ADVANCE RESEARCH JOURNAL OF MULTIDISCIPLINARY DISCOVERIES
ISSN : 2456-1045
VOL.36 I ISSUE-1 I CHAPTER-6
PUBLISHER : INTERNATIONAL JOURNAL FOUNDATION (IJF)

All Rights Reserved

Mathematical Modeling of the Alcoholysis process of secondary polyethylenerephthalate with Diethylene Glycol

***A.B. Juraev[1], R.A. Khabibullaev[2], F.A. Magrupov[3], M.G. Alimukhamedov[4]**

[1,2,3,4](*Tashkent chemical-technology institute)*

ABSTRACT

This article discusses the mathematical modeling of the alcoholysis process of recycled polyethylene terephthalate. A mathematical equation of the process with factors such as hydroxyl, acid, ester number and number average molecular weight affecting the properties of hydroxyl-containing polyether polyols has been revealed. The adequacy of the model and results is shown, the deviation of indicators by the mathematical model from practical values does not exceed 5%.

Keywords : Alcoholysis process of recycled polyethylene terephthalate, input parameters, mathematical model, adequacy, comparisons.

ORIGINAL RESEARCH ARTICLE

ISSN : 2456-1045 (Online)
(ICV-CHT/Impact Value): 72.30
(GIF) Impact Factor: 5.188
Publishing Copyright @ International Journal Foundation
Journal Code: ARJMD/CHT/V-36.0/I-1/C-6/APRIL-2019
Category : CHEMICAL TECHNOLOGY
Volume : 36.0/**Chapter-** VI/**Issue** -1 (APRIL-2019)
Journal Website: www.journalresearchijf.com
Paper Received: 22.04.2019
Paper Accepted: 01.05.2019
Date of Publication: 15-05-2019
Page: 32-39

Name of the Corresponding author:
Dr. A.B. Juraev*

Tashkent chemical-technology institute , Uzbekistan

CITATION OF THE ARTICLE

Juraev A.B., Khabibullaev R.A., Magrupov F.A., Alimukhamedov M.G.; (2019) Mathematical Modeling of the Alcoholysis process of secondary polyethylenerephthalate with Diethylene Glycol; *Advance Research Journal of Multidisciplinary Discoveries;* 36(6) pp. 32-39

ADVANCE RESEARCH JOURNAL OF MULTIDISCIPLINARY DISCOVERIES

I. INTRODUCTION

Polyethylene terephthalate (PET) has made a real revolution in the world of packaging, radically changing the situation on the world market in this area of production. An important feature of PET is the relatively easy processing of its waste. High technological effectiveness of PET recycling and wide possibilities of their utilization have made them the most recyclable in the world. The main contribution to the composition of PET waste is made by plastic bottles from under drinks [1]. From 1990 to 1995 growth rates of world PET demand averaged 15% per year, from 1995 to 2000 growth averaged already 20% annually [2].

According to the prediction of PCI (PET Packaging Resin & Recycling Ltd) for 2014, about 70% of the collected PET containers will be processed into staple fibers and nonwovens, 11% into films, 12% into bottles, for food and non-food purposes. In 2013, the production of primary PET bottle prescriptions exceeded 20 million tons. According to experts, the total number of units produced from them, mainly in the form of bottles, exceeds 500 billion units. However, it is known that the reuse of 1 ton of PET saves up to 5 m^3 of the volume of landfill for waste disposal. High consumer properties of containers made of PET, provided this material with a rapid growth in the production of packaging for beverages and food products [3]. At the end of 2015, approximately 70 million tons of PET were produced and 49.3 million tons of them are used as yarns, 20.6 million tons for bottles. According to the company Statistics MRC in 2015, the PET market amounted to 36.13 billion dollars and by 2022 it could be 65.4 billion dollars. These data indicate an increase in PET in the year by 8-9% [4],[5].

PET containers are currently actively replacing such traditional types of raw materials for packaging as glass and cardboard. Extensive use of these materials, in addition to the advantages of ease of transportation, has caused to environmental pollution. This led to a search for ways to dispose of them.

Today, PET waste accounts for more than 30% of all plastics waste, 80% of which is now being recycled [6]. The main contribution to the composition of PET waste is made by plastic bottles from under drinks [7].

Recycling of this waste is carried out by physical and chemical methods. Despite the cheapness of PET processing using physical methods, methods of chemical processing, namely glycolysis, are increasingly being investigated. With this method, you can obtain the raw materials for glues, unsaturated polyesters, polyurethane foams, etc. [8]. In practice, ethylene glycol, propylene glycol, diethylene glycol and triethylene glycol, etc. are used as reagents.

For example, the authors showed that glycolysis of polyethylene terephthalate under optimal conditions (an excess of ethylene glycol (EG: PET = 5.5), under microwave exposure results in bis (*hydroxyethyl terephthalate*) with a yield of 78% for 35 minutes. Using microwave exposure, scientists have reached significant decrease in the activation energy and duration of the process [9]. The factors that determine the content of diethylene glycol in PET have been considered. It has been noted that in order to control the content of diethylene glycol in PET, it is necessary to regulate the molar ratio of ethylene glycol and purified terephthalic acid at the esterification stage [10].

It should be noted that the study of glycolysis of PET waste glycols (ethylene, diethylene, propylene glycols, etc.) was conducted by various authors [11]. In these studies, PET waste was subjected to glycolysis mainly at a ratio of 4 moles of glycol to one elementary unit of the polymer, i.e. carried out complete alcoholysis. At the same time, different authors emphasize various aspects of the overall alcoholysis process of solid PET waste.

Thus, the degree of cleavage of PET solid waste with ethylene glycol depends on two components: the first causes an increase in the rate of glycolysis according to a logarithmic dependence, the second is a slowdown exponentially and characterizes the crystallization of the material during glycolysis. The overall effective rate of the glycolysis process of PET is determined by the competing influence of these components. In the process of heating solid waste at 120–200°C, PET crystallizes, the extent of which affects the rate of glycolysis, that is, the depth of the process depends on the initial physical structure of the material.

We also investigated the process of destruction of PET waste with a wide range of the amount of destructive agent. Diethylene glycol (DEG) was used as a destructive agent [12].

Recently, in order to carry out a full analysis of processes in chemical production, more and more attention has been paid to modern methods of describing processes, in particular, mathematical modeling. Over time, more and more complicated experiments, increasing the amount of information, it is becoming increasingly difficult to analyze the data during the experiment and manage complex experimental setups.

Computer simulation allows you to determine the patterns and statistical relationships between random variables of the experiment. Establishing the connection parameters of the experiment, you can accurately describe the nature of the changes, to conduct the minimum number of experiments or to predict and identify difficult patterns of a particular part of the process [13],[14],[15].

From the analysis of literature data it can be concluded that the above processes of PET alcoholization have not been well studied, and fully described. In addition, very few works have been devoted to computer simulation of the process of PET glycolysis. For example, V.V. Oleinik et al. reported about the development of a computerized model of PET equilibrium glycolysis, followed by a distillation process.

The influence of the ratio of PET on DEG, the distillation step, the vacuum pressure on the molecular weight (MM) and the composition of the distillation mixture was studied. The changes in oligomers MM of the composition of the distilled mixture were studied. This model mainly helps to clarify the amount of distilled and low molecular weight products in the process of glycolysis. And the optimization of the process of glycolysis and the production of alcoholysis products by predetermined properties have not been described.

II. PROBLEM DEFINITION AND METHODS OF RESEARCH

The selected problem is solved with the help of experimental studies. The following substances are used for the experiments: secondary polyethylene terephthalate in the form of flakes, diethylene glycol (GOST 10136-77), the amount of the basic substance — 99.5%, 20 = 1.445. 0.7 mol e.link is added in a four-necked flask equipped with a stirrer, a circulating cooler, a thermometer, a capillary to inert gas inlet, add. SPET, 1-4 moles of diethylene glycol.

Within 10-15 minutes we raise the temperature to 100°C and turn on the stirrer, then the temperature of the reaction mass with constant stirring from 180±5 to 220±5°C. The synthesis is carried out at a constant transmission of inert gas (nitrogen). After reaching a temperature of 220 ± 5 ° C, the duration of the synthesis is 3-15 hours. In this regard, this report is devoted to the creation of a mathematical model of the process of alcoholysis of PET waste with DEG. In the process of alcoholysis, the main factors influencing on the physicochemical properties of alcoholysis products are the duration, the ratio of products, temperature and the amount of catalysts added.

These factors fully alter the properties of alcohol products. For example, an increase in the duration of the synthesis dramatically reduces the molecular weight; the ratio results in a product from solid to viscous flow; temperature and catalysts also strongly influence on the glycolysis process. These theoretical patterns are noted in the works of V.V. Korshak. In this regard, the duration, the ratio of monomers and temperature were chosen as factors influencing on the optimization of the process.

ADVANCE RESEARCH JOURNAL OF MULTIDISCIPLINARY DISCOVERIES

A series of experiments have been conducted in order to study the conditions of the formation processes of alcoholysis products. Based on the results of experiments, mathematical models were developed for obtaining PET alcohol-DEG products by the procedure described in [15], with some re-issuing of generally accepted tables (tables 2 and 4).

The value of this mathematical description lies in the fact that it: 1) gives qualitative and quantitative information about the influence of each factor; 2) allows you to calculate the value of the response function for a given mode of technological process. In addition, based on the methods of planning experiments, one can quantitatively describe the properties of complex synthesized products.

The method of a full factorial experiment makes it possible to obtain a mathematical description of a chemical process in a certain area of factor space, lying in a neighborhood of the selected point with coordinates $x_{01}, x_{02}, \dots x_{0i}, \dots x_{0n}$. Here, $i = 1 \dots n;$ where n - the number of factors.

Using a full factorial experiment, we find a mathematical description of the formation of 4 response functions: y_1 is a hydroxyl number (N_{OH}), y_2 is an ether number (NE), y_3 is an acid number (NH), y_4 is the number average molecular weight ($M_{avg.}$) in the form of equation (1).

$$y = b_0 + b_1x_1 + b_2x_2 + \cdots + b_nx_n + b_{12}x_1x_2 + \cdots + b_{(n-1)n}x_{n-1}x_n \quad \dots\dots\dots\dots \quad (1)$$

It includes the absolute term b_0, the terms as products of the regression coefficients b_i by x_i, and terms containing the pair products of the coded variables. All factors in the course of a full factorial experiment vary at two levels, corresponding to the values of the coded variables +1 and -1.

III. EXPERIMENTAL RESULTS AND EVALUATION OF THE ERRORS

Table 1 : The following table 1 shows the conditions of the experiment.

Name	Indication in the natural and coded forms	Unit of measurement	Variation level			Measurement step
			Lower	Main	Higher	
Content of DEG in the elementary link of PET at alcoholysis	M	mole	0,7	2,35	4	1,65
	x_1	-	-1	0	+1	1
Duration of alchoholysis	τ	hour	3	9	15	6
	x_2	-	-1	0	+1	1
Temperature of reaction condition	t	^{0}C	180	200	220	20
	x_3	-	-1	0	+1	1

Before planning an experiment, you need to make sure that the experiments are reproducible. For this purpose, we conducted three series of parallel experiments, the results of which (y_{j1}, y_{j2}, and y_{j3}) are summarized in Table 2.

For each series of experiments, the variance estimates were calculated by formula (s_j^2):

$$s_j^2 = \frac{1}{k-1}\sum_{i=1}^{k}\left(y_{ji} - \bar{y}_j\right)^2 \quad \dots\dots\dots\dots(2)$$

where: $\bar{y}_j$ – averaged value j – response function; i – series number; k – the number of parallel experiments conducted under the same conditions ($k = 3$).

Table 2

№	x_1	x_2	x_3	y_{11}	y_{12}	y_{13}	s_1^2	y_{21}	y_{22}	y_{23}	s_2^2	y_{31}	y_{32}	y_{33}	s_3^2	y_{41}	y_{42}	y_{43}	s_4^2
1	-1	-1	-1	6,3	6,1	6,2	0,01	458	482	506	576	2,4	2,2	2,3	0,01	572	545	533	399
2	+1	-1	-1	19,2	18,6	19,2	0,12	190	182	186	16	5,4	5,3	4,9	0,07	409	447	434	373
3	-1	+1	-1	8,2	7,8	8	0,04	383	391	411	208	3,7	3,6	3,5	0,01	414	445	449	367
4	+1	+1	-1	19,5	20,1	18,9	0,36	182	170	167	63	5,4	5,7	5,1	0,09	248	245	257	39
5	-1	-1	+1	7,4	7,6	8,4	0,28	327	340	305	313	3,1	3,3	3,2	0,01	380	388	372	64
6	+1	-1	+1	20,6	19	20,4	0,76	185	182	167	93	6,6	6,6	5,7	0,27	302	284	284	108
7	-1	+1	+1	8,7	8,5	8,6	0,01	336	336	288	768	3,5	3,3	3,7	0,04	352	362	321	457
8	+1	+1	+1	22,7	21,3	22	0,49	172	167	171	7	6,3	6,5	7	0,13	182	187	165	133

According to the formula (3) we find the calculated value of the Cochren criterion (G_p):

$$G_p = \frac{max\, s_i^2}{\sum_{i=1}^{N} s_i^2} \quad \text{.....(3)}$$

here: i – the number of experience; N – the number of experiments ($N = 8$); $max\, s_i^2$ – the maximum value of the variance; $\sum_{i=1}^{N} s_i^2$ – the sum of the variance estimates.

The critical value of the Cochren test (G=0,871) was determined with the number of degrees of freedom *f=k-1=2* from [12]. The results obtained are recorded in table 3.

Table 3 : Results of statistic processing series of experiments

Function of отклика	m槓泥 s_i^2	$\sum_{i=1}^{N} s_i^2$	G_p	G
y_1	1,33	3,37	0,395	0,871
槔$_2$	768	2044	0,376	0,871
y_3	0,27	0,63	0,429	0,871
y_4	457	1940	0,236	0,871

Thus, the fulfillment of the condition $G_p < G$ indicates that the experiments performed are reproducible (see Table 3).

Further in the table 4 we give the planning matrix of the PFE -2^3 experiment, in which the factors are given on a dimensionless scale. The bottom part shows the scalar products of factors with averaged values of output values ($\Sigma x\bar{y}_i$).

Table 4 : Experiment-planning matrix of PFE-2^3

№	x_0	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$	$\bar{y}_1$	$\bar{y}_2$	$\bar{y}_3$	$\bar{y}_4$
1	1	-1	-1	-1	1	1	1	-1	6,2	482	2,3	550
2	1	1	-1	-1	-1	-1	1	1	19	186	5,2	430
3	1	-1	1	-1	-1	1	-1	1	8	395	3,6	436
4	1	1	1	-1	1	-1	-1	-1	19,5	173	5,4	250
5	1	-1	-1	1	1	-1	-1	1	7,8	324	3,2	380
6	1	1	-1	1	-1	1	-1	-1	20	178	6,3	290
7	1	-1	1	1	-1	-1	1	-1	8,6	320	3,5	345
8	1	1	1	1	1	1	1	1	22	170	6,6	178
$\Sigma x\bar{y}_1$	111,1	49,9	5,1	5,7	-0,1	1,3	0,5	2,5				
$\Sigma x\bar{y}_2$	2228	-814	-112	-244	70	222	88	-78				
$\Sigma x\bar{y}_3$	36,1	10,9	2,1	3,1	-1,1	1,5	-0,9	1,1				
$\Sigma x\bar{y}_4$	2859	-563	-441	-473	-143	49	147	-11				

Based on the experiment-planning matrix, the regression coefficients were calculated using formulas (3-5):

$$b_0 = \frac{1}{N}\sum_{i=1}^{N} \bar{y}_i; \quad (3)$$

$$b_j = \frac{1}{N}\sum_{i=1}^{N} x_{ij}\bar{y}_i; \quad (4)$$

$$b_{lm} = \frac{1}{N}\sum_{i=1}^{N} x_{il}x_{im}\bar{y}_i; \ (l \neq m) \quad (5)$$

To determine the significance of the regression coefficients, we calculate the experiment error ($S_{(y)i}$) and the Student's criteria (t_i) respectively, using formulas (6-7) with the number of experiments *N=8* and the number of parallel experiments *k=3*:

$$S_{(y)i} = \sqrt{\frac{\sum(y_i - \bar{y})^2}{N \cdot k}} \quad (6)$$

$$t_i = \frac{b_i}{S_{(y)i}} \quad (7)$$

To assess the significance of the regression coefficients, the critical value of Student's criterion ($t_{кр}$) is necessary. To define it, we use the formula in Excel (=Studen't dist.(significance level; degree of freedom)). For the level of significance q=0,05 and the number of degrees of freedom *f=N(k-1)*= 16 the critical value of the Student's criterion is 2,12. We reset the values of the regression coefficients corresponding to t_i, the modulus of which is less than $t_{кр}$ and leave significant regression coefficients for the description of the mathematical model of the object under study.

The results of the calculations are entered in table 5. In table 5, in the right column, the error of experience ($S_{(y)i}$) is added to the corresponding output value y_i.

Table 5

Regression coefficients									Experiment errors$_{yi}$
№	b_0	b_1	b_2	b_3	b_{12}	b_{13}	b_{23}	b_{123}	
y_1	13,89	6,24	0,64	0,71	-0,01	0,16	0,06	0,31	0,294
y_2	278,5	-101,75	-14	-30,5	8,75	27,75	11	-9,75	9,229
y_3	4,51	1,36	0,26	0,39	-0,14	0,19	-0,11	0,14	0,162
y_4	357,38	-70,38	-55,13	-59,13	-17,88	6,13	18,38	-1,38	8,991
Student criterion									
№	t_0	t_1	t_2	t_3	t_{12}	t_{13}	t_{23}	t_{123}	
y_1	47,24	21,22	2,18	2,41	-0,03	0,54	0,2	1,05	
y_2	30,18	-11,03	-1,52	-3,3	0,95	3,01	1,19	-1,06	
y_3	27,84	8,4	1,6	2,41	-0,86	1,17	-0,68	0,86	
y_4	39,75	-7,83	-6,13	-6,58	-1,99	0,68	2,04	-0,15	
Regression coefficients value									B
№	b_0	b_1	b_2	b_3	b_{12}	b_{13}	b_{23}	b_{123}	
y_1	13,89	6,24	0,64	0,71	0	0	0	0	4
y_2	278,5	-101,75	0	-30,5	0	27,75	0	0	4
y_3	4,51	1,36	0	0,39	0	0	0	0	3
y_4	357,38	-70,38	-55,13	-59,13	0	0	0	0	4

In Table 5, in the lower right column, the number of significant coefficients of the corresponding output quantity y_i was pre-computed.

At the same time, the required mathematical models will take the form indicated in formula (8):

$$y_1 = 13,89 + 6,24x_1 + 0,64x_2 + 0,71x_3$$
$$y_2 = 278,5 - 101,75x_1 - 30,5x_3 + 27,75x_{13} \quad (8)$$
$$y_3 = 4,51 + 1,36x_1 + 0,39x_3$$
$$y_4 = 357,38 - 70,38x_1 - 55,13x_2 - 59,13x_3$$

Now we check the adequacy of the obtained mathematical models - the ability of models to describe the response surface well enough and to predict the results of experiments. For this purpose, table 6 shows the value of the regression coefficients according to a mathematical model and a laboratory experiment.

Table 6

№	x_1	x_2	x_3	Values by experiments of y_i				Value on a mathematical model y_i			
				y_1	y_2	y_3	y_4	y_1	y_2	y_3	y_4
1	-1	-1	-1	6,2	482	2,3	550	6,3	438,5	2,8	542
2	1	-1	-1	19	186	5,2	430	18,8	179,5	5,5	401,3
3	-1	1	-1	8	395	3,6	436	7,6	438,5	2,8	431,8
4	1	1	-1	19,5	173	5,4	250	20,1	179,5	5,5	291
5	-1	-1	1	7,8	324	3,2	380	7,7	322	3,5	423,8
6	1	-1	1	20	178	6,3	290	20,2	174	6,3	283
7	-1	1	1	8,6	320	3,5	345	9	322	3,5	313,5
8	1	1	1	22	170	6,6	178	21,5	174	6,3	172,7

Further we calculate adequacy of dispersion by formula (9):

$$S_i^2 = \frac{1}{N-B}\sum_{i=1}^{N}(\bar{y}_i - y_i)^2 \qquad (9)$$

here: *N* - number of choices (*N=8*); *B* - quantity of significant terms.

For determination of criterion of Fischer we will calculate dispersion of reproducibility on formula (10):

$$S^2_{repr.} = S^2_y \qquad (10)$$

We determine a calculated value of criterion of Fischer by formula (11):

$$F_p = S_i^2 / S^2_{repr.} \qquad (11)$$

To determine the critical value of the Fisher criterion (F) we use the formula in Excel (=FPAdist.(significance level; f_{1ad}; f_{2a})), when calculating it, we take the significance level q=0,05 and the coefficients $f_{1ad} = N\text{-}B$ and $f_{2ad} = k\text{-}1 = 2$.

Considering the above we make calculation of adequacy of mathematical model. Results of calculation are given in tabel 7.

Table 7 : Results of calculation of mathematical model adequacy

Parameters for adequacy calculation	y_1	y_2	y_3	y_4
Adequacy of dispersion (S^2_i)	-0,748	977,25	0,026	1366
Dispersion of reproducibility ($S^2_{repr.\,i}$)	0,0864	85,174	0,0262	80,838
Calculated value of criterion of Fischer(F_p)	-8,654	11,474	0,991	16,898
Critical value of Firesh criterion (F)	19,247	19,247	19,296	19,247

Fulfillment of condition $F_p < F$ in table 7 means the mathematical model is adequate.

Now we give the obtained equations in natural form, referring to the basic level (z_i^0), step (Δz_i), upper (z_{max}) and lower (z_{min}) level of variation of factors, using the formula (12):

$$x_i = \frac{z_i - z_i^0}{\Delta z_i}; \qquad z_i^0 = \frac{z_{max} + z_{min}}{2}; \qquad \Delta z_i = \frac{z_{max} - z_{min}}{2}; \qquad (12)$$

Making algebraic calculations, we form a mathematical model of the parameters of the products of alcoholysis - hydroxyl number y_1 (N_{OH}), ether number y_2 (N_E), acid number y_3 (N_H), number average molecular weight y_4 ($M_{aver.}$):

$$\begin{aligned} y_1 &= -3,06 + 3,78z_1 + 0,11z_2 + 0,04z_3 \\ y_2 &= 1123,64 - 229,85z_1 - 3,5z_3 + 0,84z_{13} \\ y_3 &= -1,33 + 0,82z_1 + 0,02z_3 \\ y_4 &= 1131,61 - 42,65z_1 - 9,19z_2 - 2,96z_3 \end{aligned} \qquad (13)$$

In order to test the predictive properties of these models, we conducted several laboratory experiments at points which aren't coinciding the plan of an experiment. The results of the experiments are given in table. 9.

Table 9

Parameters	Designation	Results of the experiments							
		1	2	3	4	5	6	7	8
Input factors in natural form	z_1	1	2	3	1	2	3	1,5	2,5
	z_2	5	10	12	7	9	9	8	13
	z_3	200	190	190	210	200	190	210	200
Indexes by mathematical model	y_1	9,3	13,2	17,2	9,9	13,5	16,9	11,9	15,8
	y_2	362	318	248	335	300	248	308	269
	y_3	3,49	4,11	4,93	3,69	4,31	4,93	4,1	4,72
	y_4	451	392	331	403	372	359	373	314
Results of laboratory experiments	y_1	8,9	13	17	9,5	12,9	16,8	11,5	15,3
	y_2	380	320	245	350	300	250	300	270
	y_3	3,35	4,18	5,1	3,55	4,35	4,86	3,9	4,93
	y_4	462	375	335	415	355	375	380	302
Deviation, %	y_1	4,3	1,5	1,2	4	4,4	0,6	3,4	3,2
	y_2	-5	-0,6	1,2	-4,5	0	-0,8	2,6	-0,4
	y_3	4	-1,7	-3,4	3,8	-0,9	1,4	4,9	-4,4
	y_4	-2,4	4,3	-1,2	-3	4,6	-4,5	-1,9	3,8

INTERNATIONAL RESEARCH JOURNAL OF MULTIDISCIPLINARY DISCOVERIES

As results show, a deviation of indexes on mathematical model from practical values doesn't exceed 5%. It claims a practical significance of the received model.

IV. ANALYSIS OF NUMERICAL RESULTS

Based on the regularities given in formula (13), we construct isoparametric diagrams of response surfaces in the form of spline cubes (Fig. 1).

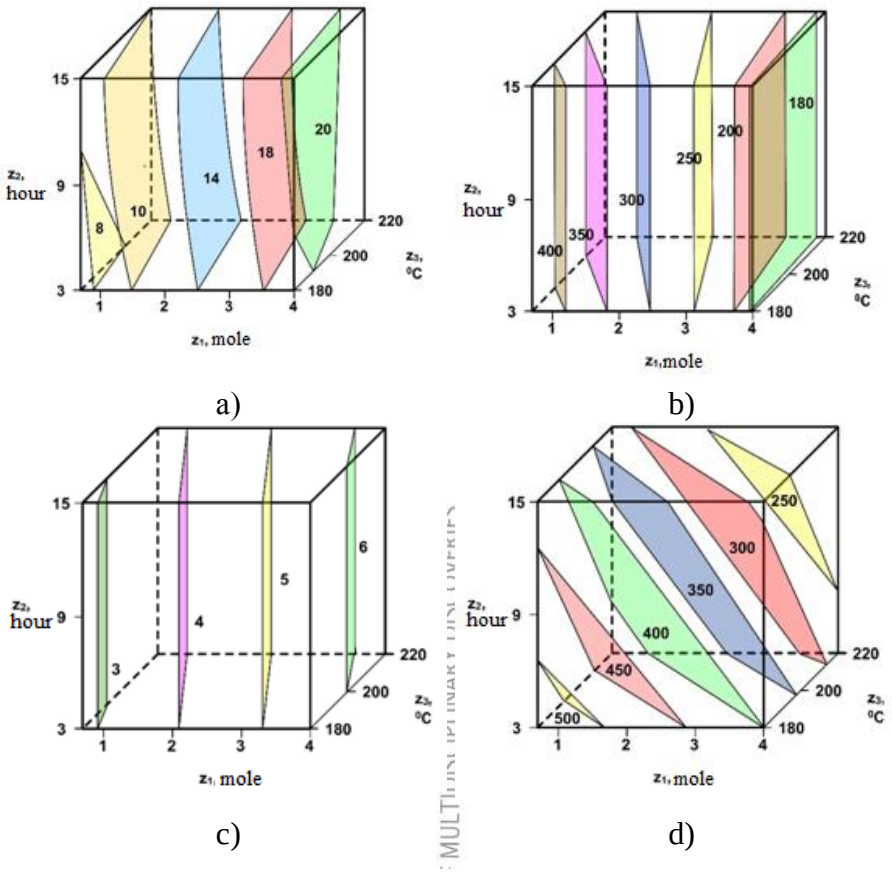

Fig. 1. Isoparametric diagrams of response surfaces of hydroxyl number (a), acid number (b), ether number (c) and molecular weight (d) of alcoholysis products of secondary polyethylene terephthalate with diethylene glycol.

As can be seen from fig. 1, the obtained mathematical model describes the change in the parameters of the alcoholysis products, depending on the content of DEG to the elementary unit of PET in the range of 0.7-4 mole, the duration of the reaction in the range of 3-15 hours and the temperature of the reaction medium in the range of 180-220°C. Putting in the mathematical model of values in the specified intervals, it is possible to predict the value of the parameters of the alcoholysis products.

As can be seen from the isoparametric diagram, the content of DEG to one elementary unit of PET mainly influences the hydroxyl number of alcoholysis products (respectively, b1=3,78 for y1; b1=-229,85 for y2; b1=0,82 for y3; b1=-42,65 for y4). But, the number average molecular weight (y4) all factors have a significant impact. This can be seen in the isoparametric diagram in fig. 1-d, in which the response surface is perpendicular to the diagonal of the cube-spline. Also, in fig. 1-b, one can observe a kind of "opening" of the response surfaces, which means an inactive change of the acid number (y_2) at low temperatures with a change in the molar ratio (x_1).

V. CONCLUSION

Thus, the obtained model is convenient for use; by giving it into a graphic form, it is possible to visualize the patterns of formation of the parameters of the alcoholysis process in the indicated intervals of the experimental parameters. The graphic view of the mathematical model turned out to be three-dimensional, since the regression coefficients describing the content of DEG to one elementary element of PET, the duration of the synthesis and the temperature of the reaction medium turned out to be significant.

VI. REFERENCES

[1] **Bedanakov A.YU., Borisov V.A., Mikitayev A.K., Keferov T.O., Davydov Ye.M., Mikitayev M.A.** Osnovnyye napravleniya pererabotki i ispol'zovaniya vtorichnogo polietilentereftalata [Bedanakov A.Yu., Borisov V.A., Mikitaev A.K., Keferov TO.O., Davydov E.M., Mikitaev M.A. The main directions of processing and use of recycled polyethylene terephthalate]. *Plasticheskiye massy*. 2007. No4, pp. 26-38.

[2] **Mitrofanov R. YU., Chistyakova YU. S., Sevodin V. P. Pererabotka otkhodov polietilentereftalata [R. Mitrofanov, Yu. S. Chistyakova, V. P. Sevodin.** Recycling of polyethylene terephthalate waste]. *Tverdyye bytovyye otkhody*. 2006. no6, pp. 12–13.

[3] **Strel'tsov Ye.** Voyna mirov v upakovke [Streltsov E. The War of the Worlds in Packing]. Polimery-dengi. 2003. no1. Available: http://polymers-money.com/journal/posting.

[4] **Masardi N., G.S.I.** PET market Overviev. CREON, Moskva. Available at: http://arpet.ru/material/4824. (accessed 18.02.2015)

[5] **Angel B.** Polyester Fibres. The 23RD PCI Consulting Group European Polyester Industry Conference, 3 October, Berlin. Available at: https://www.plastics.ru/pdf/journal/2015/ 12/PET.pdf. (01.02.2016)

[6] http://e-plastic.ru/main/articles/r11/pr02.

[7] **Plastics.ru**, 08.08.2006.

[8] **Vinogradova S.V.** *Polikondensatsionnyye protsessy i polimery* [polycondensation processes and polymers]. Moscow, Nauka publ., 2000. 373 p.

[9] **Chen F. Wang G., Shi C., Zhang Y., Zhang L., Li W.** Glycolysis kinetics of PET by microwave irradiation. J. Appl. Polym Sci. 2013. Vol.127, no4, pp. 2809-2815.

[10] **Liu-Fong, Yu Bao-hui**. Factors determining the content of diethylene glycol in polyethylene terephthalate and regulation. Zuzhi gongye= Polyester Ind. 2004. Vol.17, no3. pp.39-41.

[11] **Vaidya U.R., Nadkarni V.M.** Polyester polyols from glycolyzed PET waste: effect of glycol type on Kenetics of polyesterification. J. Appl. Polum. Sci. 1998, vol.39, no6. pp.1179-1190.

[12] **Zhurayev A.B., Nizamov T.A., Adilov R.I., Alimukhamedov M.G., Magrupov F.A.** PET soderzhashchiye bytovyye otkhody kak istochnik syr'ya dlya sinteza nenasyshchennykh poliefirov [PET containing household waste as a source of raw materials for the synthesis of unsaturated polyesters]. Plasticheskiye massy, 2011. no4. pp. 55-59.

[13] **Myshkis A.D.** *Elementy teorii matematicheskogo modelirovaniya* [Elements of the theory of mathematical modeling]. Moscow, Komkniga Publ, 2007. 192 p.

[14] **Samarskiy A.A**. *Matematicheskoye modelirovaniye: Idei. Metody. Primery* [Mathematical Modeling: Ideas. Methods Examples]. Moscow, Fizmatgiz Publ., 2001. 320 p.

[15] **Sautin S.N., Punin A.Ye.** *Mir komp'yuterov i khimicheskaya tekhnologiya* [The world of computers and chemical technology]. Leningrad, Khimiya Publ., 1991. 144 p.

ADVANCE RESEARCH JOURNAL OF MULTIDISCIPLINARY DISCOVERIES