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Mathematical simulation of process of curing auto-filler based on unsaturated polyester resin

O. G. Abdullaev[1], *Yu. U.* Toshmirzaev[1], *T. S.* Mirzaev[1], and *A. V.* Umarov[2, 3*]

[1]Namangan State University, Namangan, Uzbekistan
[2]Tashkent University of Applied Sciences, Tashkent, Uzbekistan
[3]Tashkent State Transport University, Tashkent, Uzbekistan

Abstract. In this article, with the help of mathematical modeling of the curing rate, the influence of factors directly affecting the curing processes of an auto-filler prepared based on unsaturated polyester resin was studied: the concentration of the accelerator, hardener, and temperature. When modeling the process, the accelerator, hardener, and temperature concentrations were taken as the initial (input) parameters, and the curing rate of the auto-filler at various temperatures was taken as the final (output) parameter.

1 Introduction

Paints and varnishes are multicomponent compositions applied in a liquid state to the surface of products and drying with the formation of films held by adhesion forces. Dried films are called paint coatings.

Paint coatings are widely used to cover vehicles, performing two functions - protective and decorative, i.e., technical and aesthetic. Paint coatings have significant advantages over other types of coatings, as they are easier to apply to the surface, which reduces the cost of painting work. Paint coatings have great durability; they can be applied to metal, plastics, and other materials [1, 2].

Paints and varnishes are classified according to various criteria; for example, varnishes, enamels, primers (primers), putties, and certain requirements are imposed on each class [3].

The main paints and varnishes used in vehicles include primers (primers), putties, and enamels.

This work studies the curing process of auto-filler prepared based on unsaturated polyester resin [4-7].

As you know, putties are used to level the surface to be painted and are a thick, viscous, pasty mass consisting of a mixture of fillers and pigments in a film former. Putties have a rather high viscosity than other paints and varnishes due to the higher content of solid components [8].

The bulk of the manufactured auto-filler is accounted for by the polymer composition produced based on unsaturated polyester resin [9]. One of the important parameters of an auto-filler is the curing speed after applying it to the surface.

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*Corresponding author: abdusalom@inbox.ru

When creating an auto-filler, the optimal working concentration of the accelerator in the composition of the composite material and the hardener is selected experimentally. Moreover, the paint and varnish industry produces auto-fillers of various compositions, depending on the region where they will be used.

In this regard, it becomes necessary to use the method of mathematical modeling of the auto-filler curing process since the curing speed of the auto-filler depends on the concentration of the accelerator, hardener, and ambient temperature where it is used.

2 Main parts

The object of the study is an auto-filler obtained based on an unsaturated polyester resin (PN-1 brand), cured with an accelerator (cobalt octoate), which is introduced into the composition in advance, and a hardener (methyl ethyl ketone peroxide) introduced before applying the auto-filler.

The results of experimental data on the curing of auto-fillers at various concentrations of the accelerator, hardener, and temperatures were studied by mathematical modeling using a multifactorial linear regression equation [10, 11].

Below are the experimental results of the dependence of the curing time of the auto-filler at various concentrations of the accelerator and hardener on temperature.

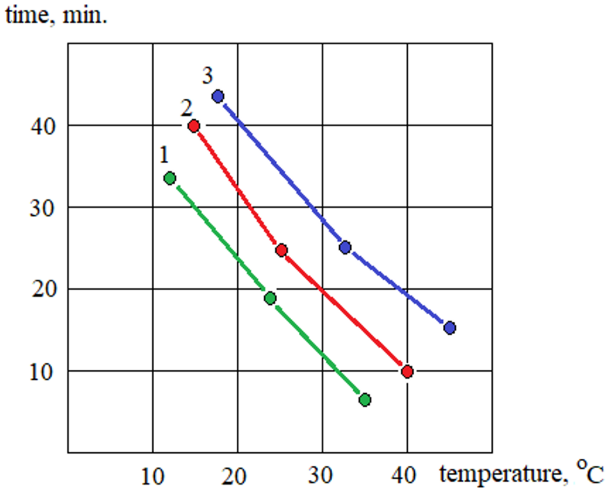

Fig. 1. Dependence of curing time of auto-filler on temperature: 1 is accelerator concentration 1.5%, hardener 1.8%; 2 is accelerator concentration 0.8%, hardener 1.6%; 3 is accelerator concentration 0.4%, hardener 1.2%.

Based on the obtained experimental data, a mathematical model has been constructed for the considered problem of determining the optimal amount of accelerator and hardener to optimize the curing time of the auto-filler at different temperatures.

Let us construct a linear regression equation for the dependence of time (t) on temperature (T), the concentration of the accelerator (x), and the hardener (y) using the least squares method.

The relationship between time, temperature, accelerator, and hardener is determined using a matrix of paired correlation coefficients using the MS Excel computer program system (table 1).

Table 1. Correlation dependence between factors of process under study

Factors	t	T	x	y
t	1			
T	-0.81	1		
x	-0.29	-0.31	1	
y	-0.27	-0.32	0.94	1

The table shows that there is a strong inverse dependence of the curing time of the auto-filler on temperature and a weak inverse dependence on the accelerator and hardener, which is associated with the occurrence of complex chemical reactions in the composite system during the curing of the auto-filler, in the presence of initiating components.

Let us assume that the multivariate linear regression equation has the form

$$t(T,x,y) = aT + bx + cy + \varepsilon \qquad (1)$$

To estimate the unknown parameters, we find the minimum value of the following sum over a, b, c, ε

$$F(a,b,c,\varepsilon) = \sum_{k=0}^{n} \left(t_i - (aT_i + bx_i + cy_i + \varepsilon)\right)^2 \qquad (2)$$

To determine the minimum of the function F(a,b,c,ε), we find its partial derivatives concerning a, b, c, ε, equate them to zero and obtain the following normal system of equations:

$$\begin{cases} \frac{\partial F}{\partial a} = -2\left[\sum_{i=1}^{n} t_i T_i - a\sum_{i=1}^{n} T_i^2 - b\sum_{i=1}^{n} x_i T_i - c\sum_{i=1}^{n} y_i T_i - \varepsilon\sum_{i=1}^{n} T_i\right] = 0 \\ \frac{\partial F}{\partial b} = -2\left[\sum_{i=1}^{n} t_i x_i - a\sum_{i=1}^{n} x_i T_i - b\sum_{i=1}^{n} x_i^2 - c\sum_{i=1}^{n} x_i y_i - \varepsilon\sum_{i=1}^{n} x_i\right] = 0 \\ \frac{\partial F}{\partial c} = -2\left[\sum_{i=1}^{n} t_i y_i - a\sum_{i=1}^{n} y_i T_i - b\sum_{i=1}^{n} x_i y_i - c\sum_{i=1}^{n} y_i^2 - \varepsilon\sum_{i=1}^{n} y_i\right] = 0 \\ \quad \frac{\partial F}{\partial \varepsilon} = -2\left[\sum_{i=1}^{n} t_i - a\sum_{i=1}^{n} T_i - b\sum_{i=1}^{n} x_i - c\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \varepsilon\right] = 0 \end{cases} \qquad (3)$$

Based on the data above in Fig. 1, construct the following auxiliary table (table 2) and, using a system of normal linear equations, compose a system of linear equations with unknown parameters a, b, c, ε.

Table 2. Auxiliary table compiled on basis of experimental data

№	t	T	x	y	x^2	y^2	T^2
1	16	45	0.4	1.2	0.16	1.44	2025
2	25	32	0.4	1.2	0.16	1.44	1024
3	43	18	0.4	1.2	0.16	1.44	324
4	10	40	0.8	1.6	0.64	2.56	1600
5	25	25	0.8	1.6	0.64	2.56	625
6	40	15	0.8	1.6	0.64	2.56	225
7	7	35	1.5	1.8	2.25	3.24	1225
8	19	23	1.5	1.8	2.25	3.24	529
9	33	12	1.5	1.8	2.25	3.24	144
∑	218	245	8.1	13.8	9.15	21.72	7721

Continuation of Table 2

№	xy	xT	xt	yT	yt	tT
1	0,48	18	6,4	54	19,2	720
2	0,48	12,8	10	38,4	30	800

3	0,48	7,2	17,2	21,6	51,6	774
4	1,28	32	8	64	16	400
5	1,28	20	20	40	40	625
6	1,28	12	32	24	64	600
7	2,7	52,5	10,5	63	12,6	245
8	2,7	34,5	28,5	41,4	34,2	437
9	2,7	18	49,5	21,6	59,4	396
∑	13,38	207	182,1	368	327	4997

Based on the above table and the system of normal equations (3), we obtain the following:

$$\begin{cases} 7721a + 207b + 368c + 245\varepsilon = 4997 \\ 207a + 9.15b + 13.38c + 8.1\varepsilon = 182.1 \\ 368a + 13.38b + 21.72c + 13.8\varepsilon = 327 \\ 245a + 8.1b + 13.8c + 9\varepsilon = 218 \end{cases} \qquad (4)$$

Having calculated this system of equations using the Mathcad program, we obtain the following results:

$$A = \begin{pmatrix} 7721 & 207 & 368 & 245 \\ 207 & 9.15 & 13.38 & 8.1 \\ 368 & 13.38 & 21.72 & 13.8 \\ 245 & 8.1 & 13.8 & 9 \end{pmatrix}, \qquad E = \begin{pmatrix} 4997 \\ 182.1 \\ 327 \\ 218 \end{pmatrix}$$

$$A^{-1} = \begin{pmatrix} 1.057x10^{-3} & 1.762x10^{-3} & 0.011 & -0.048 \\ 1.762x10^{-3} & 4.67 & -7.981 & 7.987 \\ 0.011 & -7.981 & 15.624 & -17.086 \\ -0.048 & 7.987 & -17.086 & 20.426 \end{pmatrix}, \; A^{-1}E = \begin{pmatrix} -1.099 \\ -9.498 \\ -11.739 \\ 80.689 \end{pmatrix}$$

According to the last matrix, the values of the parameters are displayed:
a=-1.099, b=-9.498, c=-11.739, ε=80.689. According to the results found above, if we replace the parameters of the multifactorial linear regression equation of the form (1) with the corresponding values, we obtain a function of the following form:

$$t(T, x, y) = -1.099T - 9.498x - 11.739y + 80.689 \qquad (5)$$

We enter the values of the corresponding factors in Fig. 1 into this function, calculate the differences and use them to determine the average error approximations to get a general idea of the quality of the model in terms of relative deviations for each observation and based on the statistical data (5), plot the function:

$$A = \frac{1}{n}\sum \left|\frac{t - t(T, x, y)}{t}\right| * 100\% = 5.968\%$$

The following is a graph of the curing reaction rate of an auto-filler versus the concentration of accelerator, hardener, and temperature.

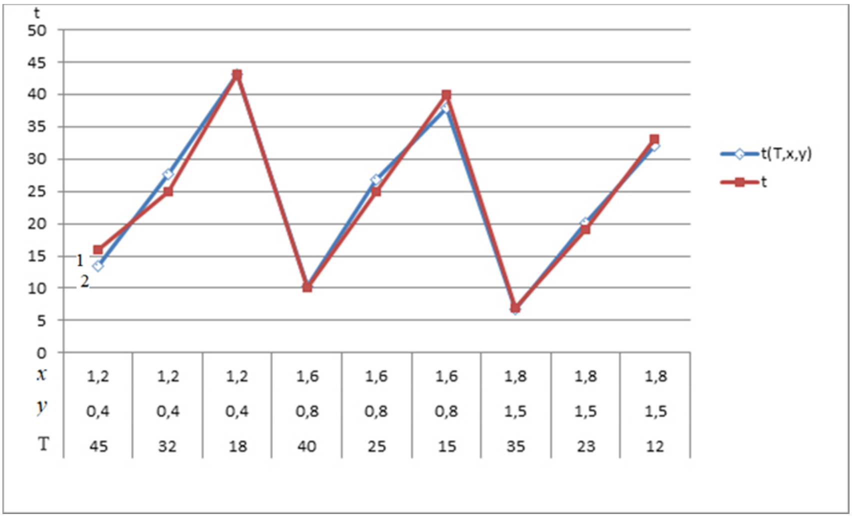

Fig. 2. Dependence of curing time on parameters x, y, and T, 1 is according to experimental, 2 is according to calculated data

From the average relative error of the above graph, it can be seen that the multivariate regression equation (4) represents the process under study with an error of 5.968%.

3 Conclusions

1. As a result of mathematical modeling of the auto-filler curing process, the function of the dependence of the curing time (reaction rate) of the composite material on the temperature of the application process and the concentration of the accelerator and hardener was determined.

2. Using this function, depending on the concentration of the accelerator and hardener (according to known x and y), which are part of the composition, it is possible to determine the rate of its curing at the operating temperature of the auto-filler, or vice versa, to determine the optimal temperature at a certain curing rate.

3. In addition, this function allows you to predetermine the amount of hardener (or accelerator) to be added at the application temperature of the auto-filler to the surface at a pre-set curing speed, according to the concentration of the accelerator (or hardener) included in the unsaturated polyester composition (when unknown one of the parameters x or y).

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