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Construction of the Regression Equation of the Electrochemical Chlorination Process of Alkylation Products with Methanol, Ethanol, and Propanol of Methyl and Dimethyl Homologues of Phenol

Abstract

The aim of the presented work is to investigate the common and different characteristics of the regularities of obtaining aromatic compounds, including C_1-C_3 alkyl derivatives of phenols, anilines and naphthols by an effective catalytic alkylation process, and to develop the chlorination of hydrogen chloride in an electrochemical system.

Experiments in the laboratory were carried out in a five-factorial design. A mathematical model of the electrolysis process of obtaining aromatic amines, phenols and naphthols by the process of heterogeneous catalytic alkylation of low molecular weight alkyl (C_1-C_3) derivatives and comparative halogenation of individual homologues in an electrochemical system has been established. The "black box" principle was used here.

Taking into account what has been said, active experimental methods were used to create the optimal mode of the electrolysis process of alkylphenols, alkyl aromatic amines, HCl. A regression equation was formulated to build a mathematical model of the process.

To assess the homogeneity of parallel experiments, the average value of variances was found, and Fisher's criterion was used to check the adequacy of the obtained results.

$U_a(X_1, X_2, X_3, X_4, X_5)$ min, $U_v(X_1, X_2, X_3, X_4, X_5)$ max and $U_b(X_1, X_2, X_3, X_4, X_5)$ max was taken for alkylamines, alkyl naphthols, alkylphenols and HCl as an optimization objective function.

A quick extraction method was used to optimize the process. For this, change steps were calculated according to all three objective functions. X_2 was taken as base factor and step was accepted as Δx_{2a}^{x} =0.5 was taken. Then the steps corresponding to the other four factors were calculated. According to the report, the optimal level of chlorination products of alkyl aromatic compounds is 82.05% by current, 72.69% by substance, and 13.01% of HCl concentration.

According to the obtained results, when X_1= 0.482 A/cm^2, X_2=4.5 A/l, X_3=38.8 ^{0}C, X_4 = 19.8 %, X_5 = 6 V, the output of the chlorination product of alkyl aromatic compounds according to the current is 82.05 %.

Keywords: *hydrogen chloride, electrochemical chlorination, phenols, alkylphenol, catalytic alkylation, alkyl-aniline, alkyl aromatic*

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Metanol, etanol və propanol ilə fenolun metil və dimetil homoloqlarının alkilləşmə məhsullarının elektrokimyəvi xlorlaşdırma prosesinin reqressiya tənliyinin qurulması

Xülasə

Təqdim olunan işin məqsədi aromatik birləşmələrin, o cümlədən fenolların, anilinlərin və naftolların C1–C3 alkil törəmələrinin effektiv katalitik alkilləşmə prosesi ilə alınmasının ümumi və fərqli qanunauyğunluqlarını tədqiq etmək və hidrogen xloridin elektrokimyəvi sistemdə xlorlaşdırılmasını inkişaf etdirməkdir.

Laboratoriya təcrübələri beş faktorlu dizayn əsasında aparılmışdır. Aşağı molekullu alkil (C1–C3) fenol törəmələrinin və onların homoloqlarının heterogen katalitik alkilləşməsi və ayrı-ayrı homoloqların elektrokimyəvi sistemdə müqayisəli halogenləşməsi prosesi ilə aromatik aminlərin, fenolların və naftolların elektroliz prosesinin riyazi modeli qurulmuşdur. Burada “qara qutu” prinsipi tətbiq edilmişdir.

Qeyd olunanları nəzərə alaraq, alkilfenolların, alkilaromatik aminlərin və HCl-in elektroliz prosesinin optimal rejimini yaratmaq üçün aktiv eksperimental metodlardan istifadə olunmuşdur. Prosesin riyazi modelini qurmaq üçün reqressiya tənliyi tərtib edilmişdir.

Parallel təcrübələrin homogenliyini qiymətləndirmək üçün dispersiyaların orta qiyməti tapılmış və alınmış nəticələrin adekvatlığını yoxlamaq üçün Fişer kriteriyasından istifadə edilmişdir.

Alkilaminlər, alkilnaftollar, alkilfenollar və HCl üçün optimallaşdırma məqsəd funksiyası kimi aşağıdakılar qəbul edilmişdir:

Ua(X1, X2, X3, X4, X5) min, Uv(X1, X2, X3, X4, X5) max və Ub(X1, X2, X3, X4, X5) max.

Prosesin optimallaşdırılması üçün sürətli çıxarış metodu tətbiq edilmişdir. Bunun üçün bütün üç məqsəd funksiyası üzrə dəyişmə addımları hesablanmışdır. X2 baza faktor kimi götürülmüş və addım $\delta = 0.5$ qəbul edilmişdir. Daha sonra digər dörd faktor üçün uyğun addımlar hesablanmışdır.

Hesabat üzrə alkil aromatik birləşmələrin xlorlaşdırma məhsullarının optimal səviyyəsi cərəyan üzrə 82.05%, maddə üzrə 72.69% və HCl konsentrasiyası üzrə 13.01% təşkil etmişdir.

Alınan nəticələrə görə, X1 = 0.482 A/sm², X2 = 4.5 A/l, X3 = 38.8°C, X4 = 19.8%, X5 = 6 V olduqda, alkil aromatik birləşmələrin xlorlaşdırma məhsulunun çıxımı cərəyan üzrə 82.05% təşkil edir.

Açar sözlər: *hidrogen xlorid, elektrokimyəvi xlorlaşdırma, fenollar, alkilfenol, katalitik alkilləşmə, alkilanilin, alkilaromatik birləşmələr*

Introduction

Among the researches in the field of petrochemicals, one of the interesting things is the production of aromatic amines and phenols by the process of heterogeneous catalytic alkylation of low molecular weight alkyl (C_1-C_3) derivatives and their comparative halogenation of individual homologues in an electrochemical system. There are no joint studies in the presented field in the literature. However, there is a large literature on the alkylation of phenols as well as anilines separately. It should also be noted that there are significant differences in the composition and structure of the catalytic systems used in the alkylation of phenols with C_1-C_3 alcohols and the catalysts used in the interaction of aromatic amines with alcohols (Agaev, 2022, pp. 11-13). In this regard, the development of catalytic systems with optimal and universal acid-basic properties in the interaction of acidic phenols and basic anilines with C_1-C_3 alcohols is not easy and requires a special approach (Muradov, 2020, pp. 25-27). A similar issue is considered important in the electrochemical chlorination of alkyl phenols and alkylanilines in the presence of HCl solution.

The aim of the presented work is to investigate the common and different characteristics of the regularities of obtaining aromatic compounds, including C_1-C_3 alkyl derivatives of phenols and anilines by the effective catalytic alkylation process, and the development of chlorination with hydrogen chloride in an electrochemical system.

Methodology

Experiments in laboratory conditions were performed in a five-factor model. First, we need to build a mathematical model of the electrolysis process of obtaining low molecular mass alkyl (C_1-C_3) derivatives of aromatic amines and phenols by heterogeneous catalytic alkylation and comparative halogenation of individual homologs in an electrochemical system. The "black box" principle was used here. The mathematical model (mathematical description) of the process is sought in the following form:

$$U_i = f(X_1, X_2, \dots, X_n), \qquad i = 1,2,\dots, n \qquad (1)$$

In the model (1), active and passive experimental methods are used to determine the values of the coefficients of the variables. It is known that getting a more accurate mathematical model with active experimental methods is possible. One of these methods is the multifactorial experiment method (Sautin, 1975, p. 115; Muradov, 2004, pp. 69-73).

Taking into account the above, active experimental methods were used to create the optimal mode of the electrolysis process of HCl for the halogenation of alkyl phenols and alkyl aromatic amines. To build a mathematical model of the process (1), the regression equation is sought in the following form.

$$U = v_0+v_1x_1+ v_2x_2+ v_3x_3+ v_4x_4+ v_5x_5+ v_{12}x_1x_2+ v_{13}x_1x_3+ v_{14}x_1x_4+ v_{15}x_1x_5+ v_{23}x_2x_3+ +v_{24}x_2x_4+ v_{25}x_2x_5+v_{34}x_3x_4+ v_{35}x_3x_5 + v_{45}x_4x_5 + v_{123}x_1x_2x_3 + v_{124}x_1x_2x_4 + v_{125}x_1x_2x_5 + +v_{134}x_1x_3x_4 + v_{135}x_1x_3x_5 + v_{145}x_1x_4x_5 + v_{234}x_2x_3x_4 + v_{235}x_2x_3x_5 + +v_{245}x_2x_4x_5+ v_{345}x_3x_4x_5 \qquad (2)$$

Here, according to the variables x_1, x_2, x_3, x_4, x_5, the anode current density X_1, the amount of current supplied to the process X_2, the temperature of the electrolyte X_3, the density of the background electrolyte X_4, and the process voltage X_5 are determined by the following formulas:

$$X_1 = \frac{x_1 - x}{\Delta x_1}; \quad X_2 = \frac{x_2 - x}{\Delta x_2}; \quad X_3 = \frac{x_3 - x}{\Delta x_3}; \quad X_4 = \frac{x_4 - x}{\Delta x_4}; \quad X_5 = \frac{x_5 - x}{\Delta x_5} \tag{3}$$

The main characteristics of the five-factor experiment are given in table 1.

Table 1.
The main characteristics of the experiment.

Characteristics	X_1, A/cm^2	X_2, A□hrs.	X_3, ^{0}C	X_4, %	X_5, V	Concentration of Chlorine, %	Output Regarding Electrical Current	Output Regarding Substances
1. Main Level	0.35	3.5	50	12.5	6	15	70	73
2. Interval of change	0.25	2.5	30	7.5	2	5	5	5
3. Upper level	0.6	6	80	20	8	20	85	90
4. Lower level	0.1	1	20	5	4	10	62	65

The variation of coded variables - factors, the results of parallel experiments conducted accordingly, and dispersions are given in table 2.

Table 2.
Results of the Experiment.

№	X_1	X_2	X_3	X_4	X_5	Alkyl Phenol Output Regarding Electrical Current											
						U_1, %	U_{2mid}, %	$C_ç$, mid	S^2_{1j}	U_{12}, %	U_{1or}, %	M_{output}, mid	S^2_{2j}	U_{21}, %	U_{22}, %	C_{HCl}, %	S^2_{j3}
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	-	-	-	-	-	77.9	80.0	78.95	2.205	80.63	82.21	81.42	1.2482	19.02	19.76	19.39	0.2738
2	+	-	-	-	-	68.44	69.06	68.75	0.1922	70.9	71.7	71.3	0.32	17.14	18.52	17.83	0.9522
3	-	+	-	-	-	61.9	63.6	62.75	1.445	65.84	66.48	66.16	0.2048	14.83	16.09	15.46	0.7938
4	+	+	-	-	-	64.1	63.8	63.95	0.045	68.12	66.72	67.42	0.98	11.18	9.9	10.54	0.8192
5	-	-	+	-	-	77.26	75.64	76.45	1.3122	80.8	81.96	81.38	0.6728	10.99	9.43	10.21	1.2168
6	+	-	+	-	-	63.7	63.1	63.4	0.18	67.14	68.06	67.6	0.4232	18.65	17.11	17.88	1.1858
7	-	+	+	-	-	76.4	76.9	76.65	0.125	80.96	79.48	80.22	1.0952	14.86	16.22	15.54	0.9248
8	+	+	+	-	-	83.5	86.1	84.8	3.38	90.5	89.38	89.94	0.6272	10.91	12.49	11.7	1.2482
9	-	-	-	+	-	69.21	71.09	70.15	1.7672	74.1	72.58	73.34	1.1552	10.5	9.88	10.19	0.1922
10	+	-	-	+	-	65.7	66.5	66.1	0.32	70.34	69.1	69.72	0.7688	18.22	17.28	17.75	0.4418
11	-	+	-	+	-	64.53	64.97	64.75	0.0968	68.17	66.71	67.44	1.0658	13.82	12.7	13.26	0.6272
12	+	+	-	+	-	71.9	72.3	72.1	0.08	75.9	76.84	76.37	0.4418	10.9	9.98	10.44	0.4232
13	-	-	+	+	-	74.8	73.8	74.3	0.5	76.81	78.33	77.57	1.1552	10.56	9.64	10.1	0.4232
14	+	-	+	+	-	64.12	63.18	63.65	0.4418	65.09	66.37	65.73	0.8192	17.8	16.08	16.94	1.4792
15	-	+	+	+	-	63.58	61.82	62.7	1.5488	66.82	65.56	66.19	0.7938	13.87	15.25	14.56	0.9522
16	+	+	+	+	-	72.3	70.6	71.45	1.445	75.53	73.95	74.74	1.2482	12.94	11.54	12.24	0.98
17	-	-	-	-	+	83.6	83.34	83.47	0.0338	87.81	87.27	87.54	0.1458	19.2	20.68	19.94	1.0952
18	+	-	-	-	+	68.56	69.32	68.94	0.2888	71.98	73.34	72.66	0.9248	17.56	18.68	18.12	0.6272
19	-	+	-	-	+	68.4	69.84	69.12	1.0368	72.93	74.71	73.82	1.5842	15.7	16.98	16.34	0.8192
20	+	+	-	-	+	66.24	65.64	65.94	0.18	68.84	69.58	69.21	0.2738	10.51	11.73	11.12	0.7442
21	-	-	+	-	+	77.95	76.33	77.14	1.3122	79.88	80.78	80.33	0.405	10.23	11.63	10.93	0.98
22	+	-	+	-	+	73.12	74.6	73.86	1.0952	76.55	75.75	76.15	0.32	19.2	18.64	18.92	0.1568

23	-	+	+	-	+	66.7	67.86	67.28	0.6728	72.49	70.27	71.38	2.4642	17.22	15.24	16.23	1.9602
24	+	+	+	-	+	68.81	69.93	69.37	0.6272	72.93	72.21	72.57	0.2592	13.1	11.42	12.26	1.4112
25	-	-	-	+	+	66.18	64.98	65.58	0.72	69.12	67.96	6.54	0.6728	10.16	10.92	10.54	0.2888
26	+	-	-	+	+	62.7	62.18	62.44	0.1352	66.41	65.05	65.73	0.9248	17.87	18.69	18.28	0.3362
27	-	+	-	+	+	69.45	68.63	69.04	0.3362	72.82	71.78	72.3	0.5408	13.85	14.89	14.37	0.5408
28	+	+	-	+	+	65.92	67.36	66.64	1.0368	70.16	71.08	70.62	0.4232	10.89	11.81	11.35	0.4232
29	-	-	+	+	+	68.24	69.48	68.86	0.7688	71.1	72.66	71.88	1.2168	10.2	11.78	10.99	1.2482
30	+	-	+	+	+	79.62	78.14	78.88	1.0952	82.03	83.85	82.94	1.6562	17.82	17.32	17.57	0.125
31	-	+	+	+	+	75.23	76.73	75.98	1.125	80.25	79.07	79.66	0.6962	12.67	14.09	13.38	1.0082
32	+	+	+	+	+	83.66	85.42	84.54	1.5488	90.59	88.85	89.77	1.5138	19.34	20.64	19.99	0.845

The accuracy of the experiment is checked regarding Cochran’s criterion:

$$G_p = \frac{\max S_j^2}{\sum_{j=1}^{N} S_j^2} \quad (4)$$

For Alkyl Phenol:

$$G_{p1} = \frac{2.05}{27.0968} = 0.0813 \quad (5)$$

For HCl:

$$G_{p2} = \frac{2.4642}{27.041} = 0.0911 \quad (6)$$

$$G_{p3} = \frac{1.9602}{25.543} = 0.07674 \quad (7)$$

$$N = 32$$

$$f = K - 1 = 2 - 1 = 1 \quad (8)$$

$$G_{cəd} = 0.389$$

$$G_{p1} = 0.0813 < G_{ced} = 0.389$$

$$G_{p2} = 0.0911 < G_{ced} = 0.389 \quad (9)$$

$$G_{p3} = 0.07674 \prec C_{ced} = 0.389$$

G_{ced} is equal to 0.389 (Kurzin, 2022, p. 78; Zakgeim, 2014, p. 304; Isgandarov, 2007, p. 226; Ostrovsky, 2008, p. 424; Kurzin, 2022, p. 78) according to the number of experiments (N = 32) and degree of freedom (*f=k-1=2-1=1)*. In both cases, $G_p < G_{ced}$ is being met; therefore, the experiment can be considered satisfactory.

To assess the homogeneity of parallel experiments, the average value of dispersions is calculated:

$$S_{ya}^2 = \frac{1}{N}\sum_{j=1}^{N} S_j^2 = \frac{1}{32} \cdot 27.0968 = 0.8468 \quad (10)$$

$$S_{ув}^2 = \frac{\sum S_i^2}{N} = \frac{1}{32} \cdot 27.041 = 0.8450 \quad (11)$$

$$S_{yc}^2 = \frac{1}{N}\sum_{j=1}^{N} S_j^2 = \frac{1}{32}\cdot 25.543 = 0.7982 \qquad (12)$$

The dispersion of average values of the parallel experiments is calculated as follows:

$$f = N\cdot(k-1) = 32\cdot(2-1) = 32 \qquad (13)$$

$$S_{\bar{y}a}^2 = \frac{S_{ya}^2}{k} = \frac{0,8468}{2} = 0.4234 \qquad (14)$$

$$S_{\bar{y}в}^2 = \frac{S_{yв}^2}{k} = \frac{0.845}{2} = 0.4225 \qquad (15)$$

$$S_{\bar{y}c}^2 = \frac{S_{yc}^2}{k} = \frac{0.7982}{2} = 0.3991 \qquad (16)$$

The error in determining the regression coefficients is calculated by the following formula:

$$S_a = \sqrt{\frac{S_{\bar{y}a}^2}{N}} = \sqrt{\frac{0.4234}{32}} = 0.113 \qquad (18)$$

$$S_в = \sqrt{\frac{S_{\bar{y}в}^2}{N}} = \sqrt{\frac{0.4225}{32}} = 0.1149 \qquad (19)$$

$$S_в = \sqrt{\frac{S_{\bar{y}в}^2}{N}} = \sqrt{\frac{0.3991}{32}} = 0.1120 \qquad (20)$$

The value of Student's criterion is t = 2.09 (Radchenko, 2014, pp. 232-234; Salman, 2017, pp. 1-19; Ostrovsky, 2012, p. 432; Ostrovsky, 2005, p. 394; Radchenko, 2011, p. 376), where the confidence coefficient is $R = 0.95$ and the degree of freedom is $f=N\square(k-1) = 32\square(2-1) = 32$. Then:

$$S_a\cdot t = 0.115\cdot 2.09 = 0.2404$$
$$S_в\cdot t = 0.01147\cdot 2.09 = 0.2401 \qquad (21)$$
$$S_c\cdot t = 0.1120\cdot 2.09 = 0.2341$$

Since the yield of chlorination products of alkyl aromatic compounds according to the current, as well as the HCl residue are influenced by the same factors in the experiment, the mathematical expression of both can be sought in the form of the polynomial shown in (2). The regression coefficients included in the polynomial are calculated as follows (Agaev, 2022, pp. 11-13; Belozerova, 2015, pp. 23-29; Belozerova, 2014, pp. 6-23; Malysheva, 2021, pp. 68-76; Aung, 2020, pp. 62-71).

$$в_0 = \frac{1}{N}\sum_{j=1}^{N} y_i$$

$$в_i = \frac{1}{N}\sum_{j=1}^{N} x_{ji} y_i$$

$$в_{im} = \frac{1}{N}\sum_{j=1}^{N} x_{ji} x_{jm} y_i; \ (i \neq m)$$

$$в_{imk} = \frac{1}{N}\sum_{j=1}^{N} x_{ji} x_{jm} x_{jk} y_i; \ (i \neq m \neq k) \quad (22)$$

$$в_{imkc} = \frac{1}{N}\sum_{j=1}^{N} x_{ji} x_{jm} x_{jk} x_{jc} y_i; \ (i \neq m \neq k \neq c)$$

$$в_{imkc} = \frac{1}{N}\sum_{j=1}^{N} x_{ji} x_{jm} x_{jk} x_{jc} x_{je} y_i; \ (i \neq m \neq k \neq c \neq e)$$

According to the comparison given in Appendix 1, the mathematical model depending on the value of the variables is obtained as follows:

$$U_1=70.84-23.98x_1-5.914x_2+0.207x_3+1.03x_4+4.248x_5+11.873x_1x_2- 0.437x_1x_3+ +0.403x_1x_4-2.191x_1x_5+0.082x_2x_3-0.029x_2x_4+0.089x_2x_5-0.017x_3x_4-0.063x_3x_5- -0.405x_4x_5+ 0.016x_1x_2x_3-0.127x_1x_2x_4-0.184x_1x_2x_5+0.091x_1x_3x_5+0.138x_1x_4x_5-0.003x_2x_3x_4-0.007x_2x_3x_5+0.047x_2x_4x_5+0.005x_3x_4x_5$$

$$U_2=68.839-20.62x_1-5.936x_2+0.333x_3+1.384x_4+5.022x_5+12.347x_1x_2-0.487x_1x_3+ +0.093x_1x_4-2.771x_1x_5+0.074x_2x_3-0.041x_2x_4+0.142x_2x_5-0.022x_3x_4-0.082x_3x_5- -0.465x_4x_5+0.021x_1x_2x_3-0.114x_1x_2x_4-1.304x_1x_2x_5+0.095x_1x_3x_5+0.202x_1x_4x_5- -0.002x_2x_3x_4-0.006x_2x_3x_5+0.048x_2x_4x_4+0.005x_3x_4x_5$$

(23)

$$U_3=18.245+8.485x_1+0.059x_2-0.122x_3-0.543x_4+1.005x_5-4.272x_1x_2+0.094x_1x_3+ +0.465x_1x_4-2.142x_1x_5+0.013x_2x_3+0.035x_2x_4-0.073x_2x_5+0.005x_3x_4-0.007x_3x_5- -0.026x_4x_5+0.208x_1x_2x_5-0.007x_1x_3x_4+0.02x_1x_3x_5+0.074x_1x_4x_5$$

In the regression equation, the calculated values using the coded values of the variables, the values obtained from the experiment, and their mean squared differences are used.

In order to test the preciseness of the obtained values, Fisher's criterion is used (Malysheva, 2019, pp. 148-153; Shishkova, 2017, pp. 28-30).

The adequacy dispersion value is calculated for both expressions as follows:

$$S_{ad}^2 = \frac{N}{N-B}\sum_{j=1}^{N}\left(y_j^p - y_j^э\right)^2 \quad (24)$$

where $f = N - B$ is the degree of freedom. The adequacy dispersion values:

$B_a=24; \quad B_b=22, B_c=16$

$$f_{ada} = N - B = 32 - 24 = 8; \quad f_{adв} = 32 - 22 = 10; \quad f_{adc} = 32 - 16 = 16$$

$$S_{ada}^2 = 28.906; \quad S_{adв}^2 = 22.505; \quad S_{adc}^2 = 5.727 \quad (25)$$

Here, $B_a=24$, $B_v=22$, *and* $B_c = 16$ are the total number of regression coefficients in the first, second, and third expressions, respectively.

Fisher's criterion values and degrees of freedom are obtained as follows:

$S_{ad1} = 3.8329$; $S^2_{\bar{y}_a} = 0.8468$

$S_{ad2} = 3.295$; $S^2_{\bar{y}_b} = 0.8450$

$S_{ad3} = 2.234$; $S^2_{\bar{yc}} = 0.7982$

$$F_{pa} = \frac{\max\left(S^2_{ada}, S^2_{\bar{y}a}\right)}{\min\left(S^2_{ada}, S^2_{\bar{y}a}\right)} = \frac{3.8329}{0.8468} = 4.526 \quad (26)$$

$$f_a = N - B_a = 32 - 25 = 7 \quad (27)$$

$$F_{pв} = \frac{\max\left(S^2_{adв}, S^2_{\bar{y}в}\right)}{\min\left(S^2_{adв}, S^2_{\bar{y}в}\right)} = \frac{3.295}{0.8450} = 3.899 \quad (28)$$

$$f_в = N - B_в = 32 - 22 = 10 \quad (29)$$

$$F_{pc} = \frac{\max\left(S^2_{adc}, S^2_{\bar{yc}}\right)}{\min\left(S^2_{adc}, S^2_{\bar{yc}}\right)} = \frac{2.234}{0.7982} = 2.798 \quad (30)$$

$$f_c = N - B_c = 32 - 16 = 16$$

As can be seen, the adequacy of both statements is proved from the comparison of the table and calculated values.

To get the natural mathematical model, expressions (3) between coded and natural values are used:

$$X_1 = 54x_1 - 1{,}4; \quad X_2 = 0{,}4x_2 - 1.4;$$
$$X_3 = 0{,}033x_3 - 1{,}667; \quad X_4 = 0.133x_4 - 1{,}667; \quad (31)$$
$$X_5 = 0.5x_5 - 3$$

Following expressions are obtained from the application of the results in the system (23):

$$U_1=70.87-0.574x_1-0.433x_2+2.21x_3-1.052x_4+0.82x_5+2.48x_1x_2+1.24x_1x_3+1.48x_1x_4+ +1.45x_2x_3+1.51x_2x_4-0.27x_2x_5+0.515x_3x_4+0.59x_3x_5+0.854x_4x_5+0.3x_1x_2x_3-0.6x_1x_2x_4- -1.48x_1x_2x_5+1.38x_1x_3x_5+ +0.52x_1x_4x_5-1.4x_2x_3x_4-0.94x_2x_3x_5+1.75x_2x_4x_5+2.26x_3x_4x_5$$

$$U_2=74.43-0.52x_1+2.33x_3-1.14x_4+0.89x_5+2.61x_1x_2+1.2x_1x_3+1.7x_1x_4+1.49x_2x_3+ +1.55x_2x_4+0.45x_3x_4+0.44x_3x_5+x_4x_5+0.41x_1x_2x_3-0.54x_1x_2x_4-1.63x_1x_2x_5+1.44x_1x_3x_5+ +0.76x_1x_4x_5-1.32x_2x_3x_4-0.83x_2x_3x_5+1.77x_2x_4x_5+2.67x_3x_4x_5$$

$$U_3=14.51+0.67x_1-0.84x_2-0.64x_4+0.51x_5-1.89x_1x_2+0.93x_1x_3+1.03x_1x_4+0.26x_1x_5+ +0.99x_2x_3+0.66x_2x_4+0.77x_3x_4+0.26x_1x_2x_5-0.41x_1x_3x_4+0.3x_1x_3x_5+0.28x_1x_4x_5$$

Conclusion

In the optimization, we take $U_a(X_1,X_2,X_3,X_4,X_5) \rightarrow \min$, $U_v(X_1,X_2,X_3,X_4,X_5) \longrightarrow \max$ and $U_v(X_1,X_2,X_3,X_4,X_5) \rightarrow \max$ as the objective function for alkyl phenol and HCl, respectively (Gupta, 2020, pp. 129-139; Meshalkin, 2019, pp. 709-718; Liyi Zh., 2017, pp. 366-375; Yazovtseva, 2024, pp. 211-223).

A quick extraction method is used to optimize the process. To do this, the change steps are calculated according to all three objective functions. X_2 is taken as the base factor and the step is considered as ΔX^*_{2a} =0.5. Then the steps corresponding to the other four factors are calculated:

$$\gamma_a = \frac{\Delta X^*_{2a}}{в_2 \Delta X_2} = \frac{0,5}{-0,4331 \cdot 2.5} = -4.4618 \qquad (32)$$

Steps:

$$\begin{aligned} &\Delta X^*_{2a} = 0.5 \\ &\gamma_a = \frac{\Delta X^*_{2a}}{b_2 \Delta X_2} = \frac{0.5}{-0.4331 \cdot 2.5} = -0.4618 \\ &\Delta X^*_1 = \gamma_1 \cdot в_1 \cdot \Delta x_1 = -0.4621 \cdot (-0.574) \cdot 0.25 = 0.066; \\ &\Delta X^*_3 = \gamma_1 \cdot b_3 \cdot \Delta X_3 = -0.462 \cdot 2.207 \cdot 30 = -30.6; \\ &\Delta X^*_4 = -0.462 \cdot (-1.052) \cdot 7.5 = 3.65 \\ &\Delta X^*_5 = -0.462 \cdot 0.818 \cdot 2 = -0.755 \end{aligned} \qquad (33)$$

Table 3 depicts the results of the report with calculated steps starting from the zero level for the factors. According to the report, the optimal level of chlorination products of alkyl aromatic compounds regarding electrical current was 82.05%, regarding substance was 72.69 %, and regarding the concentration of HCl was 13.01%.

Results

According to the obtained results, when X_1= 0.482 A/cm^2, X_2=4.5 A/l, X_3=38.8 ^{0}C, X_4 = 19.8 %, X_5 = 6 V, the yield of the chlorination product of alkyl aromatic compounds according to the current is 82.05 %. At this time, the concentration of HCl in the solution decreases from 20% to 13.01%.

Table 3.

Results of the experiment regarding quick extraction.

№ and characteristics of the experiment	X_1	X_2	X_3	X_4	X_5	Y_1	Y_2	Y_3
a_i	0.462	0.4331	2.207	1.052	0.818			
$a_i \Delta X_i$	0.1155	1.083	66.21	7.89	1.636			
Step of Change	0.066	0.5	30.6	3.65	0.755			
Value of rounding	0.066	0.5	30.6	3.65	0.755			
Zero level	0.35	3.5	50	12.5	6			
Interval of Change	0.25	2.5	30	7.5	2			
Experiments								
1	0.416	4	19.4	16.15	5.245	76.35	71.213	12.993
2	0.482	4.5	38.8	19.8	6	82.5	72.69	13.01
3	0.548	5	58.2	23.45	6.755	91.69	77.01	14.2

References

1. Agaev, A. A., Muradov, M. M., Murshudlu, N. A., & Gadzhieva, Kh. A. (2022). Alkylation of 3,4-dimethylphenol with propanols in the presence of palladium-containing zeolites. *Oil Refining and Oil Chemistry. Scientific and Technical Achievements and Advanced Experience*, (2), 11–13.

2. Aung, M. T., Abbas, S. A., Zhukova, N. A., & Chernokul'skiy, V. V. (2020). Models for managing data collection processes in Internet of Things networks with a dynamic structure. *Computational Nanotechnology*, (3), 62–71. https://doi.org/10.33693/2313-223X-2020-7-3-62-71
3. Belozerova, A. R., Belozerov, S. V. (2014). Approach to the construction of heuristic algorithms for analyzing the quality of experimental data on neutron activation measurements. *Heuristic Algorithms and Distributed Computing, 1*(4), 6–23.
4. Belozerova, A. R., Komarova, E. S., Melnikov, B. F., & Pivneva, S. V. (2015). Some issues of modeling of design technology of new reactors based on the physicochemical properties of MOX-fuel. *Frontier Materials & Technologies*, (2–1), 23–29.
5. Gupta, N., Khosravy, M., Patel, N., & Dey, N. (2020). Mendelian evolutionary theory optimization algorithm. *Soft Computing, 24*(4). https://doi.org/10.1007/s00500-020-05239-2
6. Isgandarov, A. D., Tagiyev, R. G., & Yagubov, G. Y. (2007). *Optimization methods*. Baku.
7. Kurzin, A. V., & Evdokimov, A. N. (2022a). *Optimization methods: Completion of practical assignments*. Saint Petersburg.
8. Kurzin, A. V., & Evdokimov, A. N. (2022b). *Optimization methods: Performance of practical tasks*. Saint Petersburg.
9. Liyi, Z., Chao, X., & Teng, F. (2017). Improved ant colony optimization algorithm based on RNA computing. *Automatic Control and Computer Sciences, 51*, 366–375.
10. Malysheva, T. V. (2019). Use of automated information systems in managing environmental sustainability of manufacturing industries. *Problems of Mechanical Engineering and Automation*, (2), 148–153.
11. Malysheva, T. V. (2021). Development of an algorithm for optimizing energy consumption in chemical-technological systems based on statistical training. *Computational Nanotechnology, 8*(1), 68–76. https://doi.org/10.33693/2313-223X-2021-8-1-68-76
12. Meshalkin, V. P., Bogomolov, B. B., Boldyrev, V. S., & Zubarev, A. M. (2019). Intelligent logical information algorithm for choosing energy and resource-efficient chemical technologies. *Theoretical Foundations of Chemical Engineering, 53*(5), 709–718.
13. Muradov, M. M. (2004). Construction of the regression equation of the process of condensation of propylene chlorohydrin by dilute hydrochloric acid. In *Proceedings of the Republican Scientific Conference "Modern Problems of Informatization, Cybernetics and Information Technologies"* (Vol. III, pp. 69–73). Baku.
14. Muradov, M. M., Gatamov, M. M., Prosochkina, T. R., & Agaev, A. A. (2020). Chlorination of p-cresol in an electrochemical system. *Bashkir Chemical Journal, 27*(3), 25–27.
15. Ostrovsky, G. M., & Ziyatdinov, N. N. (2012). *Optimization of technical systems*. KNORUS.
16. Ostrovsky, G. M., Volin, Y. M., & Ziyatdinov, N. N. (2005). *Optimization in chemical technology*. Fan.
17. Ostrovsky, G. M., Volin, Y. M., & Ziyatdinov, N. N. (2008). *Methods of optimization of chemical-technological processes*. KDU.
18. Radchenko, S. G. (2011). *Methodology of regression analysis*. Korniychuk.
19. Radchenko, S. G. (2014). Plans of experiments of multi-purpose use. In *Proceedings of the 9th International Scientific and Practical Conference "Mathematical and Imitation Modeling of Systems (MODS 2014)"* (pp. 232–234). Chernihiv.
20. Salman, A., & Khan, A. (2017). Fuzzy goal programming-based ant colony optimization algorithm for multi-objective topology design of distributed local area networks. *Neural Computing and Applications, 28*, 1–19.
21. Sautin, S. N. (1975). *Planning an experiment in chemistry and chemical technology*. Chemistry.
22. Shishkova, N. A. (2017). Genetic algorithm as an optimization method. *Problems of Science, 1*(5), 28–30.
23. Yazovtseva, O., Gubaydullin, I., Peskova, E., & Usmanova, A. (2024). Parallel algorithm for computer simulation of burning off sulfurous deposits from a cylindrical catalyst grain. In

Communications in Computer and Information Science (Vol. 2241). Springer, 211-223. https://doi.org/10.1007/978-3-031-73372-7_15
24. Zakgeim, A. Y. (2014). *General chemical technology: An introduction to the modeling of chemical-technological processes* (3rd ed.). Logos.

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