Full Factorial Design of Production of Hydrogen Gas at Sodiumborohydride with Cobalt Catalyst

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Abstract

Energy should be transportable, stockable and not be harmful to the environment so that it can be utilizable in today’s conditions. Regarding all these properties hydrogen energy has an importance for our future. Hydrogen can be produced in numerous ways. In the study we deal with hydrogen has been produced from sodium borohydride by using cobalt catalyst. In addition, the mathematical model of this production has been formed by using full factorial design in particular parameters. In the study, NaBH₄, Co catalyst, temperature and time parameters have been accepted as variable. The composed hydrogen gas has been determined to rise with the increase of NaBH₄, Co and temperature.

Key Words: Hydrogen, Full factorial desing, Mathematical modelling, cobalt, catalyst.

1. Introduction

A large proportion of available energy in our world is supplied by oil, natural gas, coal and wood. Approximately 80% of our energy need is still supplied by oil, natural gas and coal which are fossil fuels [Veziroğlu and Barbir.,1998]. Today energy should be transportable, stockable and harmless to the environment in order to be utilizable. Nowadays one of the significant fossil fuels used is coal. Coal is found compressed under soil. There was a substantially coal resource in the world; however a part of it lies under the fertile agricultural lands. The fertile agricultural lands are eradicated during mining coal. Moreover, transportation of coal also causes incremental costs. In view of all these factors coal cost is an energy resource that shows increase [Luther., 1984]. Further, a lot of effects of fossil originated oil and coal which are harmful to the environment have been determined. Fossil fuels substantially consist of carbon and hydrogen, there may be a trace of sulphur and bullet within the body of fuel. As a result of fossil fuels burning, carbon and sulphur, ash, goudron and many harmful compounds regarded as to be poisonous occur. These compounds diffuse to the atmosphere. Then these substances damage to soil by turning into rain, acids and the other hazardous wastes, and by precipitating. This situation affects adversely agricultural products and all livings particularly human beings [Veziroğlu and Barbir.,1998].

Carbon dioxyde composed in consequence of coal and oil burning is utilized by plants. However, all of it cannot be utilized by plants if produced too much, and the surplus results in global warming by accumulating in the atmosphere [Aslan.,2004]. Fossil fuel resources are not infinite and these resources cannot be recycled. Energy need is increasing steadily. The chief reason of this is increase in demand for energy as a result of increasing population and rising of life standards. It is thought that oil and natural gas resources will run out in 25 years in view of existing developments. Further, the consumption increase of them will affect the environment adversely [Veziroğlu and Barbir.,1998; Fulkerson.W et al., 1990].

Lots of studies have been being held in order to meet the increasing energy need. A large proportion of these studies are related to solar energy, wind energy, water energy, wave energy, tide energy and ocean thermal energies.
The energies we talk about here except nuclear energy are the natural origin renewable sources that are not harmful to the environment. The studies about them are going on. As for nuclear energy it is an energy source which is still disputed on, a complete consensus has not been provided over it yet. The source of nuclear energy is under the earth crust, it is a nonrenewable energy and when its source runs out this energy will be used up too. Besides, nuclear wastes create a great danger. Despite all these negations nuclear energy is still used in a lot of countries to provide a great deal of energy need. The last accidents happened in Fukushima Nuclear Plant after the tsunami incident occurred in Japan has brought to the minds the question of “Is nuclear energy safe?”.

Ever-increasing energy need enforces human beings to find new energy resources. One of these energy resources is hydrogen. Hydrogen has a lot of superior properties in comparison with fossil fuels. Hydrogen is environment-friendly and it doesn’t destroy nature during its extraction. Further, hydrogen can actively be utilized in energy generation with so many methods such as flame burning, catalytic burning, electrochemical transformation and hydride according to its target. Still, 1 gram hydrogen gas composes a 11-litre volume in the normal atmospheric pressure so it should be stocked in high-pressure in a pressure pot. The utmost obstacle about the common usage of hydrogen is the problems related to its storage and transportation. The studies about these problems are going on fast.

Unlike fossil fuels hydrogen can be produced from renewable energy sources easily. Producing hydrogen with water electrolysis is a known method. Besides, hydrogen can be produced from natural gas, biotechnical methods from solar energy [Riis et al., 2006]. The ability of using hydrogen as fuel in internal combustion engines has caused these kinds of works to increase in automotive industry. Hydrogen is used both in internal combustion engines as fuel and in fuel cell. Stored hydrogen fuel cell is magnanimous in this field as both capacity and battery life [Sossina., 2003].

In order to make the hydrogen energy usage common, improving systems able to store safe, in small compass in high quantity hydrogen has a great importance. Nowadays depending on the hydrogen usage fields it can be stored in solid matters as gas, liquid, or metal hydrides, chemical hydrides, nanotubes. When examining the storage conditions of hydrogen it has been observed that metal hydrides have utilisable features. Under the suitable conditions, as from NaBH₄ 0.213 g H₂ from NaH 0.084 g H₂ and from LiH 0.254 g H₂ per gram is obtained NaBH₄'s has a greater energy storage capability compared to other metal hydrides [Kojima et al., 2002].

In company with a suitable catalyzer sodium borohydride reveals two times hydrogen than that it stores as a result of the hydrolysis in water [Zhang et al., 2007; Guella et al., 2006].

NaBH₄ and NaBO₂ solutions not being combustible, using sodium metaborate in reproducing sodium borohydride, controlling reaction speed, materializing hydrogen gas obtaining even in the low temperatures, and providing hydrogen production with low cost great quantity are the most significant advantages of sodium borohydride usage [Raj et al., 2007; Wu et al., 2005; Sclapbach and Züttel., 2001; Grochala and Edwards., 2004]. The usage of low-cost catalyst in the extraction of hydrogen gas from sodium borohydride is significant in terms of economical. Cobalt is a cost efficient catalyst. Sodium borohydride is moisture sensitive in solid form and it swiftly spoils. However, the aqueous strong basic solutions of sodium borohydride are stable and they can be stocked quite a while. Sodium borohydride in this solution converts into sodium metaborate (NaBO₂) by getting off hydrogen gas when it is contacted with the convenient catalysts [Kojima et al., 2002; Kim et al., 2004; Amendola, et al., 2004]. The excitation control of hydrogen is easy. Apart from that, the sodium metaborate occurred can be converted into borohydride again [Kojima et al., 2002].

The control of hydrogen generation from sodium borohydride under favour of catalyst, the extraction of it in the requested conditions and amount are important for the production process to be able to work. Therefore, the modelling of hydrogen generation has great importance. In the study conducted, full factorial desing method has been used for the formation of the mathematical model of hydrogen generation. This method has been used in many studies. In the conducted study, full factorial design method has been utilized in overcoming “anionic red dye” in aqueous solutions [Cestari et al., 2008]. In another study, full factorial design method has been utilized in recuperating boronin aqueous solutions by absorption [Öztürk and Kavak., 2004]. In the other study, erosion durability of automotive clearcoats has been studied by full factorial desing method [Trezona et al., 2000].
2. Experimental

2.1. Materials

Co(NO₃)₂·6H₂O(%99) and sodium borohydride (98%) from Aldrich have been used as received. Deionized water has been distilled by water purification system. All glass ware and Teflon coated magnetic stir bars have been cleaned with acetone, followed by copious rinsing with distilled water before drying in an oven.

The reaction has been made reel in a 10 mL glass reactor. To hold reaction temperature steady, constant temperature circulator has been utilized. In all experiments, the reaction has been fulfilled in a 10 mL volume. The parameters used in the study have been indicated in Table-1.

The extraction of Co catalyst and hydrogen gas from NaBH₄ occurs according to the following reaction.

\[
\text{NaBH}_4 + 2\text{H}_2\text{O} \rightarrow \text{NaBO}_2 + 4\text{H}_2 \quad \Delta H = -300 \text{ kJ.mol}^{-1}
\]

2.2. Methods

In the full factorial design method all the combinations in the maximum and minimum level of the ranges are taken into consideration. Applying full factorial desing method is found by the formula of

\[
N = n^k
\]

the experiments that will be done \(k\) numbered variable and for \(n\) numbered level.

In the study done we have 4 variable values, \(k=4\). If these 4 factors change in two levels including maximum and minimum the number of experiments that must be done will be \(N=2^4=16\).

We have four factors in the study done consisting of \(Z_1, Z_2, Z_3\) and \(Z_4\). The range of these factors are as below:

\[
Z_{1\text{ min}} \leq Z_1 \leq Z_{1\text{ max}}, \quad Z_{2\text{ min}} \leq Z_2 \leq Z_{2\text{ max}}, \quad Z_{3\text{ min}} \leq Z_3 \leq Z_{3\text{ max}}, \quad Z_{4\text{ min}} \leq Z_4 \leq Z_{4\text{ max}}
\]

As is seen, each \(Z_k\) changes between its own maximum and minimum values like \(Z_{1\text{ min}}\) and \(Z_{1\text{ max}}\) (\(k=1,2,3,4\)) as indicated before, 16 experiments should be held in order to take mathematical model as the number of factors are 4.

Initially the following calculations are done:

\[
\begin{align*}
Z_k^0 &= \frac{Z_k^\text{max} + Z_k^\text{min}}{2}, \quad k = 1,2,3,4 \\
\Delta Z_k &= \frac{Z_k^\text{max} - Z_k^\text{min}}{2}, \quad k = 1,2,3,4
\end{align*}
\]  

Here \((Z_1^0, Z_2^0, Z_3^0, Z_4^0)\) point is called the center of experimental design. \(\Delta Z_k\) is the changeability value of sufficient variable. Here the minimum values of \(Z_{r-s}\) have been indicated with \(-1\) and maximum values have been shown with \(+1\) in table 1. Henceforward, in dimensionless coordinate system

\[
\begin{align*}
Y_x &= a_0 + a_1X_1 + a_2X_2 + a_3X_3 + a_4X_4 + a_{12}X_1X_2 + a_{13}X_1X_3 + a_{14}X_1X_4 + \\
&+ a_{23}X_2X_3 + a_{24}X_2X_4 + a_{34}X_3X_4 + a_{123}X_1X_2X_3 + a_{124}X_1X_2X_4 + a_{134}X_1X_3X_4 + \\
&+ a_{234}X_2X_3X_4 + a_{1234}X_1X_2X_3X_4
\end{align*}
\]

Mathematical model as above is composed. \(a_1, a_2, a_3, a_4, a_{12}, a_{13}, a_{14}, a_{23}, a_{24}, a_{34}, a_{123}, a_{124}, a_{134}, a_{234}\) and \(a_{1234}\) coefficients of the model calculated with the formula

\[
a_j = \frac{1}{N} \sum_{i=1}^{N} X_{ji} Y_i, \quad i=1, 16,
\]

and \(a_0\) coefficient is found with the formula
Table 1. The plan of full factorial design for four factors

<table>
<thead>
<tr>
<th>Experiment Number</th>
<th>X₁</th>
<th>X₂</th>
<th>X₃</th>
<th>X₄</th>
<th>Z₁</th>
<th>Z₂</th>
<th>Z₃</th>
<th>Z₄</th>
<th>Y₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>Z₁ min</td>
<td>Z₂ min</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₁</td>
</tr>
<tr>
<td>2.</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>Z₁ max</td>
<td>Z₂ max</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₂</td>
</tr>
<tr>
<td>3.</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>Z₁ min</td>
<td>Z₂ max</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₃</td>
</tr>
<tr>
<td>4.</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>Z₁ max</td>
<td>Z₂ max</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₄</td>
</tr>
<tr>
<td>5.</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>Z₁ min</td>
<td>Z₂ max</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₅</td>
</tr>
<tr>
<td>6.</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>Z₁ max</td>
<td>Z₂ max</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₆</td>
</tr>
<tr>
<td>7.</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>Z₁ min</td>
<td>Z₂ max</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₇</td>
</tr>
<tr>
<td>8.</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>Z₁ max</td>
<td>Z₂ max</td>
<td>Z₃ min</td>
<td>Z₄ min</td>
<td>Y₈</td>
</tr>
<tr>
<td>9.</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>Z₁ min</td>
<td>Z₂ min</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₉</td>
</tr>
<tr>
<td>10.</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>Z₁ max</td>
<td>Z₂ min</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₀</td>
</tr>
<tr>
<td>11.</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>Z₁ min</td>
<td>Z₂ max</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₁</td>
</tr>
<tr>
<td>12.</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>Z₁ max</td>
<td>Z₂ max</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₂</td>
</tr>
<tr>
<td>13.</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>Z₁ min</td>
<td>Z₂ min</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₃</td>
</tr>
<tr>
<td>14.</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>Z₁ max</td>
<td>Z₂ min</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₄</td>
</tr>
<tr>
<td>15.</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>Z₁ min</td>
<td>Z₂ max</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₅</td>
</tr>
<tr>
<td>16.</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>Z₁ max</td>
<td>Z₂ max</td>
<td>Z₃ max</td>
<td>Z₄ max</td>
<td>Y₁₆</td>
</tr>
</tbody>
</table>

\[ a_0 = \frac{1}{N} \sum_{i=1}^{N} Y_i \]  \hspace{1cm} (6)

After that, four parallel experiments are held in experiment centre, namely at the point of \((Z_1^0, Z_2^0, Z_3^0, Z_4^0)\) and the values \(Y_1^0, Y_2^0, Y_3^0\) and \(Y_4^0\) out parameters are calculated pursuant to them. Then the average values of these out parameters are found:

\[ \bar{Y}^0 = \frac{\sum_{u}^{4} Y_u^0}{4} \]  \hspace{1cm} (7)

Henceforward

\[ S_i^2 = \frac{\sum_{u}^{4} (Y_u^0 - \bar{Y})^2}{4} \]  \hspace{1cm} (8)

And

\[ S_{a_u}^2 = \frac{S_i^2}{16} = \frac{S_i^2}{4} \]  \hspace{1cm} (9)

are calculated. By taking the calculated values into consideration and by using Student criteria,

\[ t_m = \frac{|a_m|}{S_{a_u}} \]  \hspace{1cm} (10)

it is found \(t=\text{N}-(\text{n}+1)=16-2-1=13\), \(t_p(f) = f(13) = 2.16\) from specific Student criteria table for these values by using \(P=0.05\) condition for the formula and the mathematical model in formula and, another formula. If each calculated \(t_m\) value with formula is larger 2,16, these values are utilized in the model of \(Y_s\), and the rest, namely the values that are smaller than 2,16 aren’t utilized. Henceforward, variances may be in in the mathematical model.

Then the validity of new model is checked by Fisher criteria :

\[ F = \frac{S_2^2}{S_1^2} \]  \hspace{1cm} (11)
From hence

\[ S_2^2 = \frac{\sum_{i=1}^{16} (Y_i - \bar{Y}_i)^2}{N} \]  \hspace{1cm} (12)

The mathematical model in Y, composed in dimensionless coordinate system cannot exactly enable true process. To compose the valid mathematical model of natural process, the following change of variable formula is utilized in Y model:

\[ X_j = \frac{Z_j - Z_j^0}{\Delta Z_j}, \text{ j=1, 2, 3, 4.} \]  \hspace{1cm} (13)

After notable mathematical conversions, mathematical model is generally taken as follows in natural coordinate system:

\[ Y = \sum_{j=1}^{4} b_j Z_j^4 + b_{123} Z_1 Z_2 Z_3 + b_{125} Z_1 Z_2 Z_4 + b_{134} Z_1 Z_3 Z_4 + b_{234} Z_2 Z_3 Z_4 + b_{1234} Z_1 Z_2 Z_3 Z_4 \]  \hspace{1cm} (14)

Here are the obtained new values in the wake of altering the values and the formula in b0, b1, b2, b3, b4, b12, b13, b14, b23, b24, b123, b124, b134, b234 and b1234.

\section*{3. Results and Discussion}

Let’s compose the mathematical model of process with the method we explained before.

\[ \text{NaBH}_4 + 2\text{H}_2\text{O} \rightarrow \text{NaBO}_2 + 4\text{H}_2 \quad \Delta H = -300 \text{kJ.mol}^{-1} \]  \hspace{1cm} (15)

The attempts have been made for operating ranges, intervals and this value is decided. Here in:

\[ Z_1 - \text{NaBH}_4 \text{ amount, with mM ; } \quad Z_3 - \text{Temperature, with } ^{\circ}\text{C ;} \]
\[ Z_2 - \text{Catalyst amount, with mM ; } \quad Z_4 - \text{time; with minute, has been shown.} \]

The change intervals of Z1, Z2, Z3 and Z4 parameters are as follows:

\[
\begin{align*}
100 & \leq Z_1 \leq 500 \\
0.5 & \leq Z_2 \leq 2.5 \\
20 & \leq Z_3 \leq 40 \\
3 & \leq Z_4 \leq 20
\end{align*}
\]  \hspace{1cm} (16)

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

\[ Y = 29.93725 + 5.432X_1 + 9.174X_2 + 16.38125X_3 + 16.18475X_4 + 2.17425X_1X_2 + 3.18025X_1X_3 + 4.78925X_1X_4 + 6.333X_2X_3 + 5.185X_2X_4 + 9.70375X_3X_4 + 2.6305X_1X_3X_4 + 2.189X_2X_3X_4 + 2.704X_2X_3X_4 + 3.8655X_2X_3X_4 + 3.8655X_2X_3X_4 + 1.65425X_1X_2X_3X_4 \]  \hspace{1cm} (17)

4 parallel experiments have been held at the point of \((Z_1^0, Z_2^0, Z_3^0, Z_4^0)\) which is the center of Full factorial design plan so as to assess the values of Y, model by Styudent criteria. The centre of our experiment plan is the point consisting of \((300; 1.5; 30; 11.5)\) coordinates. The result of these 4 parallel experiments conducted in this central point as follows:

\[ Y_1^0 = 30,301; \quad Y_2^0 = 33,5588; \quad Y_3^0 = 30,458; \quad Y_4^0 = 32,982. \]  \hspace{1cm} (18)

From hence

\[ \bar{Y}^0 = \frac{Y_1^0 + Y_2^0 + Y_3^0 + Y_4^0}{4} = 31,82495 \]  \hspace{1cm} (19)

\[ S_1^2 = 2,133994 \] is found by using formula.

It is found as \(S_{ma} = \frac{S_1^2}{\sqrt{16}} = \frac{2,133994}{4} = 0,533499\) from formula. Since the found \(S_{ma}\) is a quite small number, all \(t_m\) numbers having valency with formula have become larger than \(t_p(f)=2,16\) number.
And this indicates that all the found coefficients \( a_0, \ a_1, a_2, a_3, a_4, a_{12}, a_{13}, a_{14}, a_{23}, a_{24}, a_{34}, a_{123}, a_{124}, a_{134}, a_{234} \) are effective. Thus, all the coefficient values of model are utilizable. For example, let’s check whether the coefficients of the numbers of \( a_0, a_1 \) and \( a_{1234} \) are utilizable or not:

\[
\begin{align*}
\text{For } a_0: & \quad t_0 = \frac{|a_0|}{S_{a_0}} = \frac{29,93725}{0,533499} = 56,11491306 \gg 2,16 \\
\text{For } a_1: & \quad t_1 = \frac{|a_1|}{S_{a_1}} = \frac{5,432}{0,533499} = 10,18183727 \gg 2,16 \\
\text{For } a_{1234}: & \quad t_{1234} = \frac{|a_{1234}|}{S_{a_{1234}}} = \frac{1,65425}{0,533499} = 3,1007558 \gg 2,16
\end{align*}
\]

The utility of the other coefficient values has been determined with this method, and it has been seen that all of them are utilizable.

Experimental errors were determined by the formula

\[
S_0 = \frac{\sum_{i=1}^{N} \sum_{k=1}^{M} (Y_{ik} - \bar{Y})^2}{N(M-1)}
\]

(21)

where \( N \) – a number of experiments; \( M \) – a number of parallel experiments; \( k \) – a number of factors (in the given case \( N=16, M=3 \) and \( k=4 \)).

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 \( \bar{Y} \), statistically does not exceed the errors of the experiment \( S_2^2 \).

Tabulated values of Fisher criterion for \( P=0.05 \) is \( f_1=N-k-1=11, \ f_2=M-1=2 \). Therefore \( F_{1-1}(f_1,f_2) = 19.41 \). Fisher criterion was calculated from the formulas (11) and (12). \( S_2^2 = 9,1204 \).

As \( F= 4.825927 \) and \( F_{1-1}(f_1,f_2) = 19.41 \), the mathematical model of production of hydrogen gas at sodiumborohydride with cobalt catalyst in dimensionless system of co-ordinates adequately describes the experiment carried out. Co-ordinate of centre of a plan in full scale \( (Z_1^0, Z_2^0, Z_3^0, Z_4^0) \) and variation units \( (\Delta Z_1, \Delta Z_2, \Delta Z_3, \Delta Z_4) \) with respect to axes \( Z_1, Z_2, Z_3, Z_4 \) were calculated with the formulas (3) and tabulated in Table 2.

Table 2. Calculated values of \( Z_i^0 \) and \( \Delta Z_i \)

<table>
<thead>
<tr>
<th>( Z_1^0 )</th>
<th>( Z_2^0 )</th>
<th>( Z_3^0 )</th>
<th>( Z_4^0 )</th>
<th>( \Delta Z_1 )</th>
<th>( \Delta Z_2 )</th>
<th>( \Delta Z_3 )</th>
<th>( \Delta Z_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>1.5</td>
<td>30</td>
<td>11.5</td>
<td>200</td>
<td>1</td>
<td>10</td>
<td>8.5</td>
</tr>
</tbody>
</table>

In order to take the mathematical model of the process in natural coordinate system, It has been benefited from change of variable operation as the following:
After altering variable values in the formula and after making some notable mathematical abbreviations by using, the following mathematical model has been composed in natural coordinate system:

\[
Y_{3i} = \frac{Z_1 - Z_1^0}{\Delta Z_1} = \frac{Z_1 - 300}{200} \\
X_2 = \frac{Z_2 - Z_2^0}{\Delta Z_2} = \frac{Z_2 - 1.5}{1} = Z_2 - 1.5 \\
X_3 = \frac{Z_3 - Z_3^0}{\Delta Z_3} = \frac{Z_3 - 30}{10} \\
X_4 = \frac{Z_4 - Z_4^0}{\Delta Z_4} = \frac{Z_4 - 11.5}{8.5} = \frac{2Z_4 - 23}{17}
\] (23)

After altering variable values in the formula and after making some notable mathematical abbreviations by using, the following mathematical model has been composed in natural coordinate system:

\[
Y_{3i} = -4.992424 + 0.01691Z_1 + 1.79647Z_2 + 0.31981Z_3 - 0.53721Z_4 - \\
- 0.00982Z_1Z_2 - 0.00053Z_1Z_3 + 0.00049Z_1Z_4 + 0.05145Z_2Z_3 - 0.36479Z_2Z_4 + \\
+ 0.04202Z_2Z_4 + 0.000196Z_1Z_3Z_4 - 0.00163Z_1Z_4 + 0.000013Z_2Z_4 + \\
+ 0.016283Z_2Z_3Z_4 + 0.000097Z_1Z_2Z_4 + \frac{0.04202}{Z_1Z_2Z_3Z_4}
\] (24)

The values and the relevance of the mathematical models of the experiment conducted taken in dimensionless coordinate system and besides in natural coordinate system have been given in Figure 1. As is seen from the figure, the values of basic materials acquired in both dimensionless coordinate system and in natural coordinate system are fairly close. Therefore, the process can be studied in larger parameters by using the composed mathematical model.

4. Conclusions

The usage of mathematical models looms large in the optimization and control of chemical processes. Therefore, the mathematical models of chemical processes are to be found. With the usage of the notable mathematical models of chemical processes, it will be possible to check the performance of these processes automatically.

In this study, the formation of the mathematical model of cobalt catalyst and hydrogen gas extraction from sodium borohydride by using full factorial desing method has been studied. Firstly, the basic parameters of chemical process have been selected. What parameters selected will remain stable and what parameters will be variable factors have been determined. Thus, the mathematical model of four-factor test such as the amount of NaBH₄, the amount of catalyst, temperature and time has been composed.

Firstly, the valency of the coefficient of mathematical model composed in the dimensionless coordinate system has been checked by Student criteria, and it has been founded that all the coefficients can be used. Then the mathematical model of chemical process in real coordinate system has been composed by transacting change of variable. The validity of mathematical model composed in real coordinate system has been calculated by Fisher criteria, and it has also been shown in graphic form.

It has been determined that the achievement of the mathematical model and hyrogen gas acquired in the wake of the study conducted in definite parameters and in required amounts is possible.
**Figure 1:** Graphical display of the validity of the process: $Y_{exp} -$ values received experientially; $Y_{x\ model} -$ calculated values in dimensionless coordinate system by mathematical model; $Y_{z\ model} -$ calculated values in natural coordinate system by mathematical model.

**Table 3. Full factorial design plan and resentful values of parameters**

<table>
<thead>
<tr>
<th>Parameters in dimensionless coordinate system</th>
<th>Natural coordinate system</th>
</tr>
</thead>
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<tr>
<td>EXP NO. $X_0$ $X_1$ $X_2$ $X_3$ $X_4$ $X_5$ $X_6$ $X_7$ $X_8$ $X_9$ $X_{10}$ $X_0$ $X_1$ $X_2$ $X_3$ $X_{10}$ $Y_{exp}$ $Y_{x\ model}$</td>
<td>$Z_0$ $Z_1$ $Z_2$ $Z_3$ $Y_{z\ model}$</td>
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References