

APPLICATION OF GENETIC ALGORITHMS TO DETERMINE HEAVY METAL IONS SORPTION DYNAMICS ON CLINOPTILOLITE BED

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In the last decade a growing interest was observed in low-cost adsorbents for heavy metal ions. Clinoptilolite is a mineral sorbent extracted in Poland that is used to remove heavy metal ions from diluted solutions. The experiments in this study were carried out in a laboratory column for multicomponent water solutions of heavy metal ions, i.e. Cu(II), Zn(II) and Ni(II). A mathematical model to calculate the metals' concentration of water solution at the column outlet and the concentration of adsorbed substances in the adsorbent was proposed. It enables determination of breakthrough curves for different process conditions and column dimensions. The model of process dynamics in the column took into account the specificity of sorption described by the Elovich equation (for chemical sorption and ion exchange). Identification of the column dynamics consisted in finding model coefficients β , K_E and D_{eff} and comparing the calculated values with experimental data. Searching for coefficients which identify the column operation can involve the use of optimisation methods to find the area of feasible solutions in order to obtain a global extremum. For that purpose our own procedure of genetic algorithm is applied in the study.

Keywords: sorption dynamics, genetic algorithm, heavy metal ions, clinoptilolite

1. INTRODUCTION

Natural zeolites have excellent adsorption capacity and differ considerably from other adsorbents. The group includes clinoptilolite, mordenite, chabazite, erionite and phillipsite. Unlike silica gel or activated carbon, zeolites have a unique crystalline structure which enables them to very specifically adsorb particles of certain sizes.

Zeolite crystalline framework is arranged in an interconnecting lattice structure. The arrangement of these elements in a zeolite crystal creates a porous structure with interconnecting channels, which is one of the main qualities of a good adsorbent. Clinoptilolite is a natural aluminosilicate mineral with a skeleton structure and large pores filled up with large ions (Ca, Mg, Na, K) and water particles.

Zeolites have been used to remove impurities and heavy metal ions from aqueous solutions for several years (Gomonajet et al., 1998; Kurowski, 1978). Possible applications of clinoptilolite are still extensively studied (Erdem et al., 2004; Sprynski et al., 2005), also by Polish researchers (Kosobucki et al., 2007; Petrus and Warchol, 2005). It is also important that clinoptilolite can be used for heavy metals sorption on an industrial scale e.g. (Chojnacki et al., 2004).

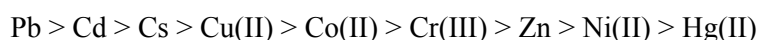
Water usually contains several dissolved substances. One of the most important factors affecting water quality is the presence of metals, and particularly the presence of heavy metals (Duffus, 2002). Those

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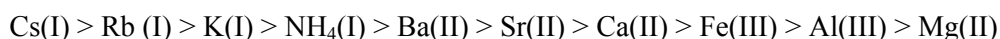
that directly affect living organisms are without doubt the most toxic ones (Linnik, 1998). Their removal from aqueous solutions is a key problem in the field of environment, human health and life protection. Several physical and chemical methods are available for removal of heavy metal ions from water, and these include chemical precipitation and filtration, coagulation, ion exchange, membrane processes and adsorption.

In recent years adsorption has become increasingly popular because materials applied in the process are manufactured using innovative methods. They have the special properties required for the adsorption of heavy metal ions.

Studies into ion removal on zeolite have revealed that ions are removed as a result of ion exchange and adsorption processes that occur at the same time. Zamzow et al., (1990) defines the following selectivity sequence of clinoptilolite for the adsorbed heavy metal ions:



The sequence confirming higher selectivity of clinoptilolite for monovalent ions the so-called exchange sequence was defined by Mercer and Ames (1976):



Sodium form of clinoptilolite has been found particularly selective for heavy metals, with the method of substituting sodium with metal of crucial importance. Zeolite should be subjected to exchange and regeneration processes several times so as to ensure that all mobile ions have been replaced by sodium ions. The presence of calcium and magnesium ions may negatively influence the effectiveness of heavy metals removal. Additionally, metals present in water solution as different complexes do not undergo ion exchange. Alkaline earth metals have also been the subject of many studies (Tarasevich et al., 2006).

2. EXPERIMENTAL STUDIES ON SORPTION EQUILIBRIUM AND DYNAMICS IN THE COLUMN

The studies were conducted on the product prepared with natural zeolite by Inwest Holding Polska Sp. z o.o. named ZEOKlin. Clinoptilolite is the main component of the sorbent 84% (cristobalite 9%, plagioclase 7%). Grain fractions of 1-3 mm in size and the density of 2160 kg/m³ were used for the studies. Clinoptilolite was washed with distilled water to remove any physical impurities and then dried at 105°C to eliminate the so-called zeolite water. The modification involved soaking for 24 hours in 3% NaCl solution, washing with distilled water until chloride ions have been eliminated and then drying at 105°C. The chemical processing was aimed at increasing clinoptilolite ion exchange ability which enables elimination of all cations from crystalline network channels. The sodium form of clinoptilolite that is particularly selective for heavy metal ions is obtained in that way. The selected equilibrium and kinetics results obtained with the material prepared as described above have been presented in the paper Tomczak and Sulikowski (2010).

Reagents used for chemical modification and preparation of solutions were manufactured by Chempur (Poland). Demineralised water and a proper metal salt were used to prepare adsorbate solution, and included CuSO₄×5H₂O, NiSO₄×6H₂O, ZnSO₄×7H₂O.

The experimental set up comprised a glass column of 3.45 cm in diameter and 70 cm in length. The column was each time filled with dry sorbent of a controlled mass approximately 60 g up to a specified bed height $h_0 = 58.8$ cm. Before proper measurement had been made, the bed was conditioned by washing it down with demineralised water. The solution was supplied to the column using a pump from the bottom upward to the top of the bed single pass and removed from the system. The selected

strategy ensured a constant concentration at the column inlet $c_0 = 20 \text{ mg/dm}^3$; 40 mg/dm^3 ; 50 mg/dm^3 ; 45 mg/dm^3 (for volumetric flow rate $Q = 0.8 \text{ dm}^3/\text{h}$) and $c_0 = 40 \text{ mg/dm}^3$ (for $Q = 0.8 \text{ dm}^3/\text{h}$; $2.4 \text{ dm}^3/\text{h}$; $4.0 \text{ dm}^3/\text{h}$).

At controlled time intervals samples were taken at the column outlet and analysed using Dionex ICS-1000 ion chromatograph.

3. MODELLING OF ADSORPTION DYNAMICS

For the purpose of modelling of adsorption dynamics the following assumptions have been made: the adsorption process is isothermal – recommended for media of a low concentration e.g. for water purification so that minor thermal effects can be neglected, the bed is uniformly packed, the fluid is incompressible and of constant viscosity, adsorbate flow rate over the entire column height is constant, mass transfer resistance is observed in both phases, mass transport is related with plug flow of the fluid and axial dispersion (parallel to the direction of fluid flow), radial dispersion is negligible, the concentration of feed fluid is constant, concentration in the sorbent changes according to the adsorption kinetics equation appropriate for a given adsorbate-adsorbent system.

Changes of the concentration in the fluid $c(t, x)$ and adsorbent $q(t, x)$ will then be a function of time and distance from the inlet. Mass balance between the fluid flow and the bed is achieved under the following conditions:

- initial $c_i(0, x) = 0$,
 $q_i(0, x) = 0$,
- boundary $c_i(t, 0) = c_{0i}$ for $t > 0$ (constant c_{0i} concentration at the column inlet),
- adsorption kinetics equation is the same at each column section.

It is a new and original approach. It was verified experimentally for different adsorption systems by the author (Tomczak, 2011a).

Equation (1) represents a general mass balance with the assumptions presented above. The equation is well known and often cited in the literature (Babu and Gupta, 2005; Chen et al., 2003; Gupta and Babu, 2009; Kamio et al., 2002; Molga, 2008; Sag and Aktay, 2001):

$$u_0 \frac{\partial c_i(x, t)}{\partial x} + (1 - \varepsilon) \rho_s \frac{\partial q_i(x, t)}{\partial t} + \varepsilon \frac{\partial c_i(x, t)}{\partial t} = \varepsilon D_{eff_i} \frac{\partial^2 c_i(x, t)}{\partial x^2(x, t)} \quad (1)$$

D_{eff_i} coefficient needs to be discussed further. The coefficient is called the effective dispersion coefficient (and includes axial dispersion). The coefficient consists not only of molecular diffusion effects, which *notabene* are negligible, but mainly of dispersion effects resulting from turbulence flow as a result of column packing and flow effects.

It should be noted that process time and the analysed column height are interconnected. The two analysed column points, both for the fluid and the adsorbent, are time shifted to each other. To facilitate interpretation of results the introduction of the following variable is suggested:

$$\xi = u_0 t - x \quad (2)$$

x – distance between the two column heights considered.

After the substitutions which is described in the publication (Tomczak, 2011) Equation (1) takes the following form:

$$-\frac{dc_i}{d\xi} + \rho_s \frac{dq_i}{d\xi} = \frac{\varepsilon D_{eff_i}}{u_0(1 - \varepsilon)} \frac{d^2 c_i}{d\xi^2} \quad (3)$$

Sorption kinetics is studied equally frequently in the literature for example (Gök et al., 2008; Pérez-Marín et al., 2007). Sorption kinetics can be described by means of different equations depending on the sorbent-sorbate system (Tomczak, 2011a). For a given system the kinetic equation should be verified empirically or it can be taken from the literature.

For chemisorption and mixed sorption that is the case for clinoptilolite, Elovich equation is applied (Chang and Juang, 2005; Suguna et al., 2010):

$$\frac{dq_i}{dt} = K_{E_i} e^{-\beta_i q_i} \quad (4)$$

which may be defined as follows:

$$\frac{\partial q_i}{\partial t} = u_0 \frac{dq_i}{d\xi} = K_{E_i} \exp(-\beta_i q_i) \quad (5)$$

Therefore adsorption value q_i is obtained at any point within the column:

$$q_i(\xi) = \begin{cases} \frac{1}{\beta_i} \ln(\alpha_i \xi + 1) & x < u_0 t \\ 0 & x \geq u_0 t \end{cases} \quad (6)$$

where

$$\alpha_i = \frac{K_{E_i} \beta_i}{u_0} \quad (7)$$

Substituting Equation (6) to Equation (5) results in the following form:

$$\frac{dq}{d\xi} = \frac{1}{\beta} \frac{\alpha}{\alpha \xi + 1} \quad (8)$$

The concentration of a selected species in the water solution at the different column height may be calculated:

$$\begin{cases} c_i = c_{0i} + \frac{\rho_s}{\beta_i} \ln\left(\frac{\alpha_i \xi + 1}{\alpha_i \xi_0 + 1}\right) - \frac{\varepsilon D_{eff} \alpha_i \rho_s}{\beta_i u_0 (1 - \varepsilon)} \left(\frac{1}{\alpha_i \xi + 1} - \frac{1}{\alpha_i \xi_0 + 1} \right) & x < u_0 t \\ c_i = 0 & x \geq u_0 t \end{cases} \quad (9)$$

ξ_0 variable corresponds to the column inlet and takes the following form:

$$\xi_0 = u_0 t \quad (10)$$

The identification of column dynamics consists of finding model coefficients β_i , K_{E_i} , D_{eff} in inverse problem based on measurement data. The coefficient values will be related with the best match of the model and the real object i.e. column operation. The subject function is presented in the form of Equation (13). The search for coefficients identifying column operation may be completed with the use of optimisation methods that search a space of admissible solutions in order to find a global extremum. In the publication, genetic algorithm was used for this task.

4. THEORETICAL BASICS OF GENETIC ALGORITHM

Methods of searching for global extrema are of fundamental importance in optimisation calculations. There are many methods of global optimisation such as subset construction, penalty functions, Simplex methods, Monte Carlo methods, Tabu search or simulated annealing, etc. Genetic algorithm (GA) also belongs to a class of global optimisation tools. It allows for searching the space of acceptable solutions, and is based on the mechanisms of natural selection and inheritance (it is inspired by biological models of evolution), using the evolutionary principle of survival of the fittest and random exchange of information (Fogel, 1994; Davis, 1991). The key feature of living organisms is their ability to reproduce and transfer their genetic information to later generations. Observing nature inspired scientists to design artificial systems having properties similar to those characteristic for natural systems for the purpose of technology and IT. John Holland was the first to apply genetic algorithms for the purpose of optimisation (Holland 1968; 1987), yet the pioneer works date back to late 1960s (Whitly, 2001).

Genetic algorithms are based on evolutionary change of individual features as a result of reproduction and adaptation to new environment conditions and selection i.e. taking advantage of better chances of survival and reproduction of stronger or better adapted individuals. The mechanism, imitating the nature and transformed into operations on numbers, has been successfully applied in many fields. Calculation methods in genetics and evolution developed independently in many countries and at different levels. It was probably related to the adaptation of the existing and effective solutions for new calculation tasks. Rutkowska et al., (1997) defines the three main directions of development:

- evolution strategies (Germany),
- evolutionary programming (USA),
- genetic algorithms.

In recent years the differences have gradually disappeared and the solutions have become similar as regards similar stages of calculations (Kamiński et al., 2005). A genetic algorithm generally comprises several stages, namely initialisation, reproduction, mutation and selection whose aim is to exchange genetic material, introduce a new genetic factor and select best individuals for further reproduction.

Initialisation is the first stage of an algorithm and involves random selection of I_R vectors (parents). Each coordinate of a vector $\mathbf{X}_k=(x_{1k}, \dots, x_{nk})$ is selected at random from a pool comprising an expected solution. It is assumed that genes representing a given feature are individual coordinates of the vector, while the vector itself is the equivalent of a chromosome i.e. a set of features.

At the *reproduction* stage offsprings may be produced as a result of crossover, one-point exchange of some of the chromosomes and cloning to preserve the parents' original genetic material.

Crossover takes place according to an adopted procedure, usually at random, with the assumed probability of random selection of individuals to exchange (recombine) genes. In the application at hand each member of the mating pool is mated with another. Then each of the offsprings produced as a result of reproduction is subjected to mutation.

Mutation involves multiplying each coordinate of a vector (individual) by mutation factor being a pseudorandom number.

At the *selection* step the selected quality function is the verification criterion. In most cases the problem may be reduced to searching for a minimum or maximum value of an objective function. Parents for the next generation are selected from the population members with a pre-defined criterion.

Subsequent generations i.e. the calculation process comprising reproduction, mutation and selection continue until an acceptable value of the objective function is returned.

The problem of searching for a global maximum of De Jong's function was selected as an example to test the proposed genetic algorithm method. The function is defined as follows:

$$F(x_1, x_2) = \sum_{k=1}^{25} \frac{1}{k + (x_1 - A(1, k))^6 + (x_2 - A(2, k))^6} \quad (11)$$

where: $A = [32, -16, 0, 16, 32, -32, -16, 0, 16, 32, -32, -16, 0, 16, 32, -32, -16, 0, 16, 32, -32, -32, -32, -32, -32, -16, -16, -16, -16, -16, 0, 0, 0, 0, 16, 16, 16, 16, 16, 32, 32, 32, 32, 32]$

Function (11) has several local maxima. 3D image is presented in Fig. 1. The coordinates of vectors x_k were selected at random from $\langle -18, 18 \rangle$ range. Calculations were made to search for a global maximum using three methods: with the proposed algorithm, gradient descent and simplex, for the purpose of testing our own procedure of genetic algorithm.

It was assumed that the solution to the problem is located within the Ω set

$$\Omega = \{x : x_1, x_2 \in \langle -18, 18 \rangle\} \quad (12)$$

Calculations with the use of the proposed method were made with 20 parents in the initial population. Satisfactory results were obtained after 6 subsequent generations. An attempt at identifying the global maximum of the function (11) by gradient and simplex methods failed to produce a satisfactory result in spite of several tens of calculation runs for a randomly selected starting point.

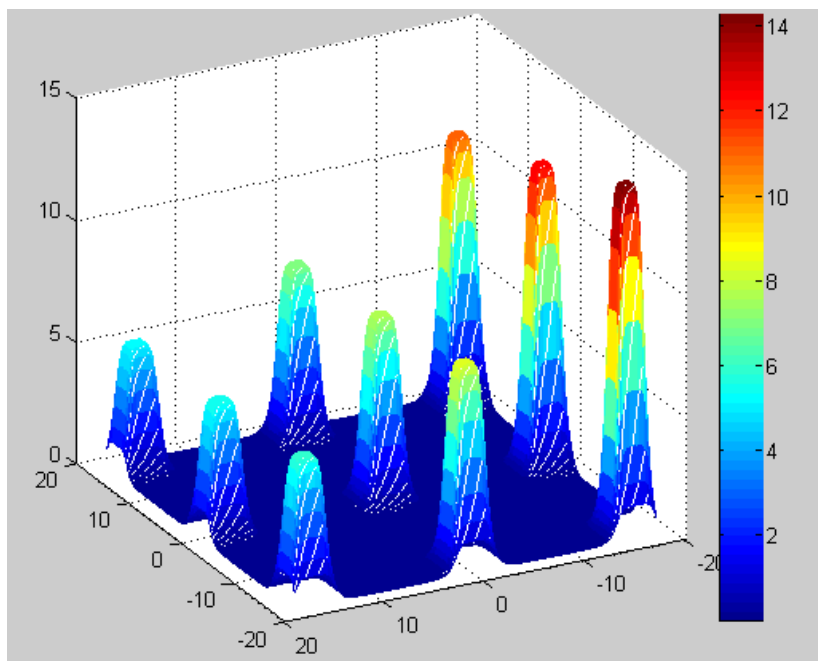


Fig. 1. Graphical representation of function with many local maxima

Genetic algorithms are often applied to solve optimisation problems in combination with artificial neural networks: learning in Kohonen networks (iris flowers), searching for weights in SNN, searching for optimal neuronal activation function, solving 0-1 optimisation problems, fast learning neural networks or fuzzy neural networks learning. Special applications include development of optimal strategy for power plant operation, ship collision avoidance, searching for physical process descriptions, selection of optimal stock portfolio, selection of biomedical data (Kaminski and Tomczak, 1998), or search for global extrema (Tomczak and Kaminski, 2008).

For calculations related to the adsorption model in the column, the objective function was defined as follows

$$F(\beta_i, K_{E_i}, D_{eff_i}) = \min \sum_{k=1}^p (c_{obl,k} - c_{exp,k})^2 \quad (13)$$

As mentioned before, the aim of the implemented GA-based optimisation procedure was to select model coefficients β_i , K_{E_i} , D_{eff_i} . In inverse problem parameter values (e.g. equilibrium concentration in the sorbent, diffusion coefficients, reaction rate constants) are estimated by the best fit between the model output and experimental data.

For all GA calculations the following parameters were assumed:

Number of parents	$l_r = 20$
Number of generations	$l_p = 20$ (subsequent generations)
Coding	floating point
Initialisation	random selection of coordinates (individuals) from a pre-defined range
Mutation	pseudorandom number generator of normal distribution
$xr = randn * alf + 1$	where
	xr – pseudorandom number
	alf – coefficient changed in subsequent generations
	$alf^{i+1} = alf^i \cdot (ip - i + 1) / ip$
	$randn$ – pseudorandom number generator N(0,1)
	mean 0 and standard deviation 1
result → new individuals	
Reproduction	each member of the population is crossed over with another (parents are included in the population)
	Assuming that the same couple produces offsprings twice, population number will be
	$L = 2 \cdot l_r^2 + l_r$
Crossover	one-point crossover point at 1/3 of length of a chromosome
Selection	hard (the strong survive and the weak die out)

5. CALCULATION AND EXPERIMENTAL RESULTS

During the first stage measurements were made for $c_0 = 50 \text{ mg/dm}^3$ and volumetric flow rate $Q = 0.8 \text{ dm}^3/\text{h}$. Based on satisfactory statistical evaluation (Cu(II) - $R^2 = 0.929$; Zn(II) - $R^2 = 0.936$; Ni(II) - $R^2 = 0.990$) it was confirmed that adsorption kinetics in the column meets Elovich model. As mentioned before, the equation is recommended for describing process kinetics in the case of chemisorption and ion exchange.

Figures 2-5 compare the concentration at the column outlet (experimental data – open symbols) with those calculated based on the model as per Equation (9) for various parameters of column operation. The highest adsorption was noted for copper ions, with lower adsorption recorded for zinc ions and the lowest for nickel ions.

Table 1 presents a statistical evaluation of model calculations for each metal ion – coefficients K_E , β , D_{eff} and α identified in the model. The following statistical factors were taken into consideration:

- sum of squares

$$Sum = \sum_{k=1}^p (y_{exp,k} - y_{cal,k})^2 \quad (14)$$

- coefficient of determination (R squared)

$$R^2 = 1 - \frac{\sum_{k=1}^p (y_{exp,k} - y_{cal,k})^2}{\sum_{k=1}^p (y_{exp,k} - y_m)^2} \quad (15)$$

where

$$y_m = \frac{\sum_{k=1}^p y_{exp,k}}{p} \quad (16)$$

- mean square error

$$\delta_m = \sqrt{\frac{\sum_{k=1}^p (y_{exp,k} - y_{cal,k})^2}{p}} \quad (17)$$

Fig. 6 presents breakthrough curves for copper, zinc and nickel ions for three column heights $h_0 = 1$ m, 1.5 m and 2 m. The results for the laboratory column height $h_0 = 0.588$ m, for the same operation parameters have already been presented in Fig. 4. An analysis of breakthrough curves indicates that the column height is of practically no importance for nickel ions as the concentration at the outlet quickly reaches saturation concentration. For the component that is most rapidly sorbed (copper ions) the period of effective column operation is clearly dependant on its height. For $h_0 = 1$ m breakthrough is observed as early as after approximately 400 minutes and for $h_0 = 2$ m after 1500 minutes.

Table 1. Clinoptilolite – Cu(II)+Zn(II)+Ni(II). Specification of model coefficients and statistical evaluation of model approximation

c_0 [mg/dm ³]	Q [dm ³ /h]	Ion	K_E [mg/g·min]	β [g/mg]	D_{eff} [m ² /min]	α [1/m]	SUM	R^2	δ_m
40	0.8	Cu(II)	4.4485e-4	0.11518	1.4975e-4	3.589e-3	1.7796	0.90177	0.3699
		Zn(II)	4.8883e-4	0.5940	4.1246e-5	2.036e-2	1.9851	0.99067	0.3907
		Ni(II)	1.0686e-1	17.9005	4.2138e-1	1.341e+2	21.5952	0.99244	1.2888
	2.4	Cu(II)	1.1469e-3	1.2276	7.1812e-4	3.290e-2	28.7291	0.94298	1.6949
		Zn(II)	1.0302e-3	2.7893	8.1157e-4	6.716e-2	33.8464	0.95719	1.8397
		Ni(II)	1.3313e-3	13.0637	5.1323e-3	4.064e-1	18.0587	0.98482	1.3438
	4.0	Cu(II)	1.6005e-3	1.58902	4.9900e-5	3.566e-2	11.8376	0.98035	1.3004
		Zn(II)	1.2374e-3	2.42243	1.4218e-3	4.204e-2	14.3645	0.98074	1.4325
		Ni(II)	3.0437e-3	10.6369	7.1804e-4	4.539e-1	4.11701	0.99621	0.7906
50	0.8	Cu(II)	5.1831e-4	0.49404	7.4789e-5	1.795e-2	14.1735	0.92913	1.3310
		Zn(II)	5.4729e-4	2.05171	6.6210e-5	7.873e-2	55.3161	0.93652	2.6295
		Ni(II)	6.0470e-3	96.6396	4.2369e-1	4.097e+1	35.9684	0.98965	2.1203

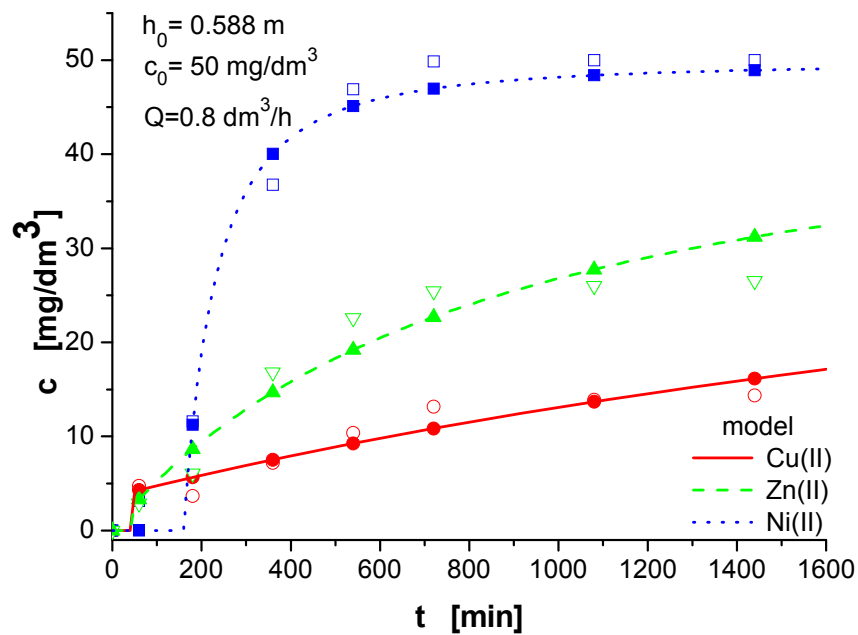


Fig. 2. Clinoptilolite - Cu(II)+Zn(II)+Ni(II): change of concentration at column outlet for $c_0 = 50 \text{ mg/dm}^3$

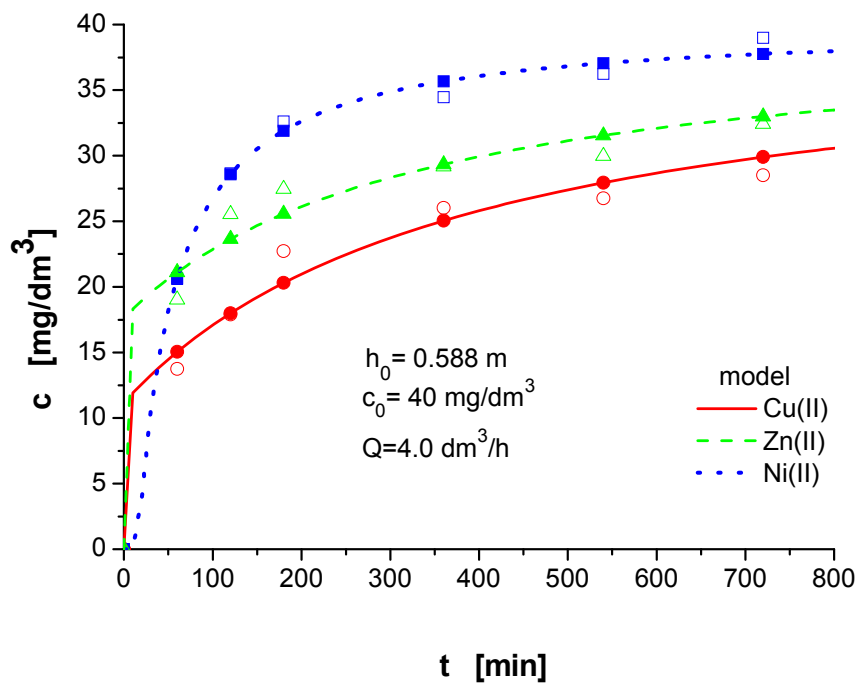


Fig. 3. Clinoptilolite - Cu(II)+Zn(II)+Ni(II): change of concentration at column outlet for $c_0 = 40 \text{ mg/dm}^3$

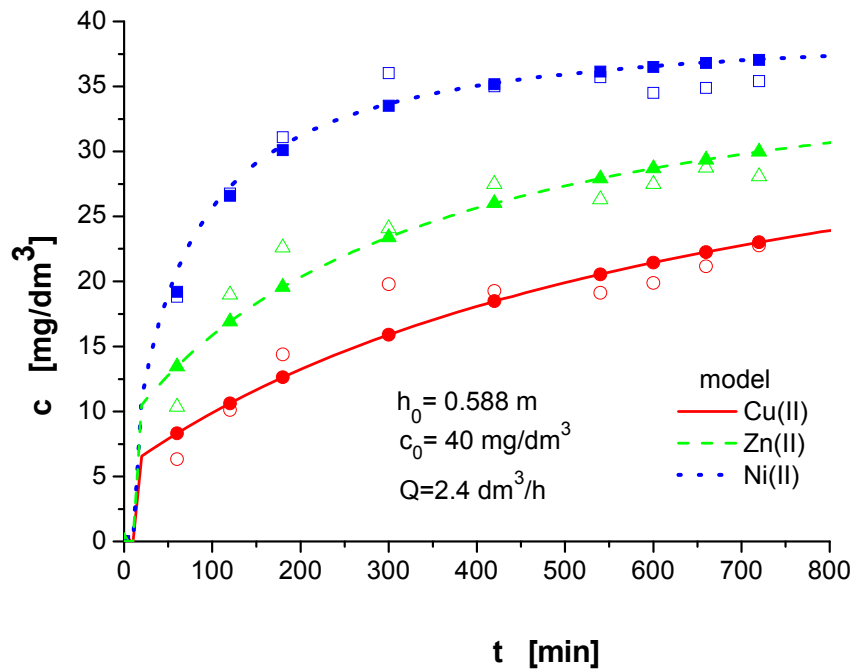


Fig. 4. Clinoptilolite - Cu(II)+Zn(II)+Ni(II): change of concentration at column outlet for $c_0 = 40 \text{ mg/dm}^3$

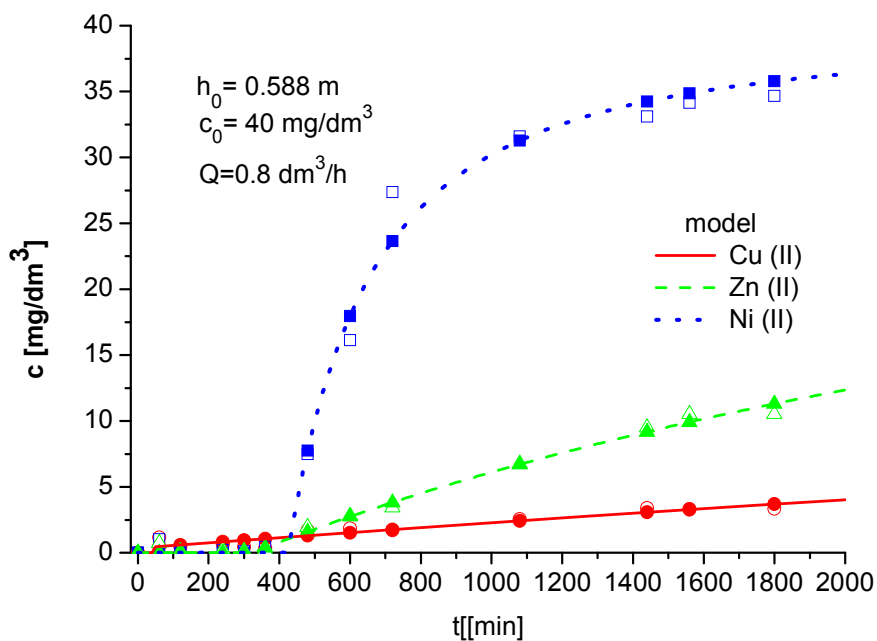


Fig. 5. Clinoptilolite - Cu(II)+Zn(II)+Ni(II): change of concentration at column outlet for $c_0 = 40 \text{ mg/dm}^3$

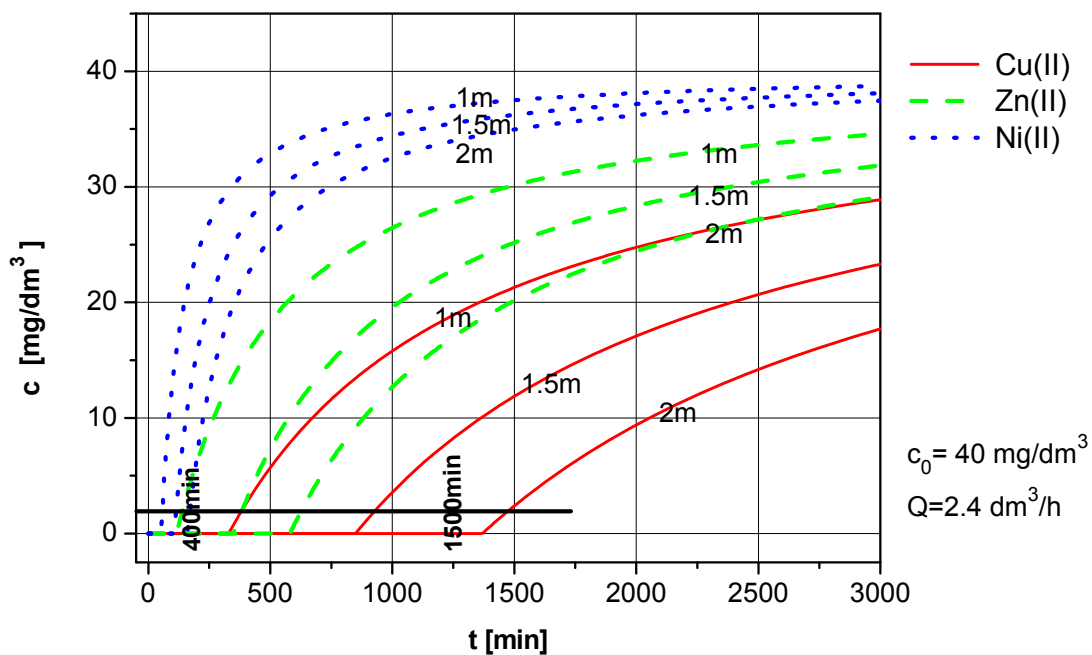


Fig. 6. Clinoptilolite - Cu(II)+Zn(II)+Ni(II): change of concentration at the outlet depending on column height

Fig. 7 presents the change in amount of adsorbed substance in the column of 1.5 m in height for the three analysed ions –Eq. (6).

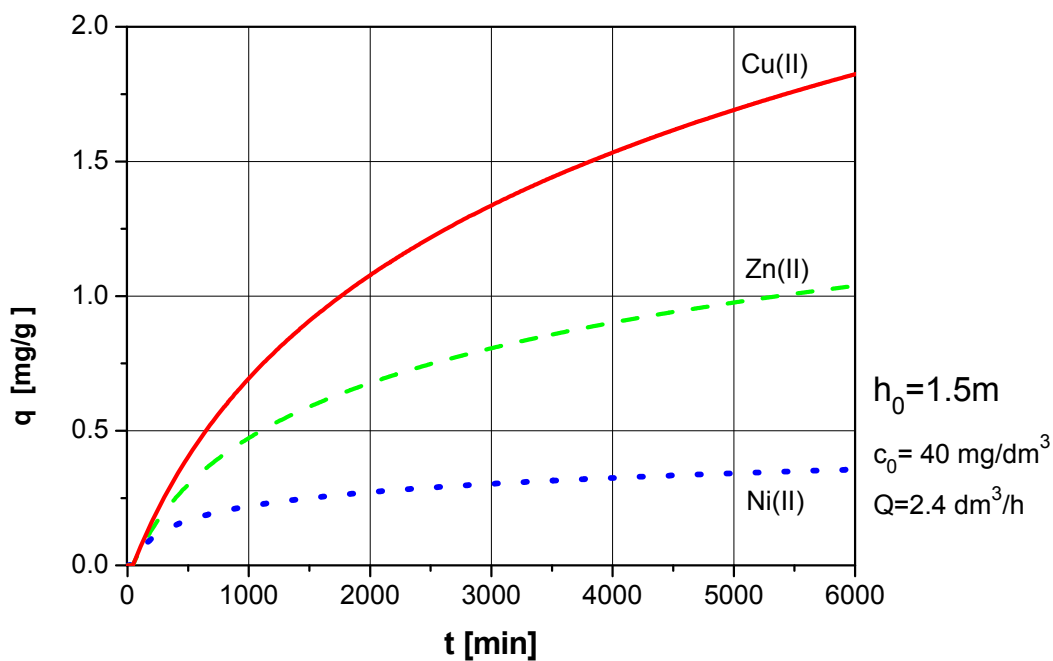


Fig. 7. Clinoptilolite - Cu(II)+Zn(II)+Ni(II): kinetics of q change in the column of $h_0 = 1.5$ m

6. CONCLUSIONS

- Optimisation in chemical and process engineering calls for new, sometimes unconventional calculation techniques. The method includes the genetic algorithm which is a random method of seeking the global minimum (extremum).
- The paper presents the authors' own modification of a classic genetic algorithm consisting of gene coding with floating point numbers. It was assumed that acceptable solutions space may be penetrated with the use of the proposed algorithm. The effectiveness of the algorithm was tested with the use of the selected test function to achieve its quick convergence. Additionally, the proposed algorithm was used to calculate three coefficients identifying column operation. The calculation quality was confirmed by a statistical evaluation.
- The effectiveness of clinoptilolite as an adsorbent of heavy metal ions was confirmed. For clinoptilolite-heavy metal ion system mixed adsorption was assumed that was based on physical interaction and ion exchange in the sequence $\text{Cu} > \text{Zn} > \text{Ni}$. The sorption kinetics was described by Elovich equation.
- Very good quality of the experimental data approximation was obtained for the calculations of column dynamics applying the proposed approach. It must be underlined that the computational effort was minimal, and the model assumptions reflected the real course of the process.
- According to the proposed model, it was easy to calculate the concentration in the fluid phase at any given point within the column for each moment of time, as well as the corresponding adsorption in the solid phase (adsorbent), which resulted in an accurate determination of the breakthrough time or column saturation.

SYMBOLS

c_i	concentration, mg/dm^3
c_{0i}	initial concentration, mg/dm^3
D_{effi}	effective diffusion (dispersion) coefficient, m^2/s
K_{Ei}	reaction rate coefficient in Elovich equation, $\text{mg}/(\text{g min})$
h_0	bed height, m
L	size of population
l_p	number of generations
l_r	number of parents
m	mass, g
p	number of experiments
Q	volumetric flow rate, dm^3/h
q_i	adsorption, $\text{mg}/\text{g d.m.}$
t	time, min
u_0	apparent velocity, m/s
x	distance, m
$y_{cal,k}$	calculated value
$y_{exp,k}$	experimental value
y_m	average value

Greek symbols

α_i	coefficient defined by Eq. (7), $1/\text{m}$
β_i	coefficient in Elovich Eq. (4), g/mg
δ_m	mean square error, mg/dm^3

ε	bed porosity, -
ξ	variable defined by Eq. (2), m
ρ_s	density of material, kg/m ³
Ω	search space, -

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