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Prediction of Multicomponent Ion-Exchange Equilibria for a Ternary System from Data of Binary Systems

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ABSTRACT

A framework is developed to provide predictions of multicomponent ion-exchange equilibria from binary data. Our input data were taken from published experimental results on the ion-exchange equilibria of the binary systems Sr^{2+}–Na^{+}, Cs^{+}–Na^{+}, and Sr^{2+}–Cs^{+} on chabazite zeolite. These systems exhibit nonideal characteristics in both solid and liquid phases. The experimental characterization has been based on the reaction equilibrium constants and the activity coefficients in both phases. The activity coefficients of the exchanger phase were obtained from the well-known Wilson model. A computer program was given in FORTRAN-77 to carry out the prediction procedure. The sum of the squares of differences between experimental and predicted points was used as a criterion for best fit. The model was also verified on systems involving the exchange of the anions SO_4^{-}, NO_3^{-}, and Cl^{-} on Amberlite IR-400. The good agreement between the experimental and predicted data showed that the proposed framework can be considered as an effective method to predict many ternary systems from binary systems.

INTRODUCTION

Multicomponent ion-exchange processes have acquired enhanced interest because of their potential applications in solving some practical problems (1). A detailed knowledge of multicomponent equilibrium data is essential for the proper understanding and development of ion-exchange processes. However, most ion-exchange selectivity and equilibrium data reported in the literature

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refer to binary ionic systems, since the number of required experimental manipulations increases enormously with each additional ionic component. In this view, the development of suitable methods for the interpolation of ternary and higher systems from a number of binary equilibrium data is very important.

Soldatov and Bickova (2) observed that the models proposed to predict multicomponent ion-exchange equilibrium behavior fall into three main classes. Models of the first class assume that the entire system behaves ideally, i.e., the activity coefficients of all components in both liquid and solid phases are equal to unity. Models of the second class assume that the presence of other counterions does not affect the equilibrium conditions existing between two exchanging counterions. The third class of models does not make either of these assumptions and so should be more accurate. The equilibrium model proposed by Klein et al. (3) is of the first class. Kataoka and Yoshida (4) proposed a model that accounted for nonidealities in the liquid phase, but assumed that the solid phase was ideal. The model proposed by Sengupta and Paul (5) recognizes that both phases in the ion-exchange system may be nonideal. The models of Bajpai et al. (6) and of El-Prince and Babcock (7) do not assume that the ionic behavior must be ideal. Their models allowed the equilibrium compositions of binary systems to be calculated by assuming that the values for the equilibrium constants were known independently. The solid phase activity coefficients were estimated using a method based upon the Wilson model (8) for excess Gibbs free energy.

A number of experimental studies have been performed to examine the equilibrium behavior of ternary ion-exchange systems. Dranoff and Lapidus (9), Pieroni and Dranoff (10), and Bajpai et al. (6) studied various systems using Dowex 50W-X8 resin. Soldatov and Bickova (2) used Dowex 50W-X12 resin with four ternary systems involving NH^4, H^+, and either Li^+, Na^+, K^+ or Cs^+. The anionic system NO_3^-–SO_4^{2-}–Cl^- was studied by Smith and Woodburn (11) using Amberlite IR-400. Sengupta and Paul (5) employed another Amberlite resin, IR-200, in their studies of Zn^{2+}–Cd^{2+}–H^+ and Cu^{2+}–Ag^+–H^+ systems.

The object of the present work is to develop a framework for estimation of multicomponent ion-exchange systems from the data of binary systems. In this respect the experimental equilibrium data for the Sr^{2+}–Cs^+–Na^+ ternary system and the three related binary systems (Sr^{2+}–Na^+, Cs^+–Na^+, and Sr^{2+}–Cs^+) were modeled using the Wilson equation (8) for the solid phase activity coefficient and the extended Deby and Huckel equation (12) for the activity coefficient estimation in the liquid phase. The anionic systems SO_4^{2-}–NO_3^-, SO_4^{2-}–Cl^-, and NO_3^-–Cl^-, studied by Smith and Woodburn (11), were used to verify the proposed model to generalize the framework for both anion and cation exchanger systems.

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THERMODYNAMIC MODEL

In the case of ternary ion exchange, the problem is more complicated than in binary systems. Keeping the definitions of the standard states as same as in binary systems, there are three reference states for each phase because of the presence of three ions. Also, in contrast to the binary exchange case, three ion-exchange reactions can be written, each of which includes two of the conjugate binaries. So, for the system Sr-Cs-Na on zeolite, the equations can be written

$$Sr_s^{2+} + 2Na_z^+ \leftrightarrow Sr_z^{2+} + 2Na_s^+ \tag{1}$$

$$Cs_s^+ + Na_z^+ \leftrightarrow Cs_z^+ + Na_s^+ \tag{2}$$

$$Sr_s^{2+} + 2Cs_z^+ \leftrightarrow Sr_z^{2+} + 2Cs_s^+ \tag{3}$$

From these equations, only two are independent, and any other one can be generated by combining the other two equations.

In the equations used to define the equilibrium constant for each reaction, Smith and Woodburn (11) employed the activities of each ion rather than their liquid concentrations and solid phase mole fractions. These activities reflect the nonideality of the system.

If subscripts 1, 2, and 3 refer to strontium, sodium, and cesium, respectively, then the three equilibrium constants are defined as:

$${}^1_2K_a = \frac{(\phi_1 Y_1)(\gamma_2 m_2)^2}{(\gamma_1 m_1)(\phi_2 Y_2)^2} \tag{4}$$

$${}^3_2K_a = \frac{(\phi_3 Y_3)(\gamma_2 m_2)}{(\gamma_3 m_3)(\phi_2 m_2)} \tag{5}$$

$${}^3_1K_a = \frac{(\phi_3 Y_3)(\gamma_1 m_1)^2}{(\gamma_3 m_3)(\phi_1 m_1)^2} \tag{6}$$

A further equation involving the solid phase mole fractions can also be written:

$$Y_1 + Y_2 + Y_3 = 1 \tag{7}$$

If the free ion concentrations are known, Eqs. (4)–(7) can be used to solve the composition of the solid phase (i.e., for Y_1, Y_2, and Y_3) in equilibrium with a liquid phase of a specified composition and concentration. If the three equilibrium constants and the activity coefficients are known, then Eqs. (4)–(7) can be solved for the three unknowns. The solid phase composition calculated by solving the equations would therefore depend on which combination of the three equations is used to solve the system. Sengupta and Paul (5) suggested that the equation of the binary pairs contains the most selective ion be chosen

along with the component summation equation. Thus, since Na is the least reactive ion for the Sr–Cs–Na system, then Eqs. (4), (5), and (7) would be solved to obtain Y_1, Y_2, and Y_3.

The proposed model considers only thermodynamic nonidealities. Other nonidealities, such as Donnan uptake, restrict the application of the model to systems of low-to-moderate solution normality (i.e., TN $\leq$ 1.0 N).

LIQUID PHASE ACTIVITY COEFFICIENTS ESTIMATION

In the multicomponent solutions of industrial interest, the electrolyte concentrations are relatively high and make the activity coefficients difficult to obtain either theoretically or from experimental data. Pal (13) reported equations for the accurate estimation of the activity coefficient ratios in ion-exchange processes. Sengupta and Paul (5) applied the ionic interaction coefficients to activity calculations in mixed electrolyte solutions of ion-exchange systems. The extended Debye and Huckel equation (12) with two parameter per ionic component has been selected to calculate the single ion activity coefficient as

$$\ln \gamma_i = \frac{-A_{z_i^2} \sqrt{I}}{1 + B_{a_i} \sqrt{I}} + b_i I \tag{8}$$

Truesdell and Jones (14) calculated the parameters a_i and b_i from experimental data of salt activity coefficients. Thus, with the two parameters per ionic species and the ionic strength (I) of the solution, it is possible to estimate the activity coefficients and hence the activity of each species in a multi-component system.

EQUILIBRIUM CONSTANTS AND SOLID PHASE ACTIVITY COEFFICIENTS

Although the activity coefficients in the liquid phase can be calculated easily using Debye and Huckel extended method (12), the method required to estimate the solid phase activity coefficients, as well as the equilibrium constants, is more complicated. The procedure proposed by Smith and Woodburn (11) calculates the solid phase activity coefficients with the well-known Wilson equation:

$$\ln \phi_i = 1 - \ln\left[\sum_{j=1}^{M} Y_j \Lambda_{i-j}\right] - \sum_{K=1}^{M}\left[\frac{Y_k \Lambda_{k-i}}{\sum_{j=1}^{M} Y_j \Lambda_{k-j}}\right] \tag{9}$$

The Wilson equation is applied to the binary experimental data (15) to obtain values for the interaction parameters Λ_{i-j} and Λ_{j-i}, and then these parameters can be used in the Wilson equation for three or more component sys-

tems. To extract the values of the interaction parameters from the binary data, Smith and Woodburn defined an equilibrium quotient, λ_{A-B}:

$$\lambda_{A-B} = \frac{(\gamma_B m_B)^{ZA} (Y_A)^{ZB}}{(\gamma_A m_A)^{ZB} (Y_B)^{ZA}} \tag{10}$$

The equilibrium quotient can be expressed in terms of the equilibrium constant:

$$\lambda_{A-B} = K_{A-B} \frac{(\phi_B)^{ZA}}{(\phi_A)^{ZB}} \tag{11}$$

Substitution of the Wilson Eq. (9) into this expression for the equilibrium quotient yields

$$\begin{aligned} \ln \lambda_{A-B} &= \ln K_{A-B} - Z \\ &\times \left[1 - \ln(Y_A + Y_B\Lambda_{A-B}) - \left(\frac{Y_A}{Y_A + Y_B\Lambda_{A-B}} + \frac{Y_B\Lambda_{B-A}}{Y_B + Y_A\Lambda_{B-A}}\right)\right] \\ &+ Z_A\left[1 - \ln(Y_A\Lambda_{B-A} + Y_B) - \left(\frac{Y_A\Lambda_{A-B}}{Y_A + Y_B\Lambda_{A-B}} + \frac{Y_B}{Y_B + Y_A\Lambda_{B-A}}\right)\right] \end{aligned} \tag{12}$$

This equation contains three unknown: K_{A-B} and two interaction parameters. A minimum of three data points is needed to evaluate them. When more than three data points are available, a search procedure can be used to find the set of values of K_{A-B}, Λ_{A-B}, and Λ_{B-A} that minimize the sum of squares of the deviations between experimental equilibrium quotients from Eq. (10) and predicted equilibrium quotients from Eq. (12) for all points. This procedure can be applied to the system Sr–Cs–Na on chabazite, and the activity coefficients in the solid phase can be calculated as

$$\begin{aligned} \ln \phi_1 &= 1 - [\ln(Y_1 + Y_2\Lambda_{1-2} + Y_3\Lambda_{1-3})] \\ &- \left[\frac{Y_1}{Y_1 + Y_2\Lambda_{1-2} + Y_3\Lambda_{1-3}} + \frac{Y_2\Lambda_{2-1}}{Y_1\Lambda_{2-1} + Y_2 + Y_3\Lambda_{2-3}} + \frac{Y_3\Lambda_{3-1}}{Y_1\Lambda_{3-1} + Y_2\Lambda_{3-2} + Y_3}\right] \end{aligned} \tag{13}$$

$$\begin{aligned} \ln \phi_3 &= 1 - [\ln(Y_1\Lambda_{3-1} + Y_2\Lambda_{3-2} + Y_3)] \\ &- \left[\frac{Y_1\Lambda_{1-3}}{Y_1 + Y_2\Lambda_{1-2} + Y_3\Lambda_{1-3}} + \frac{Y_2\Lambda_{2-3}}{Y_1\Lambda_{2-1} + Y_2 + Y_2\Lambda_{2-3}} + \frac{Y_3}{Y_1\Lambda_{3-1} + Y_2\Lambda_{3-2} + Y_3}\right] \end{aligned} \tag{14}$$

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$$\ln \phi_2 = 1 - [\ln(Y_1\Lambda_{2-1} + Y_2 + Y_3\Lambda_{2-3})] - \left[\frac{[Y_1\Lambda_{1-2}}{Y_1 + Y_2\Lambda_{1-2} + Y_3\Lambda_{1-3}} + \frac{Y_2}{Y_1\Lambda_{2-1} + Y_2 + Y_3\Lambda_{2-3}} + \frac{Y_3\Lambda_{3-2}}{Y_1\Lambda_{3-1} + Y_2\Lambda_{3-2} + Y_3}\right] \quad (15)$$

Since the three equilibrium constants and all the required activity coefficients in both phases are known, the model equations may be solved to yield the unknown phase composition.

COMPUTATIONAL ANALYSIS OF THE MODEL

A computer program to carry out the prediction procedure has been designed using FORTRAN-77. The procedure used in this program is outlined in Fig. 1. The sequence of this procedure is as follow.

1. Assume trial values for thermodynamic equilibrium constants and for the binary interaction parameters.
2. Calculate the activity coefficients in the solid phase from the Wilson equation.
3. Assume trial values for the liquid phase activity coefficients (γ_A, γ_B, and γ_C). For dilute solutions in this work (TN $\leq$ IN), values ranged from about 0.7 to near unity.
4. Calculate the predicted values of m_A, m_B, and m_C from the equilibrium constants and a mass balance: $m_A + m_B + m_C = TN$.
5. Calculate the liquid phase activity coefficients γ_A, γ_B, and γ_C from the extended Debye and Huckel equation using the predicted values of m_A, m_B, and m_C.
6. Compare these values with these assumed in Step 3.
7. Repeat the above steps, varying the values of equilibrium constants and binary interaction on parameters, to minimize the difference between the experimental and predicted values of m_A, m_B, and m_C.

MODEL VALIDATION

The ion-exchange equilibria for the binary and ternary systems involving Sr^{2+}, Cs^+, and Na^+ ions on chabazite published by Robinson et al. (16) are used as input (experimental) data in this study. In their work, simulated waste solutions were used in the experimental tests to avoid variability in feed composition. The solutions were prepared by dissolving various amounts of $SrCl_2 \cdot 6H_2O$ and CsCl in demineralized water and spiked with ^{85}Sr and ^{137}Cs tracers. The concentrations of Sr and Cs in the initial solution were 0.002 and

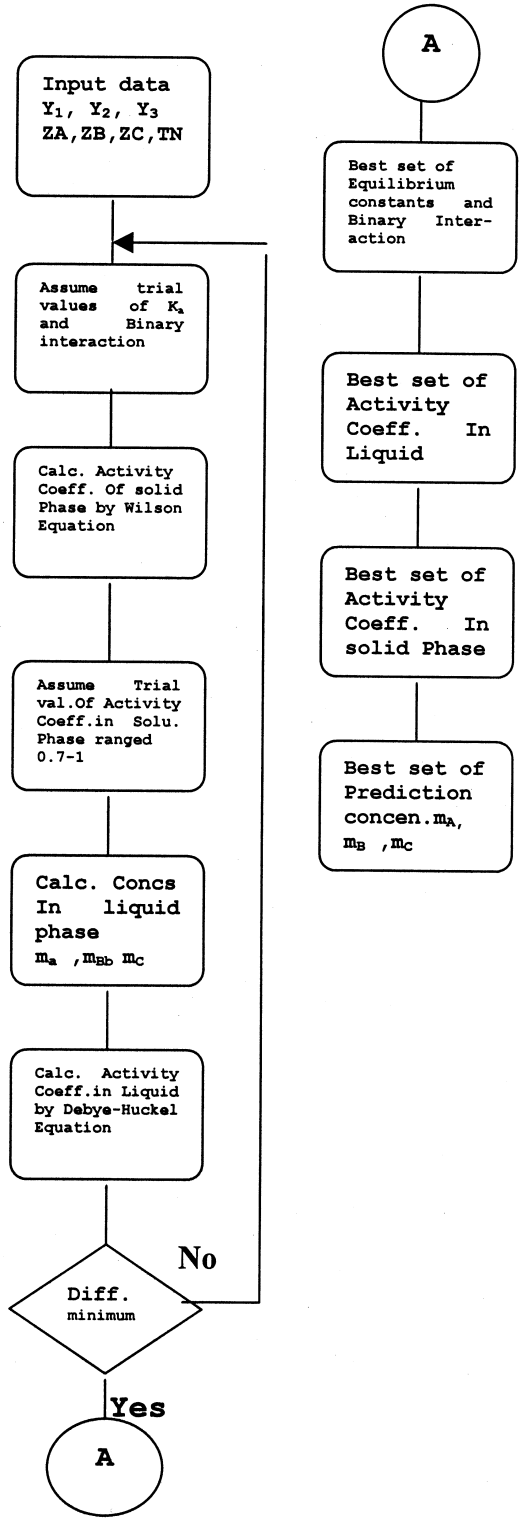

FIG. 1 Computational scheme for prediction of ternary ion-exchange equilibria from binary experimental data.

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TABLE 1
Extent of Experimental Data for the System Sr^{2+}–Cs^{+}–Na^{+}–Chabazite (16)

No. of components	Components	No. of solution/sorbent ratio
2	Sr^{2+}–Na^{+}	9
	Cs^{+}–Na^{+}	7
3	Sr^{2+}–Cs^{+}–Na^{+}	8

0.001 N, respectively. The concentrations of cations in the solution phase were measured using atomic absorption or gamma counting. The concentrations of cations in the zeolite phase were calculated from their initial and final concentrations in solution. The published data of the anionic system SO_4^{2-}–NO_3^{-}–Cl^{-} studied by Smith and Woodburn (11) using Amberlite IR-400 was used as input data to check the model validation.

RESULTS AND DISCUSSION

The extent of the data published by Robinson et al. (16) for the Sr^{2+}–Cs^{+}–Na^{+}–chabazite system is summarized in Table 1. Total solution concentrations including all components did not exceed 0.01 N for any of the data sets. All data were taken at 23°C. Equilibrium quotients were calculated for the binary data from Eq. (10). The extended Debye and Huckel equation with two parameters per ionic component (Eq. 8) was used to calculate the liquid phase activity coefficients for the ions Sr^{2+}, Cs^{+}, Na^{+}, SO_4^{2-}, NO_3^{-}, and Cl^{-} using the values of the parameters given in Table 2. Using the procedure listed in the program, the values of the equilibrium constants and the values of the Wilson interaction parameters (i.e., K_{A-B}, Λ_{A-B}, and Λ_{B-A}) were calculated and used for evaluating λ_{A-B} using Eq. (12). These λ_{A-B} values were found to match very closely with the experimental λ_{A-B} values evaluated by Eq. (10) (Table 3).

TABLE 2
Parameters for Extended Debye–Huckel Equation (12)[a]

Species	a_i	b_i	Z_i
Sr^{2+}	4.373×10^{-10}	−0.01598	2
Cs^{+}	6.217×10^{-9}	−0.04	1
Na^{+}	4.0	−0.075	1
SO_4^{-}	5.0	−0.04	−2
NO_3^{-}	3.0	0.00	−1
Cl^{-}	3.5	0.105	−1

[a] $A = 5.085$, $B = 3.281 \times 10^{9}$.

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TABLE 3
Estimates of Equilibrium Constants and Wilson Parameters for Binary Systems

Ion-exchange reaction	Equilibrium constant	Wilson parameters			R
$Sr^{2+}_{(S)} + 2Na^{+}_{(Z)} = Sr^{2+}_{(Z)} + 2Na^{+}_{(S)}$	$K^{Sr}_{Na} = 1.59$	Λ_{i-j}	Na	Sr	
		Na	1	0.112	
		Sr	7.97	1	0.13
$Cs^{+}_{(S)} + Na^{+}_{(Z)} = Cs^{+}_{(Z)} + Na^{+}_{(S)}$	$K^{Cs}_{Na} = 51$	Λ_{i-j}	Na	Cs	
		Na	1	3.95	
		Cs	0.01	1	0.1
$Sr^{2+}_{(S)} + 2Cs^{+}_{(Z)} = Sr^{2+}_{(Z)} + 2Cs^{+}_{(s)}$	$K^{Sr}_{Cs} = 0.37$	Λ_{i-j}	Cs	Sr	
		Cs	1	2.0	
		Sr	0.001	1	0.11
$SO_{4(S)} + 2NO_{3(A)} = SO_{4(A)} + 2NO_{3(S)}$	$K^{SO_4}_{NO_3} = 72.94$	Λ_{i-j}	SO_4	NO_3	
		SO_4	1	0.654	
		NO_3	3.116	1	0.17
$SO_{4(S)} + 2Cl_{(A)} = SO_{4(A)} + 2Cl_{(S)}$	$K^{SO_4}_{Cl} = 5.09$	Λ_{i-j}	SO_4	Cl	
		SO_4	1	0.228	
		Cl	3.674	1	0.19
$Cl_{(S)} + NO_{3(A)} = Cl_{(A)} + NO_{3(S)}$	$K^{Cl}_{NO_3} = 3.78$	Λ_{i-j}	Cl	NO_3	
		Cl	1	2.462	
		NO_3	0.391	1	0.14

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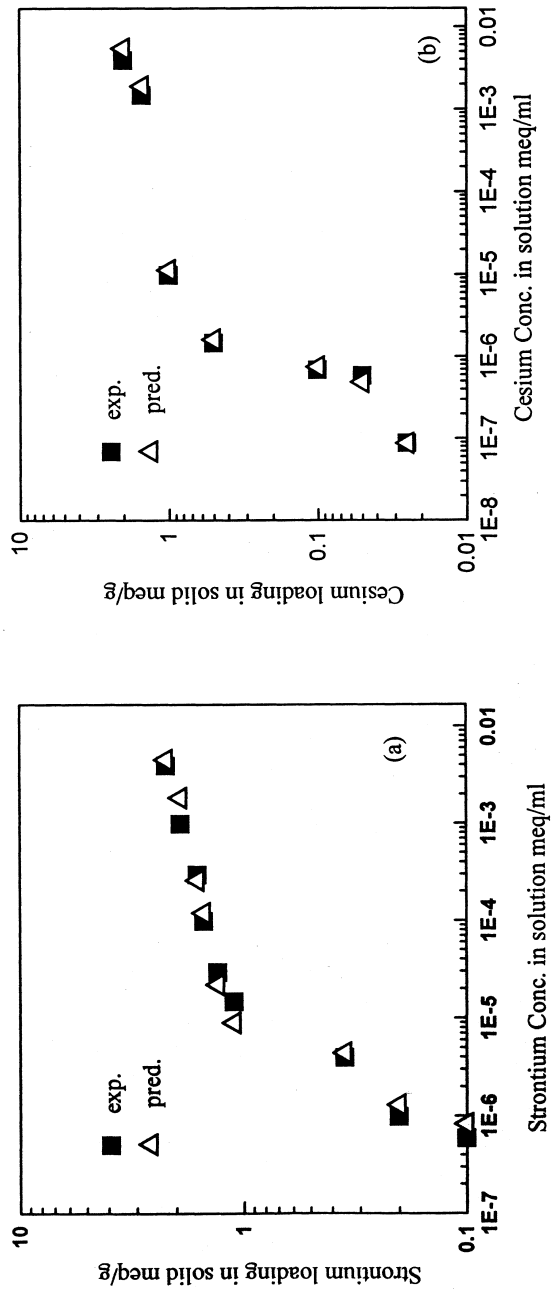

FIG. 2 Strontium–sodium and cesium–sodium isotherm with model predicted points calculated using parameter values in Table 3 (input data were taken from Ref. 16).

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The sum of squares of the differences between experimental and predicted data were used as a criterion for best fit:

$$R = \sum_{i=1}^{N} \left(\frac{C_{\text{A exp}} - C_{\text{A pred}}}{C_{\text{A exp}}} \right)$$

Figure 2 represents the Sr–Na and Cs–Na isotherms, and Fig. 3 represents the SO_4^{2-}, NO_3^-, and Cl^- isotherms. The figures show the model predicted points calculated using the data in Table 3. The set of parameter values in Table 3 was used to predict the ternary equilibrium points for experimental

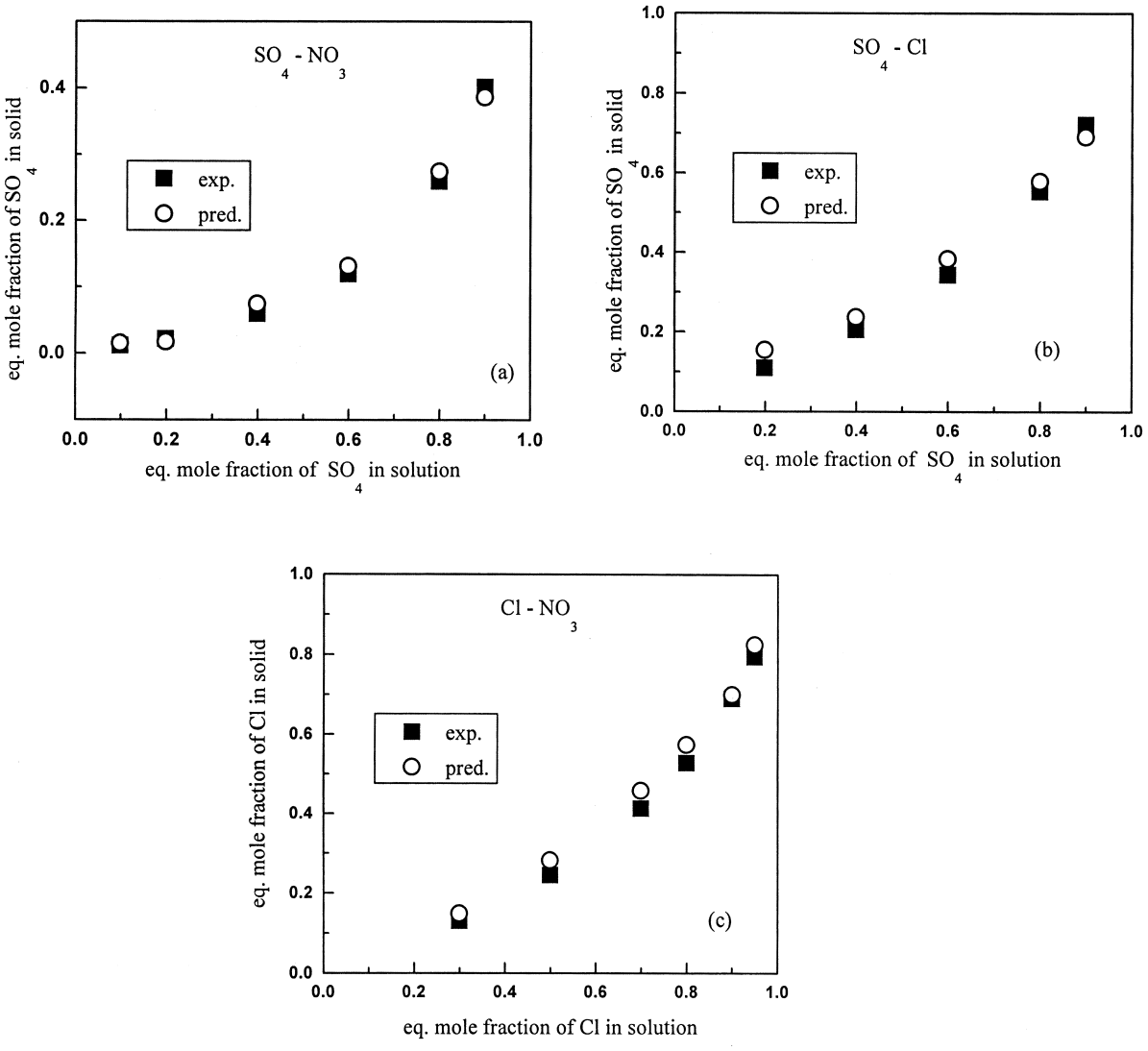

FIG. 3 Sulfate, nitrate, and chloride isotherms with model predicted points calculated using parameter valuesm in Table 3 (input data were taken from Ref. 11).

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TABLE 4
Comparison of Experimental (taken from Refs. 11 and 16) and Predicted Equilibrium Composition for the Ternary System Sr^{2+}–Cs^{+}–Na^{+} on Chabazite, and SO_4, NO_3, and Cl on Amberlite at 23°C

Equivalent mole fraction in solution						Equivalent mole fraction in zeolite			Predicted activity coefficent in zeolite		
Experimental			Predicted								
Na	Cs	Sr	Na	Cs	Sr	Na	Cs	Sr	Na	Cs	Sr
0.1	0.5	0.4	0.11	0.58	0.41	0.203	0.026	0.771	0.228	0.989	0.806
0.2	0.5	0.3	0.19	0.52	0.29	0.224	0.070	0.706	0.268	0.978	0.819
0.3	0.3	0.4	0.3	0.33	0.37	0.258	0.122	0.620	0.325	0.958	0.834
0.4	0.2	0.4	0.41	0.21	0.38	0.299	0.194	0.507	0.410	0.918	0.851
0.5	0.05	0.45	0.496	0.057	0.447	0.322	0.235	0.443	0.621	0.751	0.896
0.6	0.1	0.3	0.602	0.11	0.288	0.354	0.273	0.373	0.600	0.823	0.842
0.7	0.1	0.2	0.688	0.13	0.182	0.412	0.396	0.192	0.653	0.810	0.810
0.8	0.1	0.1	0.796	0.103	0.101	0.480	0.419	0.10	0.705	0.790	0.771
SO_4	NO_3	Cl	SO_4	NO_3	Cl	SO_4	NO_3	Cl	SO_4	NO_3	Cl
0.2	0.1	0.7	0.192	0.112	0.696	0.104	0.332	0.564	0.387	0.849	0.926
0.4	0.1	0.5	0.387	0.098	0.696	0.218	0.353	0.429	0.495	0.840	0.892
0.5	0.4	0.1	0.501	0.404	0.696	0.175	0.760	0.065	0.342	0.968	0.779
0.5	0.3	0.2	0.489	0.315	0.696	0.207	0.656	0.137	0.386	0.949	0.803
0.5	0.2	0.3	0.493	0.221	0.696	0.250	0.522	0.228	0.449	0.912	0.832
0.5	0.1	0.4	0.509	0.132	0.696	0.289	0.357	0.354	0.548	0.833	0.869
0.55	0.05	0.4	0.547	0.064	0.696	0.346	0.253	0.401	0.652	0.746	0.875
0.6	0.2	0.2	0.607	0.197	0.696	0.278	0.564	0.159	0.487	0.903	0.809

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data given by Robinson et al. (16) and experimental data given by Smith and Woodburn (11). The results are shown in Table 4. The predicted activity coefficients in the zeolite phase or the Amberlite phase for each component are also listed in Table 4. The good agreement between experimental and predicted data indicates that the applied procedure for prediction of ternary equilibrium data from binary experimental data is sound and that the iteration procedure works well.

CONCLUSION

- The prediction of ternary ion-exchange equilibrium behavior from the data of binary systems has been successfully modeled.
- The model was based on equilibrium constants for the ion-exchange reactions written in terms of liquid and solid phases activities. Liquid phase activity coefficients were calculated from the Debye and Huckel approach. Solid phase activity coefficients were calculated from the well-known Wilson equation.
- The proposed model only considers thermodynamics nonidealities, but other nonidealities such as Donnan uptake restrict the application of the model to systems of low to intermediate solution normality.
- Agreement between experimental and predicted data for the three components was good and indicated that the applied procedure for prediction is sound and that the proposed framework is an effective method to predict many ternary systems from the corresponding binary systems.
- The model may also easily be extended to the equilibrium behavior of systems higher than ternary systems.

NOMENCLATURE

K_a	equilibrium constant
γ_i	activity coefficient of ion i in solution phase
ϕ_i	activity coefficient of ion i in zeolite phase
m_i	concentration of ion i in solution phase
Y_i	mole fraction of ion i in zeolite phase
TN	total solution normality
I	ionic strength
λ_{A-B}	equilibrium quotient
Z_i	valence of ion i
Λ_{i-j}	Wilson binary interaction parameter

Subscripts

S	solution phase
Z	zeolite phase

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1 strontium
2 sodium
3 cesium

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