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MATHEMATICAL MODELLING IN SCIENTIFIC RESEARCHES OF CHEMICAL TECHNOLOGY PROCESSES

MODELOWANIE MATEMATYCZNE W BADANIACH NAUKOWYCH PROCESÓW TECHNOLOGII CHEMICZNEJ

A b s t r a c t

In this paper the features of mathematical model application for research of chemical technology objects are presented. The research of chemical and technological process of soft goods treatment in the environment of organic solvents has been presented. Effective universal composition for intensification of dry-cleaning of textile materials of different fiber composition has been elaborated by means of both theoretical and experimental investigations.

Keywords: mathematical modelling, optimization, criteria of optimization, dry-cleaning

S t r e s z c z e n i e

W niniejszym artykule przeprowadzono analizę możliwości zastosowania modelu matematycznego do badania obiektów z zakresu technologii chemicznej. Przedstawiono badanie chemiczno-technologicznego procesu obróbki wyrobów włókienniczych w środowisku rozpuszczalników organicznych. Wykonanie badań teoretycznych na modelu matematycznym oraz doświadczalnych pozwoliło na zaprojektowane efektywnej, uniwersalnej kompozycji zwiększającej możliwości chemicznego czyszczenia materiałów włókienniczych w porównaniu do środków stosowanych obecnie.

Słowa kluczowe: matematyczne modelowanie, optymalizacja, kryteria optymalizacji, chemiczne czyszczenie

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1. Introduction

In recent years in the sphere of modelling of objects of chemical and technological processes (CTP) there has been a transition tendency to the analysis and synthesis of large systems. With the growth of scales of the investigated systems their complication as objects of modelling grows, which causes a number of principles difficulties. The modern tendencies of transition to the analysis of large systems are predetermined by the requirements of reliability of prognostication of results of CTP [1].

The modern level of chemical technology is determined by two features – its basic scientific method of research and its apparatus. The research method is mathematical modelling, the studied apparatus its theory of systems and its applied part – system analysis (aggregate of methods and means of study of complex systems) [2]. Creation of effective compositions for treatment of textile materials is rather complicated problem, which requires both the knowledge of general approach to the problem, and a large number of definite questions which are directly connected with technological processes of their processing. Applying system approach it is not easy to imagine at once the task of creation the CTP on the whole, it's difficult to distinguish separate stages in solution of general problem, to set connection between them and sequence of their implementation. Basic principles of system approach are taken to two positions:

– presentation of the object as a system;
– its investigation in that aspect in which it is given as a system.

It means that the research strategy must consist in direction from the whole to the part, from the system forming relations and properties, from the structure to the elements (and not vice versa, as in the empiric approach).

The elements of the chemical and technological system are in the endless set of interconnections and interrelations. The degree of intensity of connections or relations depends on their importance. The research task is to determine, which connections are essential and determine the system, and which are not essential.

Complication of the modelling process grows in the investigation of complex systems. A complex system is difficult to be studied, that is why using experimental and theoretical modelling is rather effective. It includes analytical, empiric, numeral and discrete modelling of hydrodynamic, diffusive, mechanical and other processes of physical and chemical nature, as well as methods of processing of experimental data arrays, forming of databases and knowledge bases for characteristics of systems [1, 2].

2. The research methodology

Practical realization of directions of enhanced prediction of modelling that take place at the processing of textile materials (washing, dyeing, dry-cleaning and others) requires implementation of following stages:

1) study of properties of the object (authentication it as the management object);
2) forming of model image about the object (model forming of structure of textile material and model image of the phenomena, that is forming of the system of hypotheses about the mechanism of the phenomena which make and accompany a certain technological process);

3) formalization of information about the object – elaboration of experimental and theoretical model;
4) practical realization of the model with application of modern computing facilities.

Practice of introduction of the systems of automation has testified the importance of right solution of questions which are related to the choice of structure of model of technological process (structural authentication) and determination of model parameters (parameter authentication).

Scientific and practical researches of CTP have shown that for the construction of complex model with the high degree of prognosis and high level of approaching of dimension of modeling space to the dimension of the space of functioning of the system is necessary. From the formal point of view it means substantial growth of number of model parameters that causes some difficulties during its realization. The analysis and decoupling of the system on a number of correlated subsystems is the known principle of overcoming these difficulties and it enables to attain the necessary dimension of model for every subsystem [3].

3. The research results

The construction of a flow diagram of decoupling has enabled to apply effectively the experimental and theoretical modelling for the study of treatment of soft goods in the environment of organic solvents (Fig. 1).

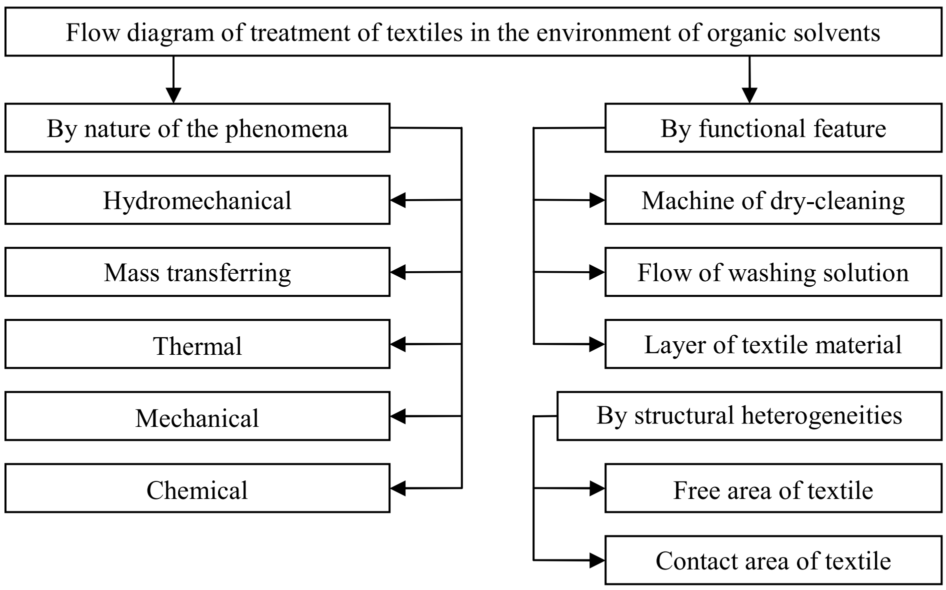

Fig. 1. Flow diagram of decoupling of chemical and technological process of treatment of textiles in the environment of organic solvents

Rys. 1. Schemat strukturalnej dekompozycji chemiczno-technologicznego procesu obróbki wyrobów włókienniczych w środowisku rozpuszczalników organicznych

The first stage included the determination of meaningful factors which influence the process of washing of wares in the conditions of dry-cleaning. For this purpose there has been used the orthogonal unsaturated plan of Plackett – Bermann, which enables to get certain estimations of linear effects of all factors with maximum possible at this number of experiments exactness identical for all effects [4].

Based on the previously determined ecollid-chemical characteristics for elaboration of washing composition it is select three SAA, which are characterized by high superficial activity, emulgation, dispersion, solubilization capabilities: phosphoxid 7, syntanol DS-10, fibre-tex 25 have been selected [5, 6].

Three-factor quadratic model has been applied for the elaboration of compositions for intensification of dry-cleaning according to the plan B3 at the second stage [1]. Approximate contents of each compound have been chosen on the basis of recommendations in relation to compositions of for intensifiers [7] which are used at the dry-cleaners of wares (tab. 1).

Table 1

Initial data for three – factor experiment

Compound component	Factor	Levels of variation			Interval of variation
		–1	0	+1	
Mass share of fibre-tex 25	X_1	0,10	0,20	0,30	0,10
Mass share of syntanol DS-10	X_2	0,05	0,10	0,15	0,05
Mass share of phosphoxid 7	X_3	0,03	0,05	0,07	0,02

For the improvement of dissolution of compositions the mixture of intersolvents: cyclohexsanol and 2-propanol in correlation 2:1, which was added to the receipt of 100 g compositions of intensification (factor of K_4).

Washing ability (MS_i %), degree of muddiness (Z %), remaining muddiness (Z_{rem} %), degree of remaining muddiness, which is expressed through additional optical density (AOD) have been chosen as the initial parameters (criteria of optimization).

The values of criteria of optimization for the calculation of mathematical models are presented in tab. 2.

The results of the experiments were processed by the special program. Models defined as: $MS_1 = f(x_1, x_2, x_3)$, $MS_2 = f(x_1, x_2, x_3)$, $AOD = f(x_1, x_2, x_3)$, $Z_{rem} = f(x_1, x_2, x_3)$ (Fig. 2) were achieved for each fabric.

For example, the mathematical model of dependence of washing ability (MS_1, %) on the indicated factors for a woolen fabric is the following:

$$MS_1 = 61{,}45 - 7{,}27x_1 + 3{,}25x_2 + 10{,}83x_3 + 4{,}34x_1x_2 +$$

$$+ 5{,}52x_1x_3 - 5{,}19x_2x_3 - 5{,}56x_1^2 + 3{,}99x_2^2 - 4{,}88x_3^2 \quad (1)$$

Table 2

Parameters of washing ability of SAA

№	Parameters of washing ability of solution of SAA for lavsan materials				Parameters of washing ability of solution of SAA for woolen materials			
	MS_1, %	MS_2, %	AOD	Z_{rem}, %	MS_1, %	MS_2, %	AOD	Z_{rem}, %
1	39,387	9,508	0,601	77,823	64,353	25,715	0,381	58,409
2	31,342	7,136	0,616	75,745	46,851	13,662	0,517	69,545
3	39,882	8,459	0,649	77,518	65,672	28,388	0,347	55,000
4	12,202	2,319	0,665	78,369	71,064	30,601	0,351	55,455
5	16,837	2,965	0,712	80,496	54,974	20,793	0,403	60,455
6	21,969	6,010	0,562	72,340	71,165	33,771	0,309	50,909
7	-4,766	-0,783	0,752	82,270	57,034	22,551	0,384	58,636
8	20,038	3,814	0,703	80,142	8,815	2,656	0,608	75,000
9	9,967	2,298	0,660	78,014	53,885	20,306	0,406	60,682
10	15,988	3,501	0,688	79,362	58,070	23,421	0,379	58,182
11	32,953	7,490	0,633	76,596	62,455	24,230	0,400	60,000
12	13,719	2,850	0,671	78,617	68,618	28,045	0,374	57,727
13	0,113	0,039	0,678	79,007	58,528	23,105	0,411	60,455
14	10,192	1,919	0,695	79,787	54,796	18,934	0,446	64,091
15	12,947	2,909	0,615	75,745	61,100	22,980	0,409	60,909

For the Lavsan fabric the mathematical model of dependence of washing ability (MS_1, %) on the indicated factors is the following:

$$MS_1 = 10,62 + 7,84x_1 - 0,13x_2 + 3,99x_3 + 5,27x_1x_2 +$$
$$+ 0,72x_1x_3 + 0,005x_2x_3 + 2,94x_1^2 + 13,30x_2^2 - 4,89x_3^2 \quad (2)$$

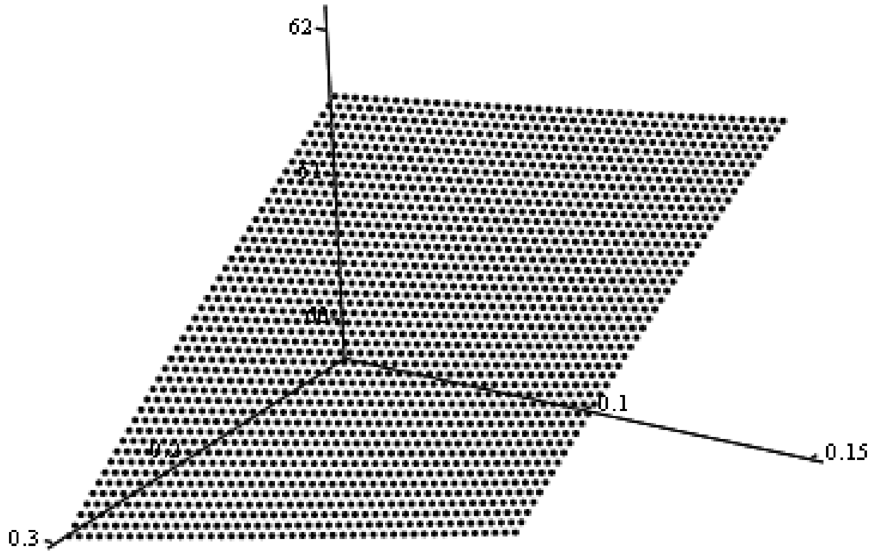

Fig. 2. Regression model of dependence of washing ability from the criteria on optimization for textile materials

Rys. 2. Model regresyjny zależności zdatności myjnej od kryterium optymalizacji dla materiałów włókienniczych

Similar models have been calculated for other criteria of optimization. All mathematical models are adequate, i.e. they can be applied with practical aims, namely for a primary objective – optimization of contents of washing composition [2]. For optimization of the composition contents the compromise task of optimization of the system of four models can be solved, and it is possible to optimize the model, for example with the washing ability. The task of optimization is formulated as follows: to determine the particles of components in washing composition for achievement of maximal washing effect, if their values belong to the range of the accepted values Φ:

$$MS_1 = f(x_1, x_2, x_3) \rightarrow \max$$
$$x_1, x_2, x_3 \in \Omega \quad (3)$$

The results of the contents of components in washing compositions are given in tab. 3.

There are differences in results for Lavsan. Foremost it is because that the coefficient of reflectivity of muddy fabric is not taken into account in equations of D. Zhuzhka and AOD. In addition, muddiness is not equally distributed on the surfaces of material, and spots on the surface of material as a result of resorption of muddiness from washing solution are seen after washing of samples.

Table 3

Compounds of washing composition (masses %)

Determination method	Wool			Lavsan		
	X_1	X_2	X_3	X_1	X_2	X_3
Kubelk-Moonk	14,5	5	6,9	29,5	14,75	6,0
Mench-Kaufmann	10	5	6,9	29,5	14,75	5,8
D. Zhuzhka	10	5	6,5	10	5	6,9
AOD	10	5	6,9	10	5	6,9

The solution of compromise task can result in finding optimum compounds of composition that has universal character of action. The compromise task is mathematically formulated as follows:

$$\begin{cases} MC_1 = f(x_1, x_2, x_3) \rightarrow \max \\ MC_2 = f(x_1, x_2, x_3) \rightarrow \max \\ \text{ДОГ} = f(x_1, x_2, x_3) \rightarrow \max \\ Z_{\text{зал}} = f(x_1, x_2, x_3) \rightarrow \min \end{cases} \qquad (4)$$
$$x_1, x_2, x_3 \in \Omega$$

As a result of optimization, an effective universal composition has been obtained. The composition can be applied for washing of pure-woolen as well as mixed fabrics. Optimal composition of contents (in mass %) is as following:

- phosphoxid 7 6,8%;
- syntanol DS-10 5,0%;
- fibre-tex 25 11,0%;
- intersolvents completion to 100%.

4. Conclusions

The work has testified that the research strategy consists of: application of the system theory and system analysis of complex CTP, as well as application of mathematical modelling as the research method. Application of mathematical methods, when studying CTP, enables to determine directions of further improvement of technology of dry-cleaning with minimum waste of time and expenses of reagents.

On the basis of scientifically substantiated system approach to the analysis of CTP of treatment of materials high-efficiency composition for intensification of dry-cleaning of textile materials has been elaborated.

Mathematical models which are characterized by the high degree of prognostication have been created with the help of modern approaches of mathematical modelling to the investigation of complex objects of chemical technology.

Realization of the results of the conducted research allows to select high-efficiency preparations for dry-cleaning of soft goods, as well as to extend possibilities of their use in different CTPs of treatment of textiles.

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