

Modelling of Fixed Bed Multicomponent Ion Exchange

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The paper presents a study of the total demineralization of dilute aqueous solutions by ion exchange using two fixed bed columns, the former with a strongly acidic resin ($R_c^- H^+$) and the second with a strongly basic resin ($R_a^+ HO^-$). A mathematical model based on a plug flow with axial dispersion and a competition between adsorption and desorption processes of ionic species was proposed to describe the multicomponent ion exchange. An experimental investigation of influence of process factors, namely feed solution composition, solution superficial velocity and operation temperature, on fixed bed breakthrough dynamics, was performed to identify the model parameters.

Keywords: ion exchange, total demineralization, fixed bed, breakthrough curves, modelling

Granular ion exchangers are successfully used in raw and waste water treatment, hydrometallurgy, analytic, inorganic and organic chemistry, food industry, medicine etc. Due to their multiple employments, the analysis of aspects concerning the solid-liquid system implied in ion exchange process was the aim of numerous research papers.

Depending on composition and concentration of feed solution, quality imposed to treated solution, investment and operation costs etc, there are various methods of phases contacting, e.g. stage wise or differential contacting, with single or multiple contact, in fixed, fluidised, stirred, moving bed [1-17]. Ion exchange in fixed bed columns is widely used in experimental researches and industrial applications due to its advantages:

- ion exchanger particles are not mechanically degraded as in case of stirred or moving beds;
- easy operation;
- possibility of coupling of process phases (service, regeneration, rinsing) in a system with continue and completely automated operation;
- rapid and total recovery of retained species by a proper selection of regeneration solution.

Characteristic performances of fixed bed ion exchange depend on various parameters, e.g. composition, concentration and flow rate of feed solution, type, total capacity and initial ionic form of ion exchanger, fixed bed height, operation temperature.

Dynamics of ion exchange between A and B contraions depends on the relative affinity coefficient of ion exchanger, K_B^A [6,8,9]:

$$\lg K_B^A = \frac{(V_B - V_A)\pi}{RT} \quad (1)$$

Correlation (1) shows a great affinity for A species at high values of osmotic pressure, π , and of difference between the volumes of hydrated ions, $V_B - V_A$, and low values of operation temperature, T . It accords with the conclusions of numerous researches that emphasised an increase of ion exchanger affinity for species with small volume and large valence absolute value.

Ion exchanger selectivity for some ions is used in applications of ion substitution, ion separation and ion removal [5,8,9]. Ion substitution refers to situations where a valuable or toxic ion is retained from a solution and

replaced by a valueless or non-toxic one. Ion separation corresponds to cases where different ions found in the influent of an ionic column are recovered and then eluted depending on ion exchanger affinity for them. Ion removal or demineralization can be partial or total and it is the best known and vast employment of ion exchangers at water or aqueous solutions treatment. Total demineralization, which is used to produce very pure water for energetic, electronic, food or pharmaceutical industries, is usually performed in an ion exchangers system consisting of a strongly acidic cationite in ionic form $R_c^- H^+$ and a strongly basic anionite in form $R_a^+ HO^-$. Ion exchange between the cations found in solution and H^+ ions is accomplished in the cationite, while the anionite retains anions existed in solution and releases HO^- ions. Accordingly, all ions are removed and replaced with water.

The aim of various research papers was to model the multicomponent mixtures separation by fixed bed ion exchange [2,14,18-25]. The models describing the fixed bed ion exchange in a cationite-anionite system can be more simple or complex depending on considered assumptions [10,15,25,26].

More sophisticated ones are based on mass balance equations, axial dispersion, film mass transfer, interparticle diffusion and complex nonlinear isotherms. To solve these models, a certain number of equilibrium and kinetic parameters must be estimated from suitable correlations by fitting experimental data determined in independent batch and dynamic studies. To avoid time-consuming and expensive experiments, simplified versions were proposed in the related literature, such as [25]:

- lumped kinetic models - which include dispersion along the column and either mass transport resistance as a lumped rate coefficient or adsorption-desorption process;
- equilibrium dispersive model - considering only dispersion while all transport resistance is neglected;
- ideal model - in which both dispersion and all transport resistance are neglected.

The present study has focused on the modelling of fixed bed ion exchange in case of total demineralization of dilute aqueous solutions containing one, two or three cations species and only an anion species, when these passed successively through a cationite and an anionite. An experimental study of influence of process factors, namely feed solution composition, solution flow rate and process

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temperature on ion exchange dynamics, described by fixed bed breakthrough curves, was performed as basis of model parameters identification.

Experimental part

Laboratory set-up shown in figure 1 was the same employed in our previous papers [27-29]. It consisted mainly of two columns with ion exchangers fixed bed, the former with a strongly acidic resin (VIONIT CS-3) and the second with a strongly basic resin (VIONIT AT-14). Feed solution stored in a vessel (1) was fed by a pump (2) into the upper part of cationic column (3) and acid effluent of this column down flowed through anionic column (4), whence completely demineralised water resulted till the column breakthrough. Electromotive force measurements of anionic column effluent, which were performed by a Cl^- electrode (5), a reference electrode (6) and a multimeter (7), were collected by a data acquisition system (8). Temperature in each ionic column was maintained at a constant value by a thermostat (9).

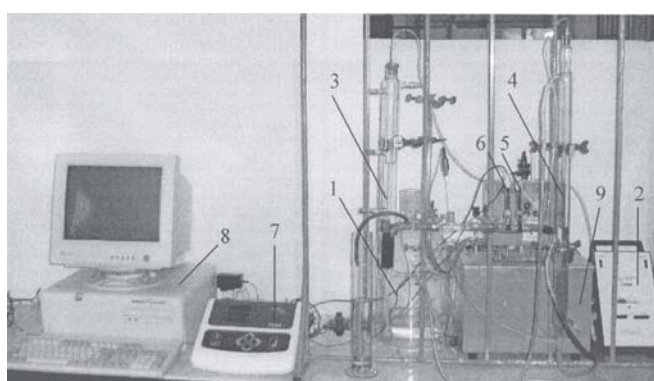
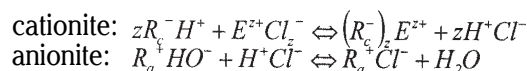


Fig. 1. Experimental set-up: 1 - storage vessel; 2 - feed pump; 3 - cationic column; 4 - anionic column; 5 - Cl^- electrode; 6 - reference electrode; 7 - Jenway 3310 multimeter; 8 - data acquisition system; 9 - thermostat

In exhausted zones of cationite and anionite, the following ion exchange reactions occur, wherein $E=Na, Ca, Al$ and $z=1, 2, 3$:



The both fixed beds of cationite and anionite had the same diameter ($d=0.025$ m), height ($H=0.22$ m), void fraction ($\varepsilon_b=0.35$) and particle diameter ($d_p=0.0015$ m). Five electrolyte solutions with the same anion concentration ($c_0=0.0085$ mol/L) and various cations concentrations (table 1) were employed as feed liquids. Experimental investigation was performed at two values of solution superficial velocity ($w_f=0.5 \cdot 10^{-3}$ m/s and $w_f=1.2 \cdot 10^{-3}$ m/s) and operation temperature ($t=30$ °C and $t=60$ °C). Time evolution of Cl^- anion concentration in anionic column effluent (breakthrough curve), $c(\tau)$, was determined on-line.

Results and discussion

Experimental breakthrough curves

Graphic representations shown in figure 2, illustrating the experimental breakthrough curves for implied solutions in various operation conditions, prove that:

- cationite selectivity for cation species increases in order: $Na^+ < Ca^{2+} < Al^{3+}$;
- breakthrough curve corresponding to solution $S4$ ($NaCl+CaCl_2$) ranges between those characteristic of solutions $S1$ ($NaCl$) and $S2$ ($CaCl_2$) and is near to that of $S1$;
- breakthrough curve corresponding to solution $S5$ ($NaCl+CaCl_2+AlCl_3$) is close by that characteristic of solution $S2$ ($CaCl_2$);
- an increase of operation temperature enhances the adsorption of Na^+ and Ca^{2+} , so that the values of breakthrough time corresponding to solutions $S1$, $S2$ and $S5$ become larger;
- an enlargement of solution superficial velocity determines a decrease of the values of characteristic breakthrough time of all implied solutions.

Modelling of fixed bed multicomponent ion exchange

A lumped kinetic model based on adsorption-desorption was proposed to simulate the fixed bed ion exchange. The underlying assumptions are as follows:

Solution \ Ion	Na^+		Ca^{2+}		Al^{3+}		Cl^-	
	$g \cdot L^{-1}$	$mol \cdot L^{-1}$	$g \cdot L^{-1}$	$mol \cdot L^{-1}$	$g \cdot L^{-1}$	$mol \cdot L^{-1}$	$g \cdot L^{-1}$	$mol \cdot L^{-1}$
$S1$ ($NaCl$)	0.1955	0.0085	-	-	-	-	0.3	0.0085
$S2$ ($CaCl_2$)	-	-	0.1700	0.0043	-	-	0.3	0.0085
$S3$ ($AlCl_3$)	-	-	-	-	0.0765	0.0028	0.3	0.0085
$S4$ ($NaCl+CaCl_2$)	0.0978	0.0043	0.085	0.0021	-	-	0.3	0.0085
$S5$ ($NaCl+CaCl_2+AlCl_3$)	0.0652	0.0028	0.0567	0.0014	0.0255	0.0009	0.3	0.0085

Table 1
IONS CONCENTRATION
IN FEED SOLUTIONS

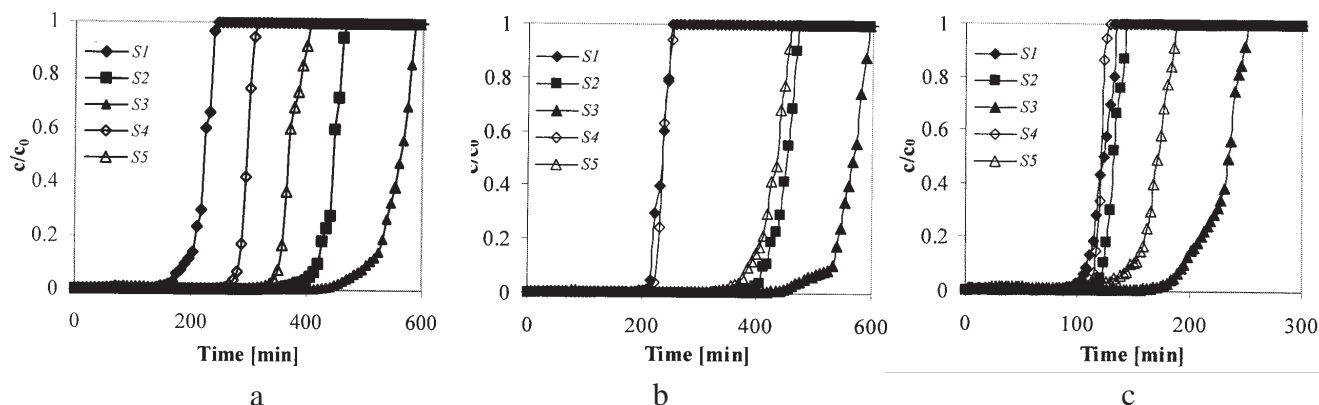


Fig. 2. Experimental breakthrough curves of Cl^- ions concentration dynamics in anionic column effluent:
a. $w_f=0.5 \cdot 10^{-3}$ m/s, $t=30$ °C; b. $w_f=0.5 \cdot 10^{-3}$ m/s, $t=60$ °C; c. $w_f=1.2 \cdot 10^{-3}$ m/s, $t=30$ °C

- cationite and anionite particles are identical and have a spherical shape with a d_p diameter;
- ion exchange in cationite occurs between H^+ ions existed in resin and i ($i=A, B, D; A=Na^+, B=Ca^{2+}, D=Al^{3+}$) cation species contained in solution; ion exchange in anionite takes place between OH^- groups found in resin and C ($C=Cl^-$) anion species existed in solution;
- ion exchanger particle is dense and small, so that ion exchange reaction occurs on its surface or in a superficial layer with small thickness;
- overall ion exchange rate of ionic species depends on the competition between species adsorption and desorption processes;
- kinetics of adsorption process is linear with respect to free active sites number of solid and species concentration in liquid phase;
- kinetics of desorption process is linear with respect to species concentration in solid phase;
- flow pattern is plug flow with axial dispersion of liquid phase;
- axial dispersion coefficient, D_p , is determined by means

of Levenspiel correlation: $Pe = \frac{w_f d_p}{D_l} = 2$;

- ion exchange is an isothermal process.
- Characteristic mathematical model of ion exchange process occurring in fixed beds of cationite and anionite is described by the following system of equations and restrictions:
- conservation equations of i and C species in liquid phase:

$$\varepsilon_b \frac{\partial c_i}{\partial \tau} + w_f \frac{\partial c_i}{\partial x} = D_l \frac{\partial^2 c_i}{\partial x^2} - v_{ex,i}(c_A, c_B, c_D, s_A, s_B, s_D) \quad (2)$$

$$\varepsilon_b \frac{\partial c_C}{\partial \tau} + w_f \frac{\partial c_C}{\partial x} = D_l \frac{\partial^2 c_C}{\partial x^2} - v_{ex,C}(c_C, s_C) \quad (3)$$

- conservation equations of i and C species in solid phase:

$$\rho_b \frac{\partial s_i}{\partial \tau} = v_{ex,i}(c_A, c_B, c_D, s_A, s_B, s_D) \quad (4)$$

$$\rho_b \frac{\partial s_C}{\partial \tau} = v_{ex,C}(c_C, s_C) \quad (5)$$

- overall ion exchange rate equations of i and C species:

$$v_{ex,i}(c_A, c_B, c_D, s_A, s_B, s_D) = k_{1i} \varepsilon_b \left(1 - \frac{1}{Q} \sum_{i=1}^3 z_i s_i\right) c_i - k_{2i} s_i \quad (6)$$

$$v_{ex,C}(c_C, s_C) = k_{1C} \varepsilon_b \left(1 - \frac{1}{Q} z_C s_C\right) c_C - k_{2C} s_C \quad (7)$$

- electroneutrality conditions in solid phase:

$$s_{H,0} = s_H + \sum_{i=1}^3 z_i s_i \quad (8)$$

$$s_{OH,0} = s_{OH} + z_C s_C \quad (9)$$

- initial conditions for j ($j=i, C$) species:

$$CII: \tau = 0 \quad 0 \leq x \leq H \quad s_j(x, 0) = 0 \quad (10)$$

$$s_H(x, 0) = s_{H,0}, s_{OH}(x, 0) = s_{OH,0}$$

$$CI2: \tau = 0 \quad 0 < x \leq H \quad c_j(x, 0) = 0 \quad (11)$$

$$CI3: \tau = 0 \quad x = 0 \quad c_j(0, 0) = c_{j,0} \quad (12)$$

- boundary conditions for j ($j=i, C$) species:

$$CLI: \tau > 0 \quad x = 0 \quad c_j(0, \tau) = c_{j,0} \quad (13)$$

$$CL2: \tau > 0 \quad x = H \quad \frac{\partial c_j(H, \tau)}{\partial x} = 0 \quad (14)$$

The mathematical model was numerically solved by an adequate finite differences method and the values of C anion concentration in column effluent, $c_C(H, \tau)$, were determined depending on preset values of rate constants, k_{1i} and k_{2i} , respectively. Minimizing the objective function described by relationship (15), wherein $c(\tau)$ is experimental concentration of C anion species in anionic column effluent, k_{1i} and k_{2i} parameter values were identified. Estimated model parameters at a value of solution superficial velocity of $0.5 \cdot 10^{-3}$ m/s are summarized in table 2.

$$f(k_{1i}, k_{2i}) = \sum_{\tau} [c_C(\tau, H) - c(\tau)]^2 \quad (15)$$

Table 2
ESTIMATED MODEL PARAMETERS AT $w_f = 0.5 \cdot 10^{-3}$ m/s

No.	Solution	i	k_{1i}		k_{2i}	
			[s ⁻¹]		[g·L ⁻¹ ·s ⁻¹]	
			30 °C	60 °C	30 °C	60 °C
1	S_1	Na^+	$1.52 \cdot 10^{-1}$	$1.59 \cdot 10^{-1}$	$0.67 \cdot 10^{-2}$	$0.54 \cdot 10^{-2}$
2	S_2	Ca^{2+}	$1.89 \cdot 10^{-1}$	$1.93 \cdot 10^{-1}$	$0.32 \cdot 10^{-2}$	$0.30 \cdot 10^{-2}$
3	S_3	Al^{3+}	$2.03 \cdot 10^{-1}$	$2.13 \cdot 10^{-1}$	$0.27 \cdot 10^{-2}$	$0.26 \cdot 10^{-2}$
4	S_4	Na^+	$1.64 \cdot 10^{-1}$	$1.65 \cdot 10^{-1}$	$0.40 \cdot 10^{-2}$	$0.38 \cdot 10^{-2}$
		Ca^{2+}	$1.75 \cdot 10^{-1}$	$1.76 \cdot 10^{-1}$	$0.37 \cdot 10^{-2}$	$0.35 \cdot 10^{-2}$
5	S_5	Na^+	$1.66 \cdot 10^{-1}$	$1.67 \cdot 10^{-1}$	$0.39 \cdot 10^{-2}$	$0.37 \cdot 10^{-2}$
		Ca^{2+}	$1.74 \cdot 10^{-1}$	$1.77 \cdot 10^{-1}$	$0.34 \cdot 10^{-2}$	$0.31 \cdot 10^{-2}$
		Al^{3+}	$1.94 \cdot 10^{-1}$	$1.97 \cdot 10^{-1}$	$0.25 \cdot 10^{-2}$	$0.24 \cdot 10^{-2}$

Data shown in table 2 emphasize according to the qualitative analysis of breakthrough curves (fig. 2) the following aspects:

- values of adsorption rate constant vary in ascending order ($k_{1Na^+} < k_{1Ca^{2+}} < k_{1Al^{3+}}$) and those of desorption rate constant in descending order ($k_{2Na^+} < k_{2Ca^{2+}} < k_{2Al^{3+}}$) from Na^+ to Al^{3+} at any value of temperature; this is in good agreement with the cationite selectivity for cation species which increases in order $Na^+ < Ca^{2+} < Al^{3+}$;
- an increase of operation temperature determines larger values of k_{1i} and smaller values of k_{2i} which produces an enhancement of ion exchange process.

Kinetic parameters identified for each cation species at the both values of operation temperature were employed to obtain the characteristic parameters of Arrhenius equation (16):

$$k_i = A_i e^{-\frac{E_i}{RT}} \quad (16)$$

Values of Arrhenius equations parameters summarized in table 3 show that:

- pre-exponential factor, A_i , and activation energy, E_i , depend on i cation species and cation species number existed in feed solution;
- activation energy of adsorption process, E_{1i} , has positive values, therefore the adsorption rate constant, k_{1i} , increases with temperature;
- activation energy of desorption process, E_{2i} , has negative values, accordingly the desorption rate constant, k_{2i} , decreases with temperature;

No.	Solution	<i>i</i>	A_{1i} [s ⁻¹]	E_{1i} [J·mol ⁻¹]	A_{2i} [g·L ⁻¹ ·s ⁻¹]	E_{2i} [J·mol ⁻¹]
1	S_1	Na^+	0.251	$1.258 \cdot 10^6$	$0.602 \cdot 10^{-3}$	$-6.071 \cdot 10^6$
2	S_2	Ca^{2+}	0.239	$1.016 \cdot 10^6$	$1.297 \cdot 10^{-3}$	$-2.271 \cdot 10^6$
3	S_3	Al^{3+}	0.346	$1.344 \cdot 10^6$	$2.288 \cdot 10^{-3}$	$-0.417 \cdot 10^6$
4	S_4	Na^+	0.180	$0.238 \cdot 10^6$	$2.264 \cdot 10^{-3}$	$-1.434 \cdot 10^6$
		Ca^{2+}	0.189	$0.191 \cdot 10^6$	$1.997 \cdot 10^{-3}$	$-1.553 \cdot 10^6$
5	S_5	Na^+	0.180	$0.218 \cdot 10^6$	$2.174 \cdot 10^{-3}$	$-1.471 \cdot 10^6$
		Ca^{2+}	0.195	$0.287 \cdot 10^6$	$1.219 \cdot 10^{-3}$	$-2.582 \cdot 10^6$
		Al^{3+}	0.221	$0.315 \cdot 10^6$	$2.174 \cdot 10^{-3}$	$-1.729 \cdot 10^6$

Table 3
ARRHENIUS EQUATIONS PARAMETERS AT
 $w_f = 0.5 \cdot 10^{-3}$ m/s

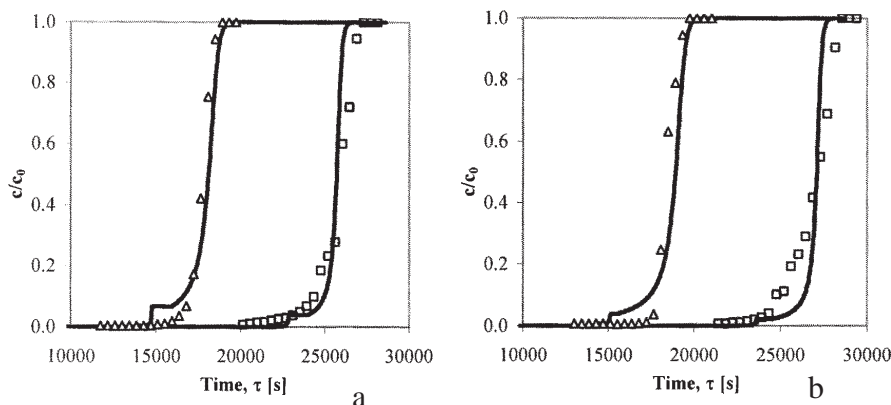


Fig. 3. Experimental (□ S_2 , △ S_4) and simulated (—) breakthrough curves of Cl^- ions concentration dynamics in anion column effluent at $w_f = 0.5 \cdot 10^{-3}$ m/s:
a. $t = 30$ °C; b. $t = 60$ °C

No.	Solution	<i>i</i>	$A_{1i,w}$ [s ⁻¹]	$E_{1i,w} = E_{1i}$ [J·mol ⁻¹]	$A_{2i,w} = A_{2i}$ [g·L ⁻¹ ·s ⁻¹]	$E_{2i,w} = E_{2i}$ [J·mol ⁻¹]
1	S_1	Na^+	$0.292 \cdot (w_f \cdot 10^3)^{0.22}$	$1.258 \cdot 10^6$	$0.602 \cdot 10^{-3}$	$-6.071 \cdot 10^6$
2	S_2	Ca^{2+}	$0.278 \cdot (w_f \cdot 10^3)^{0.22}$	$1.016 \cdot 10^6$	$1.297 \cdot 10^{-3}$	$-2.271 \cdot 10^6$
3	S_3	Al^{3+}	$0.403 \cdot (w_f \cdot 10^3)^{0.22}$	$1.344 \cdot 10^6$	$2.288 \cdot 10^{-3}$	$-0.417 \cdot 10^6$
4	S_4	Na^+	$0.210 \cdot (w_f \cdot 10^3)^{0.25}$	$0.238 \cdot 10^6$	$2.264 \cdot 10^{-3}$	$-1.434 \cdot 10^6$
		Ca^{2+}	$0.220 \cdot (w_f \cdot 10^3)^{0.25}$	$0.191 \cdot 10^6$	$1.997 \cdot 10^{-3}$	$-1.553 \cdot 10^6$
5	S_5	Na^+	$0.220 \cdot (w_f \cdot 10^3)^{0.31}$	$0.218 \cdot 10^6$	$2.174 \cdot 10^{-3}$	$-1.471 \cdot 10^6$
		Ca^{2+}	$0.227 \cdot (w_f \cdot 10^3)^{0.31}$	$0.287 \cdot 10^6$	$1.219 \cdot 10^{-3}$	$-2.582 \cdot 10^6$
		Al^{3+}	$0.257 \cdot (w_f \cdot 10^3)^{0.31}$	$0.315 \cdot 10^6$	$2.174 \cdot 10^{-3}$	$-1.729 \cdot 10^6$

Table 4
ARRHENIUS EQUATIONS PARAMETERS
DEPENDING ON SOLUTION VELOCITY

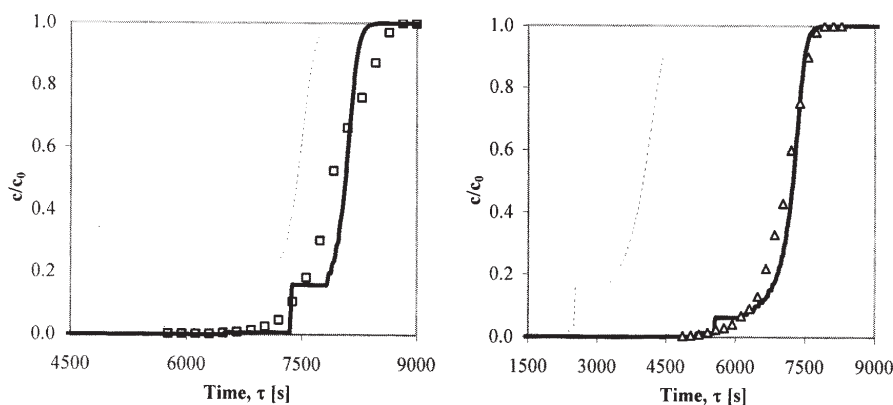


Fig. 4. Experimental (□ S_2 , △ S_4) and simulated breakthrough curves of Cl^- ions concentration dynamics in anion column effluent at $w_f = 1.2 \cdot 10^{-3}$ m/s and $t = 30$ °C:
- - - k_{1i}, k_{2i} (table 2); — $k_{1i,w} = A_{1i,w} \exp(-E_{1i}/RT)$, $k_{2i,w} = k_{2i}$ (table 4)

- larger values of pre-exponential factor, A_{1i} , indicate that the adsorption process rate is close by those characteristic of reactions occurring in liquid medium;

- smaller values of pre-exponential factor, A_{2i} , prove that the desorption process is slow, so that an equilibrium state will be reached after long time of phases contacting.

Experimental data and breakthrough curves simulated by means of estimated parameters in case of demineralization of S_2 ($CaCl_2$) and S_4 ($NaCl + CaCl_2$) solutions at $w_f = 0.5 \cdot 10^{-3}$ m/s are illustrated in figure 3. A good agreement between experimental and simulated data (errors less than 10 %) is observed.

Effect of solution superficial velocity

A power function was proposed to quantify the effect of superficial velocity, w_f , on the adsorption rate constant, $k_{1i,w}$:

$$k_{1i,w} = k_{1i,w}^0 w_f^{n_i} \quad (17)$$

Expressing the adsorption rate constant by means of Arrhenius equation (16) and considering that only the pre-exponential factor depends on w_f , eq. (17) turns into:

$$A_{1i,w} = A_{1i,w}^0 w_f^{n_i} \quad (18)$$

The values of pre-exponential factor, $A_{1i,w}$, expressed as a power function with respect of solution superficial velocity, w_f , are shown in table 4. An enlargement of the velocity power value, n_i , with number of cation species contained in feed solution is noticed. This is probably due to an adsorption enhancement of a cation species in presence of a more rapid one.

The breakthrough curves simulated according to the data presented in table 2 and table 4 in case of

demineralization of S_2 (CaCl_2) and S_1 ($\text{NaCl}+\text{CaCl}_2$) feed solutions at $w_f=1.2 \cdot 10^{-3}$ m/s and $t=30$ °C are illustrated in figure 4. A good agreement between experimental data and those simulated by means of parameters summarized in table 4 is observed.

Conclusions

For the modelling of fixed bed multicomponent ion exchange in case of total demineralization of dilute aqueous solutions, the following were achieved:

- a treatment scheme based on a ion exchangers fixed bed equipment with two ionic columns, one with strongly acidic cationite (R^+H^+) and another with strongly basic anionite (R^+HO^-), was selected;

- an experimental investigation to evidence the influence of feed solution composition (one, two or three cations species and one anion species), solution superficial velocity and operation temperature on fixed bed breakthrough dynamics was performed;

- experimental breakthrough curves showing the dynamics of anion concentration in anionic column effluent were plotted;

- a lumped kinetic model, considering plug flow with axial dispersion and finite rate of adsorption-desorption process, was proposed to describe the multicomponent ion exchange dynamics;

- the model parameters were estimated by means of breakthrough experimental data;

- simulation of process dynamic concluded that the effect of solution superficial velocity has to be quantified in adsorption rate constant of cation species;

- the proposed model predicted well the real conditions and it could facilitate ion exchange columns design and operation.

Nomenclature

A_i - pre-exponential factor of i cation species in Arrhenius equation (16), s^{-1} ;

$A_{i,w}^0$ - constant in eq. (18);

c - experimental concentration of anion species in anionic column effluent, $\text{mol}\cdot\text{L}^{-1}$;

c_0 - initial concentration of anion species in feed solution, $\text{mol}\cdot\text{L}^{-1}$;

c_j - concentration of j species in liquid phase, $\text{mol}\cdot\text{L}^{-1}$;

d - internal diameter of ionic column, m;

d_p - diameter of resin particle, m;

D_l - axial dispersion coefficient, $\text{m}^2\cdot\text{s}^{-1}$;

E_i - activation energy of i cation species in Arrhenius equation (16), $\text{J}\cdot\text{mol}^{-1}$;

H - total height of fixed bed, m;

k_{ij} - adsorption rate constant of j ionic species, s^{-1} ;

$k_{i,w}^0$ - constant in eq. (17);

k_{-j} - desorption rate constant of j ionic species, $\text{g}\cdot\text{s}^{-1}\cdot\text{L}^{-1}$;

K_B^A - affinity coefficient of ion exchanger;

n_i - constant in eq. (17) and eq. (18);

Pe - Peclet number;

Q - parameter depending on total mass capacity of resin, $\text{mol}\cdot\text{g}^{-1}$;

R - gas constant, $R=8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$;

R_a - anionite matrix;

R_c - cationite matrix;

s_j - concentration of j ionic species in solid phase, $\text{mol}\cdot\text{g}^{-1}$;

t - operation temperature, °C;

T - operation absolute temperature, K;

v_{exj} - overall ion exchange rate of j ionic species, $\text{mol}\cdot\text{L}^{-1}\cdot\text{s}^{-1}$;

V_j - volumes of j hydrated ion, m^3 ;

w_f - solution superficial (fictive) velocity, $\text{m}\cdot\text{s}^{-1}$;

x - axial coordinate in fixed bed, m;

z_j - absolute value of valence of j ionic species;

Greek letters

ε_b - void fraction of fixed bed;

π - osmotic pressure, $\text{N}\cdot\text{m}^{-2}$;

ρ_b - density of fixed bed, $\text{g}\cdot\text{L}^{-1}$;

τ - time, s.

Subscripts

b - fixed bed;

C - anion species ($C=Cl$);

ex - ion exchange;

i - cation species ($i=A, B, D$; $A=Na^+$, $B=Ca^{2+}$, $D=Al^{3+}$);

j - ionic species ($j=i, C$);

w - solution superficial velocity;

0 - initial;

1 - adsorption;

2 - desorption.

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