1^0, Z_2^0\) \& \(Z_3^0\), three collateral experiments are tested, and the values of \(Y_1^0, Y_2^0\) \& \(Y_3^0\) out parameters are computed in accordance with them. After that, the mean value of these out parameters are found:
\[
\overline{Y}^0 = \frac{\sum_{u} Y_u^0}{3} \tag{6}
\]

Thereafter
\[
S_i^2 = \frac{\sum_{u} (Y_u^0 - \overline{Y})^2}{3} \tag{7}
\]
and
\[
S_{aa} = \frac{S_i^2}{\sqrt{8}} \tag{8}
\]

's values are computed. By considering the calculated (6), (7) and (8) values, and using Student criteria.

\[
t_m = \frac{|a_m|}{S_{aa}} \tag{9}
\]

with the formula, the values found by the formula in (5) of the mathematical model in (4) are seen from private Student criteria table by using \( P=0.05 \) condition that they are \( f=2, \ t_p(f)=4.3 \) for these values. The values are utilized in the model in (4) by using the formula in (9) if each \( t_m \) value is larger than 4.3. The rest, that is the values which are lower than 4.3 are not used.

Henceforward, variances may be in the mathematical models in (4).

Thereafter, the validity of the new model is checked by Fisher criteria:
\[
F = \frac{S_2^2}{S_1^2} \tag{10}
\]

Here
\[
S_2^2 = \frac{\sum_{i=1}^{N} (Y_i - \overline{Y}_i)^2}{N} \tag{11}
\]

The mathematical model in (4) taken in dimensionless coordinate system is capable of supplying the actual process exactly. To form the valid mathematical model of natural process, the following change of variable formula in model (4) is used:

\[
X_j = \frac{Z_j - Z_j^0}{\Delta Z_j}, \quad j=1, 2, 3. \tag{12}
\]

Mathematical model is taken as the follows in natural coordinate system after certain mathematical conversions:

\[
Y_z = b_0 + b_1 Z_1 + b_2 Z_2 + b_3 Z_3 + b_{12} Z_1 Z_2 + b_{13} Z_1 Z_3 + b_{23} Z_2 Z_3 + b_{123} Z_1 Z_2 Z_3 \tag{13}
\]

These \( b_0, b_1, b_2, b_3, b_{12}, b_{13}, b_{23} \) ve \( b_{123} \) are new values taken as a result of conversion of the formula and values in (12).
2.2.2. Optimization

In the process of optimization it was used the modified Hooke-Jeeves method, which is still very effective and original. The research consists of the sequence of steps of exploring the search around the base point, beyond which, if successful, should come research to the sample. The procedure is presented below:
A) Choose the starting base point \( b_1 \) and a step length \( h_j \) for each variable \( x_j \), \( j=1, 2, \ldots, n \).
B) Calculate \( f(x) \) at the base point \( b_1 \) to obtain information about the local behavior of the function \( f(x) \). This information will be used to find a suitable search direction on the model by which we can hope to achieve a greater decrease of the function value. The function \( f(x) \) at the base point \( b_1 \) is as below:

1. It is calculated the value of the function \( f(b_1) \) at the base point \( b_1 \).
2. Each variable is changed by one step by adding length. So, we calculate the value of the function \( f(b_1+h_1e_1) \), where \( e_1 \) is a unit vector in the direction of the axis \( x_1 \). If this leads to a decrease of the value function, then, \( b_1 \) is replaced by \( b_1+h_1e_1 \). Otherwise, it is calculated value of the function \( f(f(b_1-h_2e_1)) \), and if its value is reduced, then \( b_1 \) is replaced by \( b_1-h_2e_1 \). If none of the made steps does reduces the function value, then, the point \( b_1 \) remains unchanged and considered the changes in the direction of axis \( x_2 \), i.e. it is found the value of \( f(b_1+h_2e_2) \), etc. When we examine all the variables \( n \), we will have a new base point \( b_2 \).

3. If \( b_2=b_1 \), i.e. the decrease in the function has not been reached, then, the study is repeated around the same base point \( b_1 \), but with reduced pitch length. In practice, satisfactory is the reduction step (or steps) to ten times from its initial length.
4. If \( b_2\neq b_1 \), the search is performed on the model.
C) When you search on the model, it is used information obtained in the course of the study, and the minimization of the function is completed by the search in the direction of given sample.

The procedure is as follows:
1. It is reasonable to move from the base point \( b_2 \) in the direction of \( b_2 – b_1 \) as the search in this direction has already led to decrease in the function value. Therefore, we calculate the function at the point of sample \( P_i=b_i+2(b_2 – b_1) \). In general, \( P_i=b_i+2(b_{j+1} – b_j) \).
2. Then, the study should be continued around the point \( P_1 \) (\( P_i \)).
3. If at least step c) the point 2 is of less value than in the base point \( b_2 \) (generally \( b_j+1 \)), then it is obtained a new base point \( b_3 \) (\( b_{j+1} \)).
D) To complete this process, when the step length (the length of steps) will be decreased to a predetermined low value [24].
3. Results and discussion

The mathematical model of
\[ \text{Na}_2\text{O} \cdot 2\text{CaO} \cdot 5\text{B}_2\text{O}_3 \cdot 16\text{H}_2\text{O} + 6\text{H}_3\text{O}^+ \rightarrow 2\text{Na}^{++}(\text{aq}) + 2\text{Ca}^{++}(\text{aq}) + 10\text{H}_3\text{BO}_3 + 10\text{H}_2\text{O} \]  

(14)

process has been formed by using full factorial design method with the study conducted. The mathematical model to be formed of the process will be as follows

\[ Y_z = b_0 + b_1 Z_1 + b_2 Z_2 + b_3 Z_3 + b_{12} Z_1 Z_2 + b_{13} Z_1 Z_3 + b_{23} Z_2 Z_3 + b_{123} Z_1 Z_2 Z_3. \]

Here:
- \( Z_1 \) – Hydrochloric acid concentration is denominated with mol/L;
- \( Z_2 \) – temperature is denominated with \(^0\text{C}\);
- \( Z_3 \) – solid/liquid ratio is denominated with g/mL.

reaction time has been stabilized as 5 minutes in all the experiments.

The range of \( Z_1, Z_2 \) and \( Z_3 \) parameters are as follows:

\[
\begin{align*}
0.5 & \leq Z_1 \leq 2 \\
20 & \leq Z_2 \leq 60 \\
0.02 & \leq Z_3 \leq 0.1
\end{align*}
\]

(15)

In accordance with the values given in Table 1, full factorial design long shot and the used values of parameters have been displayed in Table 4.

\[
a_j = \frac{1}{N} \sum_{i=1}^{N} X_{ij} Y_i
\]

(16)

using the formula above, the values of mathematical model to be formed in dimensionless coordinate system have been found as they are shown in (17) system.

\[
\begin{align*}
a_0 &= 3.063915 \\
a_1 &= 0.16404 \\
a_2 &= 0.561375 \\
a_3 &= 0.714313 \\
a_{12} &= 0.362485 \\
a_{13} &= 0.206658 \\
a_{23} &= 0.490343 \\
a_{123} &= 0.376693
\end{align*}
\]

(17)

Thus, the following mathematical model has been formed in dimensionless coordinate system:

\[
Y_x = 3.063915 + 0.16404 X_1 + 0.561375 X_2 + 1.714313 X_3 + 0.362485 X_1 X_2 + 0.206658 X_1 X_3 + 0.490343 X_2 X_3 + 0.376693 X_1 X_2 X_3
\]

(18)

To assess the values of (18) model with Student criteria, 3 collateral experiments have been tested at the points of \((Z_1^0, Z_2^0, Z_3^0)\) which is the centre of full factorial design plan. The centre of our experimental design is the point consisting of (1.25; 40; 0.06) coordinates. At this central point, the results of 3 collateral experiments held have been found as follows:
\[ Y_1^0 = 4,0949; \quad Y_2^0 = 4,1181; \quad Y_3^0 = 4,1412 \]  \tag{19}

Hence
\[ \bar{Y}^o = \frac{Y_1^0 + Y_2^0 + Y_3^0}{3} = 4,118067 \]  \tag{20}

\[ S_1^2 = \frac{1}{3} \sum_{n=1}^{3} (Y_u^0 - \bar{Y}^o)^2 \]  

by using the formula, the result is found as \( S_1^2 = 0,00053515 \).

\[ S_{u_n} = \frac{S_1^2}{\sqrt{8}} \]  

from the formula, the result is found as \( S_{u_n} = \frac{S_1^2}{\sqrt{8}} = \frac{0,00053515}{2,828} = 0,000189 \).

As the found \( S_{u_n} \) is a rather low number, all the values of the \( t_m \) numbers found by (9) formula are larger than \( t_0(f)=4,3 \) number. And this shows that all the found coefficient values \( a_0, a_1, a_2, a_3, a_{12}, a_{13}, a_{23} \) and \( a_{123} \) are useable. Thus,

\[ Y_x = 3,063915 + 0,16404 X_1 + 0,561375 X_2 + 1,714313X_3 + 0,362485X_1X_2 + \\
+ 0,206658X_1X_3 + 0,490343X_2X_3 + 0,376693 X_1X_2X_3 \]  \tag{18}

All the coefficient values of the model have been accepted as useable. For instance, the value of \( a_0 \) coefficient can be calculated.

\[ t_0 = \frac{|a_0|}{S_{u_n}} = 3,06395/0,000189=15959,81 >> 4,3 \text{ (usable)} \]

\[ t_{123} = \frac{|a_{123}|}{0,000189} = 3,06395/0,000189 = 1993,084656 >> 4,3 \text{ (usable)} \]  \tag{21}

Whether the other coefficient values are useable or not has been determined by this method. Henceforward, the validity of (18) mathematical model has been checked by Fisher criteria, and by (10) and (11) formulas.

Experimental errors were determined by the formula
\[ S_0 = \frac{\sum_{i=1}^{N} \sum_{k=1}^{M} (Y_{ik} - \bar{Y}_i)^2}{N(M-1)} \]  \tag{22}

where \( N \) – a number of experiments; \( M \) – a number of parallel experiments; \( k \) – a number of factors (in the given case \( N=8, M=3 \) and \( k=3 \)).

In the development of the mathematical model, its adequacy was checked by minimizing the differences of squariances of experimental \( (Y_{\text{exp}}) \) and estimated \( (Y_{\text{model}}) \) values. It is considered that the mathematical model adequately describes this particular process in the case of residual dispersion \( S_2^2 \) of the output value \( Y_i \), estimated by formula (12) relative to the average experimental values \( \bar{Y}_i \), statistically does not exceed the errors of the experiment \( S_2^2 \). Tabulated values of Fisher criterion for \( P=0.05 \) is \( f_1=N-k-1=4, f_2=M-1=2 \). Therefore \( F_{1-1}(f_1, f_2)=19.3; S_2^2 = 0.000188 \).

As \( F=0,351271 \) and \( F_{1-1}(f_1, f_2)=19.3 \) (here \( F<F_{1-1}(f_1, f_2) \)), the mathematical model of the process of deriving boric acid from ulexite mineral in dimensionless system of co-ordinates adequately describes the experiment carried out. Co-ordinate of center of a plan in full scale \( (Z_1, Z_2, Z_3) \) and variation units \( (\Delta Z_1, \Delta Z_2, \Delta Z_3) \) with respect to axes \( Z_1, Z_2, Z_3 \) were calculated with the formulas (3) and tabulated in Table 4.
Table 4. Calculated values of \( Z_i^0 \) and \( \Delta Z_i \)

<table>
<thead>
<tr>
<th>( Z_i^0 )</th>
<th>( Z_2^0 )</th>
<th>( Z_3^0 )</th>
<th>( \Delta Z_1 )</th>
<th>( \Delta Z_2 )</th>
<th>( \Delta Z_3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,25</td>
<td>40</td>
<td>0,06</td>
<td>0,75</td>
<td>20</td>
<td>0,04</td>
</tr>
</tbody>
</table>

In order to the mathematical model of the process in natural coordinate system, is has been benefited from (12) formula as follows:

\[
\begin{align*}
X_1 &= \frac{Z_1 - Z_1^0}{\Delta Z_1} = \frac{Z_1 - 1,25}{0,75} = \frac{4Z_1 - 5}{3} \\
X_2 &= \frac{Z_2 - Z_2^0}{\Delta Z_2} = \frac{Z_2 - 40}{20} \\
X_3 &= \frac{Z_3 - Z_3^0}{\Delta Z_3} = \frac{Z_3 - 0,06}{0,04} = \frac{50Z_3 - 3}{2}
\end{align*}
\]  

(23)

After the variable value in (21) formula, the following mathematical model has been formed in natural coordinate system by using (18) model and making certain mathematical simplifications:

\[
Y_z = 0,408787833 + 0,345559333Z_1 + 0,008172567Z_2 + 41,12100833Z_3 - 0,013503633Z_1Z_2 - 18,22426667Z_1Z_3 - 0,171848333Z_2Z_3 + 0,627821667Z_1Z_2Z_3
\]  

(24)

The calculated \( Y_{Z_i}^\text{model} \) values by using (24) model have been added to the last column of the Table 5.

The mathematical model values and relevance of the tested experiment results which have been formed in dimensionless coordinate system (18), and in natural coordinate system (24) has been given in figure 1.

As can be seen in the figure, the values of the derived basic materials in both dimensionless coordinate system and in natural coordinate system are rather close to each other. Therefore, the process can be researched through in larger parameters by using the formed mathematical model.

On the basis of the obtained model, it was built different graphs presented in Table 6:

\[
Y_z = 0,408787833 + 0,345559333Z_1 + 0,008172567Z_2 + 41,12100833Z_3 - 0,013503633Z_1Z_2 - 18,22426667Z_1Z_3 - 0,171848333Z_2Z_3 + 0,627821667Z_1Z_2Z_3.
\]

The acquired product amount in consequence of both models show relevance to experimental results. This demonstrates the validity of the formed mathematical model. The process can be brought under control as expected by using this mathematical model.
Table 5. Full factorial design plan and resentful values of parameters

<table>
<thead>
<tr>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Experiment number</th>
<th>Y _\text{exp}</th>
<th>Y _x \text{mod}</th>
<th>Y _z \text{mod}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment number</td>
<td>Experiment number</td>
<td>Experiment number</td>
<td>Experiment number</td>
<td>Experiment number</td>
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<td>1,31</td>
<td>0,5 20 0,02 1,306</td>
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<td>2 20 0,02 1,251</td>
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<td>2 60 0,02 1,363</td>
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<td>6,94</td>
<td>2 60 0,1 6,939</td>
</tr>
</tbody>
</table>

Figure 1. Graphical display of the validity of the process: \( Y \_\text{exp} \) – values received experientially; \( Y \_x \text{model} \) – calculated values in dimensionless coordinate system by mathematical model; \( Y \_z \text{model} \) – calculated values in natural coordinate system by mathematical model.
Table 6. Change of parameters in the specified ranges

<table>
<thead>
<tr>
<th>No</th>
<th>Change of parameters</th>
<th>No</th>
<th>Change of parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$Z_{1\text{min}} = 0.5 = \text{constant}$</td>
<td>2</td>
<td>$Z_{1\text{max}} = 2 = \text{constant}$</td>
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<tr>
<td></td>
<td>$20 \leq Z_2 \leq 60$</td>
<td></td>
<td>$20 \leq Z_2 \leq 60$</td>
</tr>
<tr>
<td></td>
<td>$0.02 \leq Z_3 \leq 0.1$</td>
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<td>$0.02 \leq Z_3 \leq 0.1$</td>
</tr>
<tr>
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<td>$Z_{2\text{min}} = 20 = \text{constant}$</td>
<td>4</td>
<td>$Z_{2\text{max}} = 60 = \text{constant}$</td>
</tr>
<tr>
<td></td>
<td>$0.5 \leq Z_1 \leq 2$</td>
<td></td>
<td>$0.5 \leq Z_1 \leq 2$</td>
</tr>
<tr>
<td></td>
<td>$0.02 \leq Z_3 \leq 0.1$</td>
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<td>$0.02 \leq Z_3 \leq 0.1$</td>
</tr>
<tr>
<td>5</td>
<td>$Z_{3\text{min}} = 0.02 = \text{constant}$</td>
<td>6</td>
<td>$Z_{3\text{max}} = 0.1 = \text{constant}$</td>
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<td></td>
<td>$0.5 \leq Z_1 \leq 2$</td>
<td></td>
<td>$0.5 \leq Z_1 \leq 2$</td>
</tr>
<tr>
<td></td>
<td>$20 \leq Z_2 \leq 60$</td>
<td></td>
<td>$20 \leq Z_2 \leq 60$</td>
</tr>
</tbody>
</table>

The graphs obtained on the basis of Table 6 are shown in Figure 2. The graphs show that the obtained mathematical model is multivariable increasing function.

For optimization, it was used the modified Hooke-Jeeves method, which is described in section 2.2.2 of this article. Since it was necessary to find the maximum value of the function $Y_z$, we used the method not to minimize, but to maximize the function. The algorithm for solving optimization (maximization) of the obtained mathematical model is given in Figure 3.

After optimization of mathematical model of the process it was obtained the following values of the arguments in which $Y_z \text{max} = 6.394061632$: $Z_1 = 2.2$; $Z_2 = 60$; $Z_3 = 0.1$. These values are again proving that the obtained mathematical model is multivariable increasing function.

### 4. Conclusions

The presence of the optimum accrual shape of the processes in numerous fields matters to. The formation of the mathematical model of the process by retaining the optimum accrual conditions of the chemical processes that occur depending upon a lot of variables enables this process to be checked automatically. In this study, reaction time as 5 minutes, stirring speed as 400 revs/minutes, and particle size as 1,205mm has been stabilized during accruing of the chemical process.

With full factorial design method, in dimensionless coordinate system

$$Y_x = 3.063915 + 0.16404 X_1 + 0.561375 X_2 + 1.714313X_3 + 0.362485X_1X_2 + 0.206658X_1X_3 + 0.490343X_2X_3 + 0.376693 X_1X_2X_3$$

model has been formed.

The model formed in natural coordinate system occurs as
Fig. 2. The obtained graphs for different values of the arguments
Finally, the optimization problem has been solved and found the optimal values of the variables to let to obtain the maximum value of function $Y_z$.

**REFERENCES**


