ION EXCHANGE EQUILIBRIA IN BINARY AND TERNARY SYSTEMS

DETERMINATION OF ION EXCHANGE PARAMETERS FOR BINARY SYSTEMS AND APPLICATION TO TERNARY SYSTEMS

BY

WILLIAM D.A. BOYER, B.ENG.

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AUTHOR:	William D.A. Boyer, B.Eng. (McMaster University)
SUPERVISOR:	Dr. M.H.I. Baird
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ABSTRACT

Ion exchange equilibrium data can be used to predict the viability of a proposed process. Ion exchange equilibria have been studied considerably since the 1950's but the complexity of the basic research has tended to reduce its direct usefulness to the practising engineer. This research has been undertaken to determine if a moderately simple method of experimentation and analysis could be applied to predict ion exchange equilibria to within limits of accuracy acceptable to engineers.

The first step in the research was to develop a simple mathematical model for a binary system to calculate the selectivity coefficient and resin capacity from batch experiments. The model was successfully applied for the exchange of Na^+ with five heavy metal ions: Ni^{2+}; Cu^{2+}; Cd^{2+}; Pb^{2+} and Zn^{2+} on a typical commercial resin (Dowex HCR-W2). The binary parameters were then used to predict the equilibrium values for several ternary systems. From these ternary experiments, it was determined that binary data can be used to predict ternary systems if the selectivity coefficients of the two ions involved are either almost equal or differed by at least a factor of five. A kinetic effect was proposed to explain the discrepancies observed between the predicted and experimental values for the intermediate ratios of selectivity coefficients of the involved ions, although further work is required to confirm this hypothesis.

Several packed bed experiments were performed to check some of the results from the binary and ternary system experiments and as exploratory work for future research. These experiments confirmed the capacity data calculated from the binary system experiments and were consistent with the trends observed in the ternary system experiments.

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Every life you touch, you change in some way. We should all strive to make that change a good one, and leave each life a little better when we leave than when first we entered.

A simple smile will often open a door that would normally remain closed to the most insistent of callers.

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NOMENCLATURE

Symbols

a	Valency of ion A
b	Valency of ion B
A	Ion in solution or resin phase
B	Ion in solution or resin phase
C	Concentration (eq/L or N)
K	Selectivity coefficient or equilibrium constant
R (reactions)	Active exchange site on resin backbone
R (equations)	Volume ratio of resin to liquid (L bulk resin/L solution)
X	Equivalent fraction of ion C in resin at equilibrium

Subscripts

$\_$	Variable applies to resin phase
a	Valency of ion A
b	Valency of ion B
A	Value of variable for ion A
A+B	Sum of values for both ions A and B
AB	Indicates selectivity coefficient for system A^{a+}-B^{b+}
AC	Indicates selectivity coefficient for system A^{a+}-C^{c+}
B	Value of variable for ion B
BC	Indicates selectivity coefficient for system B^{b+}-C^{c+}
C	Value of variable for ion C

Superscript

a	Valency of ion A
b	Valency of ion B
o	Initial value of variable (prior to exchange occurring)

CHAPTER 1: INTRODUCTION

1.1 A Brief History of Modern Ion Exchangers

Ion exchange has been in use as an industrial unit process since the early 20th century. At that time, it was used solely for water softening and made use of only natural inorganic exchange materials such as greensand and zeolites to remove the undesirable ions such as calcium and magnesium from water and replace them with the more preferable sodium ions (Helfferich, 1962). These natural exchange materials suffered from several shortcomings, limiting the applicability of ion exchange as a viable alternative to other treatment systems.

One of the biggest problems was that the materials tended to have fairly low capacities, so that large systems were needed to accomplish a given objective. They were often susceptible to harsh conditions such as high temperatures or extremes in acidity or alkalinity. The range of selectivities were restricted to only a few ions in solution, instead of all the ions, which was normally desired. These drawbacks seriously limited the application of ion exchange to a few specific areas in the water softening field.

In the 1930's, the development of synthetic organic resins allowed these shortcomings to be either eliminated or minimized (Helfferich, 1962). The new resins had much higher capacities, as much as an order of magnitude or more higher than the naturally occurring, inorganic materials previously used. The new resins were also less susceptible to the harsh environments which the natural materials could not withstand. Perhaps the biggest advantage of the new synthetic resins came with the ability to tailor the properties of the resins, including ion selectivity. Although this ability did not allow for perfect tailoring of the resins and indeed in the beginning was fairly limited, it did provide for the possibility of future resins being designed with much greater selectivity for certain ionic species over other competing species. This property is still being explored and exploited today, with ongoing research developing new resins to be used in specialized applications with high selectivities for a particular ionic species in the presence of higher concentrations of less desired ions.

With the new, broader range of applications available to ion exchange, the process has expanded beyond the water softening industry into other areas such as pollution control and precious metal recovery. A summary of some of the present industrial uses for ion exchange is presented in Table 1.1, compiled from Calmon and Gold (1979).

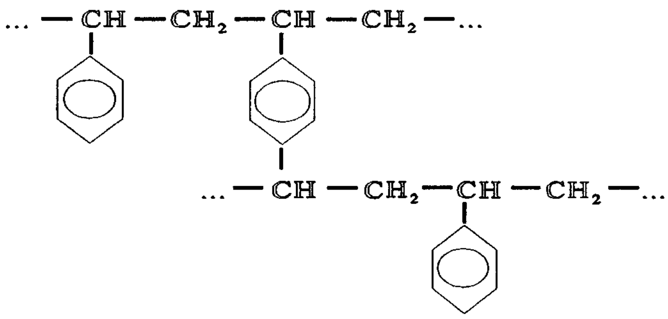
Table 1.1: Summary of Industrial Applications for Ion Exchange

Industrial Use	**Type of Resin**
Desalination of Brackish Water	Weak Base Anion/Acid Cation
Renovation of Sour Water	Weak Base Anion/Acid Cation
Secondary/Tertiary Sewage Treatment	Weak Base Anion/Acid Cation
Removal/Recovery of Heavy Metals	Strong Acid Cation
Separation/Recovery of Strong Acids from Salt Solutions	Strong Base Anion
Recovery from Plating Baths and Rinse Waters	Strong Acid Cation
Chromate Recovery from Cooling Tower Blowdown	Strong/Weak Base Anion
Mercury Removal	Strong Acid, Complexing Cation Strong Base, Complexing Anion
Precious Metal Recovery	Strong Base Anion

1.2 A General Description of Ion Exchange Resins

Present day ion exchangers are based on copolymer gels, the most popular being polystyrene cross-linked with divinylbenzene (DVB). Figure 1.1 shows a typical section of a polystyrene - divinylbenzene copolymer. The normal production of an ion exchange resin has two main steps. The first step is to form the resin particles. These particles are no more than beads of copolymer gels, with no ion exchange properties. The gels are not solid particles but instead have a porous structure and the size of the pores can be adjusted by varying the polymerization conditions.

Figure 1.1: Polystyrene - Divinylbenzene Resin



The next step introduces the active groups where the ion exchange will occur. The type of active group introduced depends on the desired function of the ion exchanger and can range from simple groups like sulphates and tertiary amines which have very little selectivity, to chelating agents which will selectively exchange with ions of one specific type above all others.

The use of a polymer gel provides several advantages. The resin particles are insoluble in an aqueous medium, allowing easy separation from the solution being treated. Because of the porous nature mentioned earlier, the resin has a much higher surface area in contact with the solution than would a solid particle of the same shape, giving the resin a much higher capacity than the solid. The porous nature allows the ions in solution to diffuse into the resin and reach the exchange sites. The mechanical strength of the particle is fairly high because the resin particle is basically one large macromolecule and the forces holding the backbone in place are covalent bonds. The mechanical strength can be adjusted by changing the cross linking of the resin; the higher the cross linking (e.g. the higher the DVB content) the stronger the resin will be. The main disadvantages of increasing the cross linking ratio are a loss in capacity and a drop in exchange rate. The factors occur because of the inability of a highly cross linked resin to swell with solvent. When a resin does not swell, the pore sizes will remain smaller than they would in the swollen state, slowing the diffusion of the ions into and out of the resin and effectively blocking off some areas of the resin from exchange. In addition, with less swelling, the osmotic pressure and stearic hindrance effects can contribute to reduced exchange capacity.

The organic macromolecule which forms the resin particle is fairly resistant to chemical attack, especially compared to the older inorganic resins. Most, if not all, resin backbones consist of saturated polymer gels, which are, because of their basic structure, resistant to chemical reactions. Even the benzene rings, which are normally reactive because of their ring structure, have their reactivity reduced by the introduction of active ion exchange sites to the rings.

1.3 Ion Exchange Reactions

The exchange of ions occurs within the ion exchange resin at points known as active sites. These active sites can be any ionogenic group which will dissociate when a solvent is introduced to the resin. The dissociation of the ionogenic group produces a fixed ionic charge and a counter ion which is of opposite charge to the fixed charge. The fixed charge remains attached to the resin particle and acts as the exchange site, while the counter ion is free to move in the solvent. The counter ions will tend to remain in the vicinity of the fixed charge to act as a counter charge and maintain the electroneutrality of the resin.

For ion exchange to occur, the active sites must have a stronger preference for the undesirable ions that are in solution than for the counter ions that are originally within the resin. The ions in solution diffuse into the resin particle and displace the counter ions from the vicinity of the fixed charge. The counter ions then diffuse out into the bulk solution. The exchange occurs in stoichiometric amounts, with ions exchanging based on their valence state, for example one calcium ion, with a charge of +2, would exchange for two sodium ions, each with a charge of +1. The exchange can be represented by the reaction equation:

$$b(R_a\text{-}A^{a+}) + aB^{b+} \rightleftharpoons a(R_b\text{-}B^{b+}) + bA^{a+} \qquad (1.1)$$

where the R- represents the active site or fixed charge on the resin backbone and A and B represent the exchanging ions, A being the more desired and B being the less desired ion in the solution. The subscripts a and b represent the number of fixed sites associated with the ions A and B.

The extent to which reaction 1.1 proceeds will depend on several factors, perhaps the most obvious factor being concentration. Since the reaction is reversible, an equilibrium point will be reached. The higher the driving force, the farther the reaction will proceed. In the case of reaction 1.1, the greater the concentration of ion

B in solution, the further the reaction will proceed to the right before equilibrium is established.

The ion exchange reaction itself is almost completely isothermal, but the equilibrium constant is dependent on temperature. The exact effects of temperature depend on how the activity coefficients of the various ions change with the temperature in both the bulk solution and in the resin. The activity coefficients are used in addition to the concentrations to account for the non-idealities in both the solution and the resin phases.

The properties of the active ion exchange groups also play a major role in determining the final equilibrium for the reaction. Depending on the selectivity of the active groups, the resin will preferentially exchange for one ion in the presence of higher concentrations of the other, driving the reaction farther to one side or the other.

To quantify the entire reaction, a selectivity coefficient has been defined as:

$$K_{AB} = (\underline{C}_A/C_A)/(C_B/\underline{C}_B) \qquad (1.2)$$

Where K is the selectivity coefficient, C is the concentration of the subscripted ion, and the underline represents the concentration of the subscripted ion in the resin phase. The concentration in the resin phase can be in any realistic units chosen to suit the individual circumstances and once selected should remain constant throughout the work. The equation given here is for the simplest case of two exchanging monovalent ions. The general case will be discussed in the next chapter.

Both the reaction and equation presented thus far refer to binary systems where there are only two ionic species competing for the exchange reaction, the species originally on the resin (the desirable ion) and the species originally in the liquid phase (the undesirable ion). This special case of a binary system is easy to quantify in terms of the selectivity coefficient, but unfortunately is not very realistic. As will be seen in the next chapter, multi-component systems with more than two competing ionic species are quantified by breaking the system into its respective binary equations and defining the binary selectivity coefficients as though the additional species were not present in the system.

1.4 Statement of Research Objectives

To characterize a resin fully would require a large number of selectivity coefficients. For this reason resins are rarely, if ever, explored in full detail. The determination of selectivity coefficients is usually only done for specific ions of interest. Dowex HCR-W2 (a strong acid cation resin produced by the Dow Chemical Company, Midland MI) was chosen as the resin for study in this project and was used in the Na^+ form. The resin was to be applied to the removal of heavy metals from mine effluent waters. To this end, the metal ions examined were Ni^{2+}, Cu^{2+}, Cd^{2+}, Zn^{2+} and Pb^{2+}.

In addition to the characterization of the resin, a method of linearly plotting the data which would allow the determination of both the selectivity coefficient and the capacity of the resin from the same graph was examined. This method also required a slight shift in the experimental procedure from the accepted procedure as presented in the literature (Helfferich, 1962).

Finally, the resin was examined in several column runs as a check of the data already obtained and as a brief exploration into possible future work.

The main objectives of this research were:

1. determination of the binary selectivity coefficients between each of the five heavy metal ions listed previously, and Na^+,
2. examination of several ternary (two heavy metal ions and Na^+) systems and the determination of the applicability of the binary data to the ternary systems,
3. comparison of the proposed method of data analysis and the results obtained to the accepted methods and values from literature, and
4. performance of several column runs and proposal for future directions of experimentation for characterizing this resin.

This thesis consists of six chapters. Chapter 1 is this brief introduction to ion exchange. The detailed review of literature pertaining to this work is presented in Chapter 2. Chapter 3 outlines the experimental procedure for objectives 1, 2 and 4, while Chapter 4 presents the results obtained. Chapter 5 discusses the results and Chapter 6 presents the conclusions drawn from those results and suggests some future areas for research. Appendices are included containing the raw experimental data, correlation information, sample calculations, calibration information and a computer program used to solve the ternary systems.

CHAPTER 2: LITERATURE REVIEW AND MODEL MANIPULATION

Ion exchange had been in use for over 30 years as an industrial operation before much interest was invested in the theoretical aspect of the process (Helfferich, 1962). Beginning in the late 1940's, scientists began to focus their attention more on characterizing the reactions of ion exchange resins in order to predict the usefulness of a given resin in a given process. This interest in characterizing resins has continued to this day.

Several of the benefits of knowing equilibrium data for a resin have been pointed out by Klein et al. (1967). Resin behaviour in a process can be predicted knowing only equilibrium data, solution feed composition and the initial composition of the resin. This allows the estimation of the technical and economic feasibility of a proposed process or the estimation of the effect of a change in operating conditions. The average solution volume before ideal breakthrough occurs in a fixed bed ion exchange column can also be predicted knowing only the information given above.

2.1 Historical Model Formulation

According to Helfferich (1962), the first attempts at prediction of the characteristics of ion exchange equilibria were done using thermodynamic principles. As cited by Helfferich (1962), the first attempt came from Kielland in 1935 then Gaines and Thomas (1953) followed with a truly rigorous thermodynamic treatment. Gaines and Thomas (1953) base their treatment on a translation of Gibbs work using the fact that at equilibrium there is one relation involving the chemical potential and valences of the ions and another that states the chemical potentials of each ion must be equal in all three phases. The third phase is the vapour phase which is virtually non-existent in ion-exchange, but it is still used in the relation.

During this time, other less rigorous equations were also being applied to ion exchange equilibria. The most general was an empirical equation similar to the Freundlich adsorption isotherm (Nachod, 1949) which evolved into the mass action law presented in Chapter One. Other equations were developed by Wiener and Jenny & Vageler (cited by Nachod, 1949) but these equations have become nothing more than historical notes.

Dranoff and Lapidus (1957) note that the primary emphasis of previous workers had been on the mass action law and on adsorption concepts to quantify ion exchange systems. In their paper (Dranoff and Lapidus, 1957), the authors look at both the mass action law and a Langmuir type adsorption isotherm for monovalent-monovalent exchange of the form:

$$\frac{C_A}{C^o_{A+B}} = \frac{\underline{C}_A/\underline{C}_{A+B}}{K_{AB}+(K_{AB}-1)\underline{C}_A/\underline{C}_{A+B}} \tag{2.1}$$

Where: C = concentration in the liquid phase
$\underline{C}$ = concentration in the resin phase
C^O = initial concentration
K_{AB} = appropriate equilibrium constant

From their work, they concluded that the above equation is more easily graphed than the (equivalent but differently written) mass action law and also provides estimates of K less sensitive to slight changes in concentrations.

Prior to the late 1950's, the majority of the work that had been done had concentrated on binary systems, which are systems with only two competing ionic species. Binary experiments had the advantages of being easy to set up experimentally and were much easier to analyse, both chemically and numerically. Experimenters did however begin to realize that binary systems were of little practical importance and work was begun on characterizing multicomponent systems. Initial work began with ternary systems and later progressed to quaternary and higher systems, but even to this day, ternary systems are still studied (Mehablia et al., 1994) as being the simplest of the multi-component systems.

The main goal of Dranoff and Lapidus (1957) was to study the equilibria in ternary systems and to determine if it was possible to predict the final equilibrium concentrations. The obstacle to these predictions was that the theory developed to date dealt only with two competing ionic species and was not easily extended to three competing species. To overcome this, they treated the ternary system as a collection of its three component binary reactions. They noted from their experimental data that the binary reactions proceeded to approximately the same equilibria in ternary systems as in binary systems. Given this observation, they state that it should be possible to predict ternary and higher systems using binary data.

Pieroni and Dranoff (1963) extended the work of Dranoff and Lapidus (1957). They also observe that the equilibria for any two ions are essentially the same in binary and ternary systems. They state many of the assumptions that were previously ignored but that must be made to treat the system in the manner of Dranoff and Lapidus (1957). The main assumption that underlies the treatment of multi-component systems as a collection of binary reactions is that the presence of the additional ions does not in any way interfere with the binary reaction being considered. Other assumptions that are made include the assumption that resin swelling effects are negligible and that activity coefficients in both the solution and resin phases are constant over the concentration ranges of interest.

Pieroni and Dranoff (1963) treat their data using the standard mass action chemical equilibria, but they also briefly mention that Donnan membrane equilibria theory can be used to treat ion exchange reactions. They note (but do not show) that if the above assumptions of negligible swelling effects and lack of solution non-idealities (constant activity coefficients) are applied to the Donnan theory, it reduces to the same expression as the mass action equilibria.

The selectivity coefficients obtained (Pieroni and Dranoff, 1963) with the mass action law tended to vary with resin loading and solution phase composition, but it was possible to assign an average value to the coefficients which would represent the data sufficiently well for engineering purposes. Any use of the selectivity coefficients thus obtained depends strongly on the absence of serious non-idealities in the system.

From the analysis of their data, Pieroni and Dranoff (1963) found that the equilibrium distributions were the same for binary and ternary systems when the systems were dilute. They also found that a single valued selectivity coefficient could be chosen for each binary system that would permit close prediction of equilibrium distributions.

Moody and Thomas (1968) primarily examine the effects of organic and aqueous-organic solvents on ion exchange systems, but they do introduce refinements to the equilibrium constant to include terms for equivalent moisture and the standard state of the resin. These terms provide better accuracy, but at the cost of increased complexity.

Much of the early work done in ion exchange suffered in several areas. Bajpai et al. (1973) note that there was a lack of information pertaining to the resin phase activity coefficients of ions in ternary systems. Most previous workers (Gaines and Thomas, 1953; Dranoff and Lapidus, 1957; Pieroni and Dranoff, 1963; Klein et al., 1967) had either implicitly or explicitly assumed that the resin phase activity coefficients were either unity or were constant over the concentration ranges being studied. This led to a simplified version of the equilibrium constant known as the modified selectivity coefficient (Bajpai et al., 1973). When the solution phase activity coefficients were also dropped, the resulting constant was termed the selectivity coefficient.

Bajpai et al. (1973) also point out that, contrary to what had been assumed in the past, the resin phase activity coefficients are affected by the presence of additional ions in multi-component systems. This then necessitates the determination of the resin phase activity coefficients for multi-component systems, in order to more accurately predict the equilibrium concentrations.

The data of Bajpai et al. (1973) showed a wide variation in the selectivity coefficients depending on the solution phase composition. When they incorporated the solution phase activity coefficient into their results, not much improvement was achieved in the predictions of the equilibrium conditions. Based on these results, they concluded that the system demonstrated a strong dependence for the resin phase activity coefficient on ionic composition.

Despite the difficulties in extending binary equations to multi-component systems, work continued in that area. Smith and Woodburn (1978) introduced a method for characterizing multi-component systems. They started with the common hypothesis that multi-component systems could be predicted from a combination of subsystems that were characterized experimentally. Their model used an equilibrium constant based on thermodynamic principles and they inferred the solution phase ionic activities from an extended Debye-Huckel treatment.

To characterize the resin phase, they used the Wilson model (Wilson, 1964) to correlate the excess Gibbs free energy. The Wilson model was itself a semi-empirical generalization of Flory and Huggins work from the early 1940's. They also note that this model has its theoretical origins in an athermal solution theory, where there is very little or no heat of reaction, which makes it easily applicable to ion exchange. Using their model, they found it possible, through the use of lower order (binary) systems, to infer all the interaction parameters required to specify a higher order (ternary and above) system.

Prior to 1974, the prediction of solution phase activity coefficients in multi-component systems using only the data from binary systems was difficult and required enormously complicated equations (Pitzer and Kim, 1974). Pitzer and Kim (1974) changed this in the last of a four paper series which provided a set of equations to solve this problem. Their derivation was based on the expression for the excess Gibbs energy. The predictions rely on a set of interaction parameters that can be determined from binary data and applied to higher order systems. Their predictions were compared to experimental data and they found extremely good agreement for the systems they studied.

Harvie and Weare (1980) applied the Pitzer correlation to predict a quaternary system. They noted that the correlation guaranteed convergence and was efficient and easy to implement. Meijer and Van Rosmalen (1984) also used the Pitzer correlation to determine ionic activity coefficients in the solution phase and found it acceptable.

Manning and Melsheimer (1983) conducted their experimental work on ion exchange membranes, but the equilibrium theory and therefore the applicable equations are the same as for ion exchange resins. As many workers had done before them, they hypothesized that binary selectivity data could be used to predict ternary ion exchange equilibria. The basis of their analysis is the Donnan equilibrium equation, which has the same definition as the mass action law and they note that the equilibrium constant so defined is a thermodynamic constant dependent only on temperature provided the activities are properly defined. They also follow the historical practice of replacing the activities with concentrations due to the difficulty of calculating the solid phase activity coefficients. This replacement results in the previously mentioned selectivity coefficient.

In order to predict the ternary equilibrium concentrations, Manning and Melsheimer (1983) used the method proposed by Klein et al. (1967) where the selectivity coefficients would be the same for a given ion pair in both binary and ternary systems. They also make the assumption of non-interference by the third competing ionic species.

To compare their ternary results with their binary work, Manning and Melsheimer (1983) plotted their ternary data as the equivalent fraction in the resin phase (the equivalent fraction of a species in the resin phase is defined as the concentration of that species divided by the total exchange capacity of the resin) on a third component free basis (e.g. $\underline{x}_A/(1-\underline{x}_C)$) vs. the equivalent fraction in the liquid phase on a third component free basis (e.g. $x_A/(1-x_C)$). The binary data were plotted as $\underline{x}_A$ vs. x_A, the equivalent fraction of A in the resin phase vs. the equivalent fraction of A in the liquid phase. Despite the apparent disagreement of the ternary data with the binary data, which was also noted by Dranoff and Lapidus (1957), both teams of experimenters found the above graphical method to provide good agreement between the binary and ternary data.

Another option mentioned by Manning and Melsheimer (1983) is a purely graphical representation of ternary data on a ternary diagram as presented by Dranoff and Lapidus (1957). They point out several problems with this approach, most notably those for monovalent-divalent exchange. In these cases, the system shows a strong dependence on total solution concentration. Another problem is the lack of a selectivity coefficient calculated from the data, the method of system characterization preferred by most other investigators.

In their conclusions, Manning and Melsheimer (1983) found that their calculated binary selectivities showed very little dependence on either the solid phase composition or the solution phase composition. Another important point they make is that multicomponent interaction effects do not seem to pose any severe problems for predicting multicomponent equilibria for relatively low ionic concentrations. The order of selectivities determined by Manning and Melsheimer (1983) followed the radii of hydration of the ions, with the smallest ion being most preferred by the resin and the largest ion the least prefered. They explain this by noting that the solid will be subjected to less swelling with the smaller ions than with the larger ions and therefore there would be less osmotic pressure from the uptake of the smaller ions.

Vasquez et al. (1986) continue the previous trend of using the equilibrium constant to characterize the systems being studied. However, their definition of the equilibrium constant is slightly modified from the traditional definition, in that they use the equivalent fraction of the ions in the solid phase as opposed to the concentration. This has the effect of changing the value and units of the equilibrium constant so that direct comparison between two equilibrium constants is not possible without first converting one. In the determination of the capacity of the resin, Vasquez et al. (1986) noted that there appeared to be a slight dependence of the capacity on the type of counterion being examined. While small, this dependence is considered as a possible source of error for equilibrium experiments and calculations.

Shallcross et al. (1988) started with the model proposed by Smith and Woodburn (1978) for characterizing ion exchange systems. They continued to use the Wilson equation for estimating the solid phase activity coefficients, but followed the work of Harvie and Weare (1980) and Meijer and Van Rosmalen (1984) by replacing the extended Debye-Huckel equation for estimating solution phase activity coefficients with the Pitzer correlation. The equilibrium constant thus defined is a function of temperature only, whereas the simpler seletivity coefficients would be a function of total liquid normality, liquid composition and the specific exchange material, in addition to the temperature.

The Smith and Woodburn model with the modification proposed by Shallcross et al. (1988) is applicable to the equilibrium calculation of systems of practical interest over extended concentration ranges (Shallcross et al., (1988). Shallcross et al. (1988) do note one drawback to the proposed model. As stated, with the activities in place of the concentrations, the model considers only thermodynamic non-idealities and ignores other non-idealities such as Donnan uptake. This restricts the model to systems with an initial concentration below 1N.

Although Shallcross et al. (1988) noted an improvement in their predictions from using the Pitzer correlation instead of the extended Debye-Huckel equation, this claim was refuted by Allen et al. (1989) who stated that the use of the Pitzer correlation 'does not, however, appear to yield results with a statistically significant improvement over the extended Debye-Huckel relation...' (Allen et al., 1989). The major drawback to this model, as noted by Allen et al. (1989), is that it requires N^2-1 parameters to fully characterize an N-component system.

Allen et al. (1989) point out that most of the work in the late 1980's was focussing on predicting multicomponent exchange equilibia with parameters obtained from binary data. This work was following three main paths. The first path was to calculate the activities in a multicomponent system directly from the binary data. The second path involved finding how the selectivity coefficients varied with changing solution concentration for a binary system and using an integral technique to apply this to determing ternary equilibrium concentrations. The final path is to determine a number of parameters that characterize a binary system and then estimate the activities in a multicomponent system using these parameters.

Allen et al. (1989) used the Wilson equation to estimate the solid phase activities and the extended Debye-Huckel equation for liquid phase activities instead of the Pitzer correlation as was done by Shallcross et al. (1988). To reduce the number of parameters required to characterize a multicomponent system, two new conditions were proposed by Allen et al. (1989). The first was a reciprocity constraint for the parameters determined in the Wilson equation. The second condition was the Hala constraint which also applies to the Wilson equation parameters. These two conditions combined reduced the number of parameters from N^2-1 to 2(N-1) without a significant loss of fit (Allen et al., 1989).

More recently, Mehablia et al. (1994) used the method of Shallcross et al. (1988) to characterize and predict their multicomponent systems, with one difference. Where the method of Shallcross et al. (1988) calculated the equilibrium constant and the interaction parameters using the same calculations, Mehablia et al. (1994) calculated the equilibrium constant separately using the approach of Gaines and Thomas (1953). This had the effect of decoupling the equilibrium constant from the interaction parameters, the coupling of the two being a problem noted by Mehablia et al. (1994). One other problem noted by Mehablia et al. (1994) was the sensitivity of the Wilson parameters to slight changes in experimental data.

Table 2.1: Summary of Reviewed Articles

Author	Year	Base Model	Proposed Modifications and Results
Gaines and Thomas	1953	Mass Action Law/ Integral Techniques	
Dranoff and Lapidus	1957	Mass Action Law/ Concentrations	Graphical representation of binary pairs, replace concentrations with normalized concentrations.
Pieroni and Dranoff	1963	Mass Action Law/ Equivalent Fractions	
Bajpai et al..	1973	Mass Action Law/ Equivalent Fractions	Inclusion of solution phase activity coefficients, little improvement found.
Smith and Woodburn	1978	Thermodynamic Equilibrium Constant / Mass Action Law	Debye-Huckel equation for solution phase activities, Wilson model for solid phase interaction parameters.
Harvie and Weare	1980	Mass Action Law	Pitzer correlation for solution phase activities.
Manning and Melsheimer	1983	Klein et al. with concentrations	Solution phase activities in place of concentrations, application to membrane ion exchange equilibrium.
Vasquez et al.	1986	Smith and Woodburn model	Capacity slightly depended on counterion. Concentration for liquid phase, equivalent fraction for solid phase.
Shallcross et al.	1988	Smith and Woodburn model	Pitzer correlation for solution phase activities. Concentration for liquid phase, equivalent fraction for solid phase.
Allen et al.	1989	Smith and Woodburn model	Hala constraint, reciprocity constraint reduces parameters from (N^2-1) to $2(N-1)$.
Mehablia et al.	1994	Shallcross et al.	Decoupling of equilibrium constant by using Gaines and Thomas approach.

The general effect of all the modifications proposed to the methods over the years has been to increase the accuracy of the predicted equilibrium concentrations. This has been offset by a corresponding increase in the complexity of the methods. More and more specialized knowledge is required to apply these methods. In the interest of the pure and applied sciences, these complications would be valid, but for engineering purposes, the levels of accuracy obtained would appear to exceed those which are required. To this end, an extremely simple model for ion exchange equilibrium will be examined to determine if it can be applied to a highly non-ideal system to within acceptable limits of accuracy.

The model that was chosen for examination was the mass action law studied by early investigators (Gaines and Thomas, 1953; Dranoff and Lapidus, 1957; Pieroni and Dranoff, 1963; Bajpai et al., 1973) with concentrations replacing both the liquid phase and solid phase activities. Also included is the assumption that the multicomponent systems can be represented by a set of pseudo-binary equations with no third ion interaction effects.

A disadvantage which has not been mentioned of all the methods presented previously is that the capacity of the resin must be determined in an experiment separate from the equilibrium runs. Given the observations of Vasquez et al. (1986) that the capacity of the resin seems to be at least slightly dependent on the counterion, this could require an excessive amount of extra experiments. As will be shown in the following derivation, the proposed experiments and analysis allow the calculation of both the selectivity coefficient and the resin capacity from the same set of data.

2.2 Binary Model Development

The purpose of the binary model is to develop a system for plotting data that would lead to a simple calculation of the selectivity coefficient and the capacity for the binary system being examined. As was mentioned in the first chapter, there are several assumptions that can be made when treating ion exchange systems. The assumptions made here are negligible resin swelling and unit activity coefficients in both the liquid and solid phase. Since perfect predictions for the data are not what is desired but merely a quick, simple and moderately accurate approach to predicting the final concentrations, the assumptions made are justified.

The development is carried out for the common case of a monovalent ion B^+ (e.g. Na^+) being exchanged with a divalent ion A^{2+} (e.g. Cu^{2+}) represented by the reaction:

$$2R\text{-}B^{+}+A^{2+} \rightleftharpoons R_2A^{2+}+2B^{+} \tag{2.2}$$

Starting with the definition of the selectivity coefficient:

$$K = \frac{\underline{C}_A}{C_A} \times \frac{C_B^2}{\underline{C}_B^2} \tag{2.3}$$

Where: C = equilibrium solution concentration in equivalents/litre
$\underline{C}$ = equilibrium resin concentration in equivalents/litre bulk resin

The bulk resin volume is used here because it is easier to measure and has more applicability to real systems.

R is then defined as the volume ratio of resin to liquid and for the uptake of A^{2+} by an initially A-free resin:

$$\underline{C}_A = \frac{C_A^o - C_A}{R} \tag{2.4}$$

Where: ° = indicates initial concentration of ionic species.

From the electroneutrality condition:

$$C_B = C_A^o - C_A \tag{2.5}$$

and:

$$\underline{C}_B = \underline{C}_B^o - \underline{C}_A \tag{2.6}$$

In this case, $\underline{C}^o_B$ is equal to the capacity of the resin because initially the resin is completely in the Na^+ form.

Combining equations 2.3 - 2.6:

$$K = \frac{(C_A^o - C_A)/R}{C_A} \times \frac{(C_A^o - C_A)^2}{(\underline{C}_B^o - (C_A^o - C_A)/R)^2} \tag{2.7}$$

Rearranging:

$$K(\underline{C}_B^o - (C_A^o - C_A)/R)^2 = (C_A^o - C_A)^3/RC_A \tag{2.8}$$

and taking the square root of both sides:

$$K^{1/2}(\underline{C}_B^o - (C_A^o - C_A)/R) = (C_A^o - C_A)^{3/2}/(RC_A)^{1/2} \tag{2.9}$$

Rearranging again:

$$(C_A^o - C_A)/R = \underline{C}_B^o - (C_A^o - C_A)^{3/2}/(RC_AK)^{1/2} \tag{2.10}$$

After collecting data on C_A^o, C_A and R, $(C_A^o-C_A)/R$ vs. $(C_A^o-C_A)^{3/2}/(RC_A)^{1/2}$ can then be graphed. Using normal linear regression, the mean value of the resin capacity ($\underline{C}_B^o$) can be determined from the intercept and the selectivity coefficient (K) can be determined from the slope ($\propto K^{-1/2}$).

Once the binary selectivity coefficients have been determined, they can be used to predict the ternary equilibrium concentrations. The ternary model does not provide a graphical result but requires a computer-aided solution of the equilibria and ion balances.

2.3 Ternary Model Development

Beginning by defining the species A and B to be the two competing heavy metal ions (both assumed to be divalent) and C to be Na^+ (initially on the resin), the two selectivity coefficients can then be written as:

$$K_{AC}=\frac{\underline{C_A}}{C_A}\times\frac{C_C^2}{\underline{C_C^2}} \tag{2.11}$$

$$K_{BC}=\frac{\underline{C_B}}{C_B}\times\frac{C_C^2}{\underline{C_C^2}} \tag{2.12}$$

Making the simplifying assumption that the resin capacity ($\underline{C}_C^o$) is constant and the same for all competing species and by applying the electroneutrality condition the result is:

$$\underline{C}_C^o=\underline{C}_A+\underline{C}_B+\underline{C}_C \tag{2.13}$$

In the liquid phase:

$$C_A^o+C_B^o=C_A+C_B+C_C \tag{2.14}$$

Performing a mass balance between the liquid phase and the resin:

$$C_A^o-C_A=R\underline{C}_A \tag{2.15}$$

$$C_B^o-C_B=R\underline{C}_B \tag{2.16}$$

$$C_C=R(\underline{C}_C^o-\underline{C}_C) \tag{2.17}$$

To solve for the final equilibrium concentrations, begin by defining:

$$X=\underline{C}_C/\underline{C}_C^o \tag{2.18}$$

where X is the equivalent fraction of ion C in the resin at equilibrium.

By combining equations 2.17 and 2.18:

$$C_C = R\underline{C}_C^o(1-X) \tag{2.19}$$

For species A, from equation 2.11:

$$K_{AC} = \frac{\underline{C}_A}{C_A} \times \frac{R^2(1-X)^2}{X^2} \tag{2.20}$$

Rearranging:

$$\underline{C}_A = \frac{K_{AC} X^2 C_A}{R^2(1-X)^2} \tag{2.21}$$

Substituting equation 2.21 into 2.15:

$$C_A^o - C_A = \frac{K_{AC} X^2 C_A}{R(1-X)^2} \tag{2.22}$$

Which rearranges to:

$$C_A = \frac{C_A^o}{1 + \frac{K_{AC} X^2}{R(1-X)^2}} \tag{2.23}$$

Similarly, for species B:

$$C_B = \frac{C_B^o}{1 + \frac{K_{BC} X^2}{R(1-X)^2}} \tag{2.24}$$

From equation 2.14:

$$C_C = C_A^o + C_B^o - C_A - C_B \tag{2.25}$$

Assuming a value for X (close to 0, which would be the case for complete stripping of the Na^+ ion), calculate C_A and C_B from equations 2.23 and 2.24, and compare the values of C_C calculated from equations 2.19 and 2.25. If these two values agree to within a preset limit of accuracy, the system has converged and the values calculated are the predicted equilibrium concentrations. If the two predicted values of C_C do not agree, adjust the value of X accordingly and resolve equations 2.19, 2.23, 2.24 and 2.25. Continue adjusting the parameter X until the two predictions of C_C do agree to within the preset limit. A short computer program was written in BASIC to solve the system and is given in Appendix A.

CHAPTER 3: EXPERIMENTAL

The experimental work was carried out in two distinct phases. The first of these phases, individual batch tests, was itself separated into two parts. First, binary exchange equilibrium parameters were measured and second, some ternary systems were used to check the validity of the model and the parameters. The second phase of the experimental work, which was not the main focus of the research, involved a few fixed bed column tests which were also used to check some of the information from the batch tests and to provide extra information for future work. For both phases, the resin studied was Dowex HCR W2, produced by The Dow Chemical Company, Midland MI.

3.1 Batch Experiments

3.1.1 Batch Apparatus

The batch experiments were carried out in 125 mL plastic Nalgene bottles which were agitated in a constant temperature shaker bath at 25±1°C. The stock feed solutions used in these experiments were prepared in 1 L volumetric flasks and divided into the plastic bottles using a 50 mL pipette.

The chemicals used for the stock solution were laboratory grade salts supplied by Fisher Chemicals. The chemicals studied were nickel sulphate, cupric sulphate, cadmium nitrate, zinc sulphate and lead nitrate. All solutions, including the initial stock solution and the final equilibrated solutions were analyzed on a Jarrel-Ash ICAP 9000, which operates on the atomic emission principle. The samples were analyzed with an Argon carrier gas with a plasma flow rate of 20 L/min, sample aspirator flow rate of 300 mL/min and sample flow rate of 5 mL/min. Four exposures were run for each sample and each exposure lasted for 15 seconds. The reported value of the concentration was the numeric average of the 4 exposures.

3.1.2 Batch Procedures

The first step in the batch experiments was to prepare the stock solution to be used in the run. The concentration of the stock solution was varied between runs, but was normally within the 0.05-0.15 eq/L range. The solution was prepared by weighing out the solid salt and dissolving the solids in distilled, deionized water in a volumetric flask and making up the volume to one litre. The pH for all solutions was approximately 5.5 and remained constant at that value throughout the experiments.

Fifty mL of solution was then pipetted into each of 18 plastic bottles for the samples and the remainder was placed in a nineteenth bottle to act as the control sample. Resin was then added to the 18 sample bottles in ratios varying from approximately 0.01 g resin/L solution to 0.1 g resin/L solution.

All 19 bottles were placed on the shaker bath and agitated for a minimum of 24 hours to allow equilibrium to be achieved. The temperature for all the runs was held constant at 25±1° C.

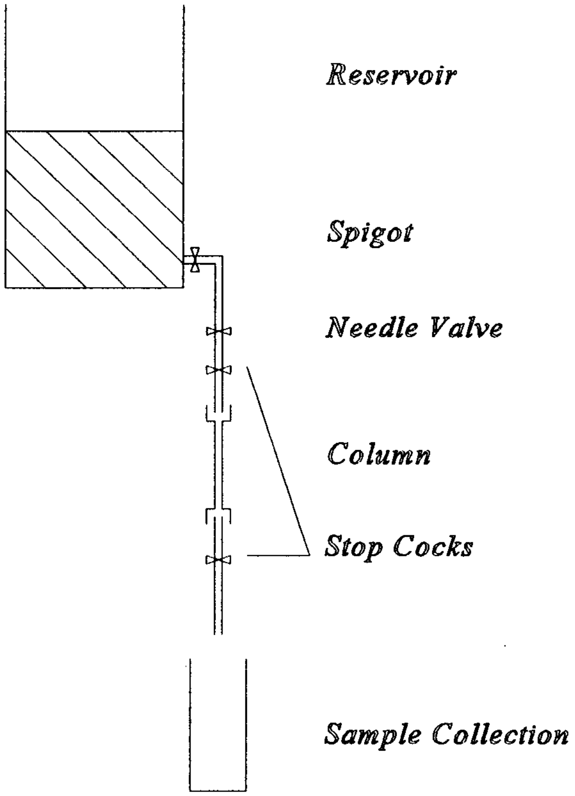
After the 24 hours, the samples were removed from the shaker bath and the solution was decanted to separate it from the resin. The solution was then analyzed by ICP. The readout was monitored for any anomalous readings that may have occurred from fine resin particles entrained in the solution being analyzed interfering with the flame of the analyzer. No such anomalies were found in any of the runs. Any solutions with concentrations outside the linear range of the detector in the ICP were diluted in order to bring the concentration within the linear range. The data were then analyzed. The raw data are given in Appendix B and the analyzed data are presented in Chapter 4.

3.2 Packed Bed Experiments

3.2.1 Packed Bed Apparatus

The column apparatus consisted of a 60 L overhead reservoir tank with a spigot, a graduated needle valve to control the flow, two stopcocks to isolate the column and a detachable column. The column was approximately 15 cm long with an internal diameter of 1.5 cm. Inside the column, a small piece of stainless steel screen was used at the bottom of the column to support the resin bed, and a plug of glass wool was placed at either end of the bed to act as a flow distributor and collector system. A diagram of the apparatus is shown in Figure 3.1 on the following page.

Figure 3.1: Diagram of Packed Bed Apparatus



3.2.2 Packed Bed Procedures

The stock solution was prepared in the reservoir by adding an appropriate amount of the solid salt to approximately 20 L of distilled, deionized water with a concentration of approximately 0.03 eq/L. The column was prepared in several steps. The screen was placed in the bottom of the column and a small plug of glass wool was placed on top of the screen. The column was then filled with distilled, deionized water to eliminate any air bubbles from the resin and to ensure good packing of the resin beads. The resin was then added to the column and a small plug of glass wool was placed on top to provide uniform flow distribution.

The needle valve was calibrated using standard procedures and the flow was set using the needle valve, prior to reconnecting the column. The column was purged of air by filling with distilled, deionized water from the bottom up before being reattached to the rest of the apparatus. The stopcock was then opened and the distilled water was allowed to pass through the column before sampling began. The column effluent was sampled at regular intervals to achieve a detailed record of the breakthrough curve and the samples were analyzed in the same manner as those in the batch experiments. Raw data are presented in Appendix C and analyzed data are presented in Chapter 4.

3.3 Safety Precautions

All standard laboratory procedures were followed with respect to safe handling of common chemicals. Safety glasses and latex gloves were worn at all times while handling chemicals in any state. Spills were contained, cleaned and disposed of in accordance with the MSDS recommendations. All solutions were disposed of in the hazardous waste collection drum.

Special precautions were undertaken when conducting the experiments involving lead. A lead assessment (Boyer, 1996) was performed as required by the Occupational Health and Safety Act before any experiments were begun. All handling of the lead containing materials (powder, solution and resin) was done in a fume hood with latex gloves and a lab coat to minimize possible exposure. Transportation of the lead containing materials was done in tightly capped plastic bottles carried in plastic pans. No spills or accidents were encountered with the lead experiments.

CHAPTER 4: RESULTS

The first phase of the batch experiments was to determine the binary ion exchange selectivity coefficients for the resin as defined in equation 2.2. The results are summarized below in Table 4.1 (with 95% C.I.) and presented in Figures 4.1-4.5.

Table 4.1: Summary of Binary Ion Exchange Selectivity Coefficients

Species	Capacity (eq/L)	Selectivity (K)	mol. wt.
Ni^{2+}	2.41±0.09	0.826±0.135	58.7
Cu^{2+}	2.18±0.10	0.694±0.132	63.5
Zn^{2+}	1.62±0.09	0.925±0.335	65.4
Cd^{2+}	1.93±0.08	1.98±0.46	112.4
Pb^{2+}	2.20±0.14	5.95±1.77	207.2

These results were then applied to predict the final resin concentrations in tertiary systems, as shown in Figures 4.6-4.17.

The packed bed operating conditions are summarized in Table 4.2 and the results are presented in Figures 4.18-4.21.

Table 4.2: Summary of Packed Bed Operating Conditions

Figure	Concentration (eq/L)			Flow Rate (mL/min)	Bed Volume (mL)	Determined Capacity (eq/L)
	Ni^{2+}	Cd^{2+}	Pb^{2+}			
4.18	0.0085	0	0	9.3	10	1.91
4.19	0.0047	0.0041	0	9.5	10	2.07
4.20	0.0046	0.0042	0	5.8	10	1.99
4.21	0.0022	0.0023	0.0027	8.5	10	2.03

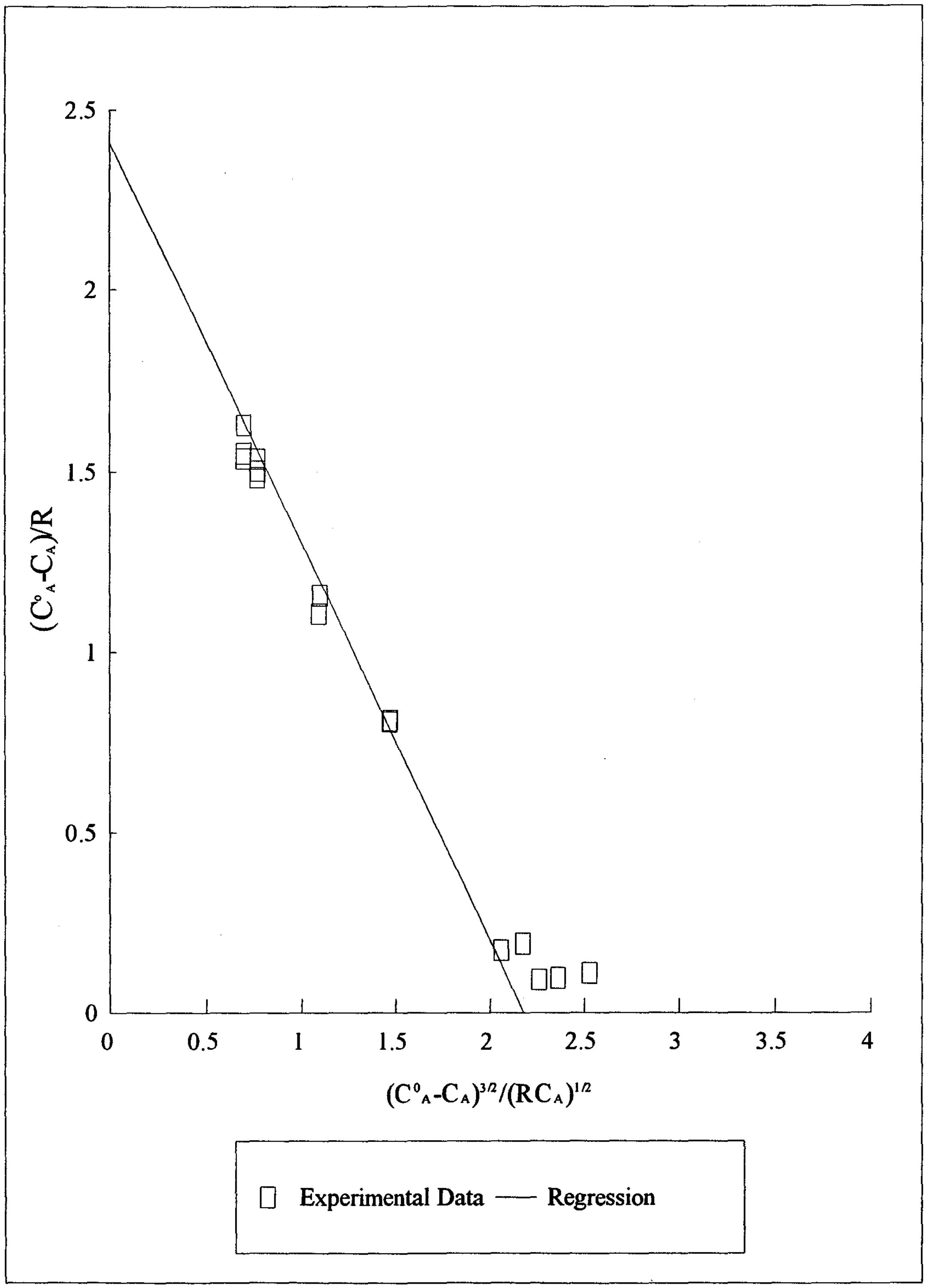


Figure 4.1: Determination of binary parameters for Ni^{2+}-Na^{+} system.

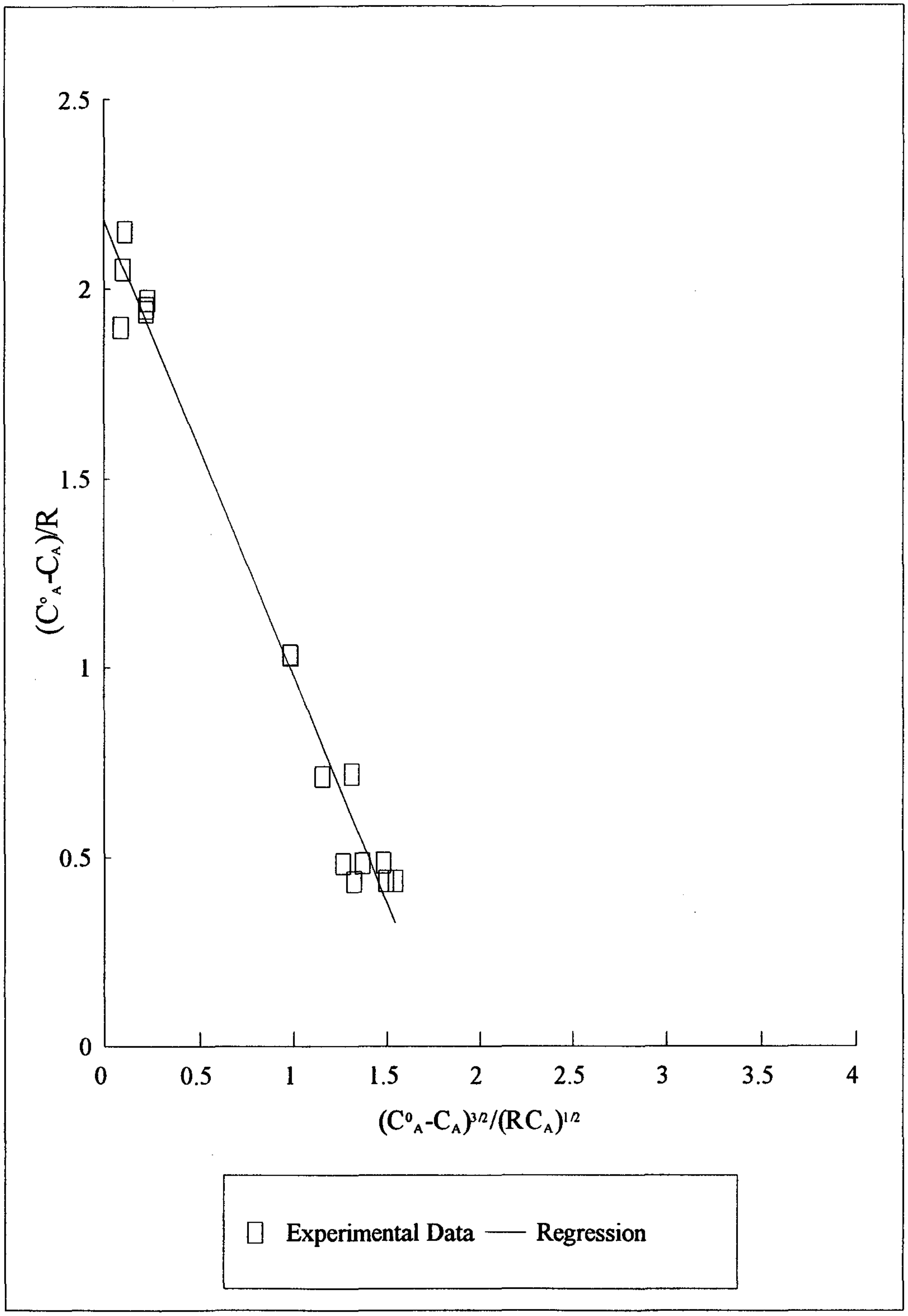


Figure 4.2: Determination of binary parameters for Cu^{2+}-Na^{+} system.

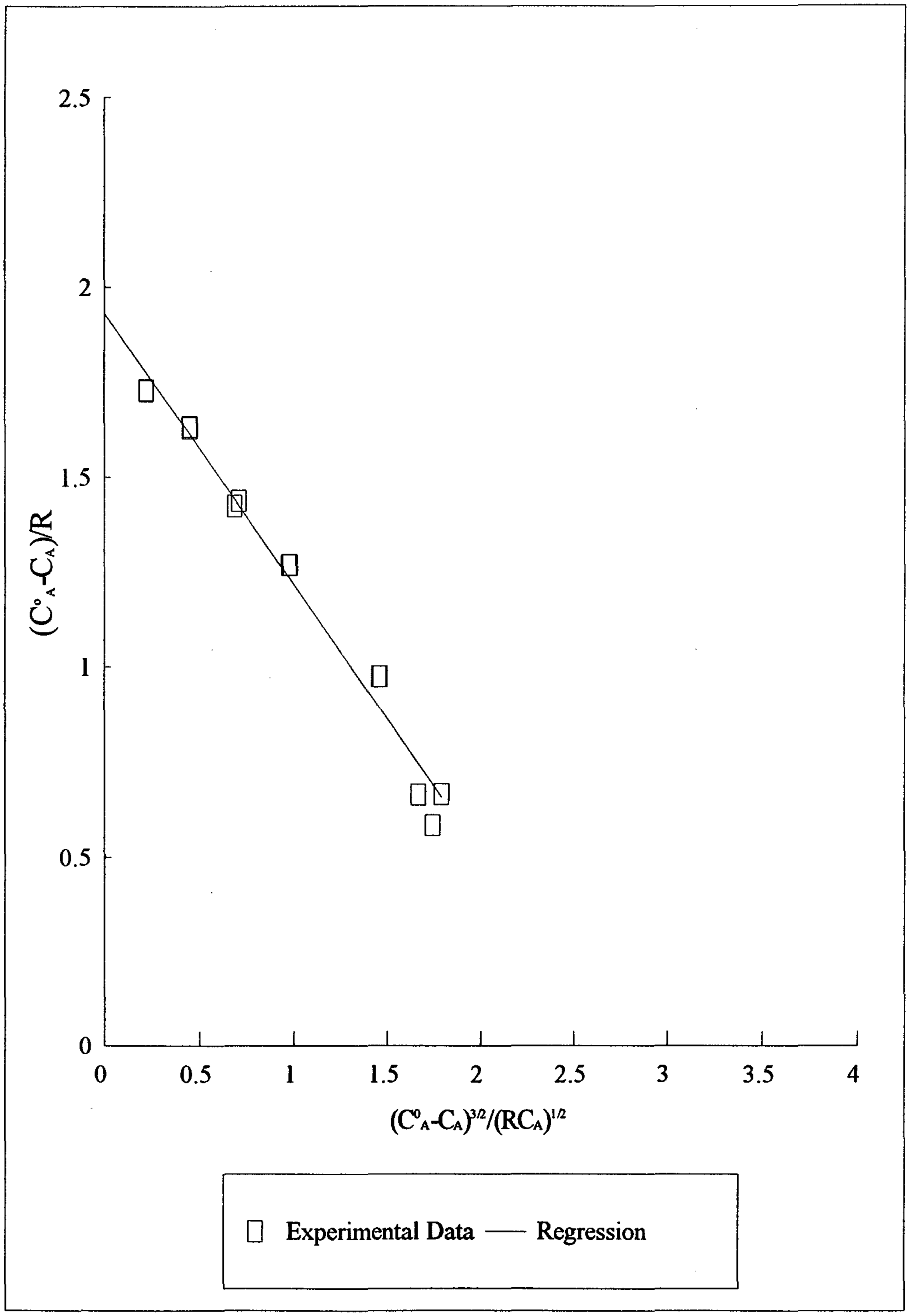


Figure 4.3: Determination of binary parameters for Cd^{2+}-Na^{+} system.

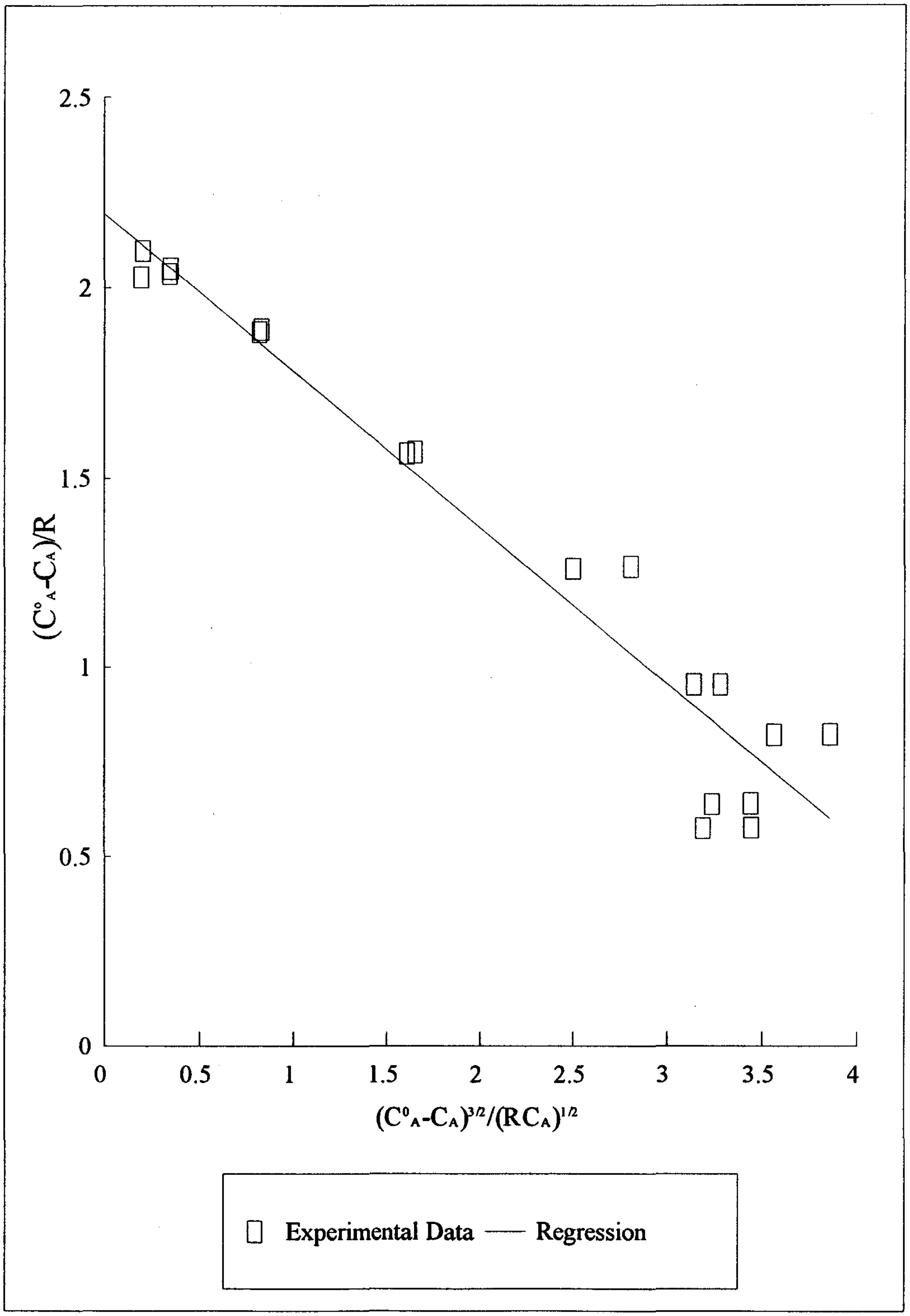


Figure 4.4: Determination of binary parameters for Pb^{2+}-Na^{+} system.

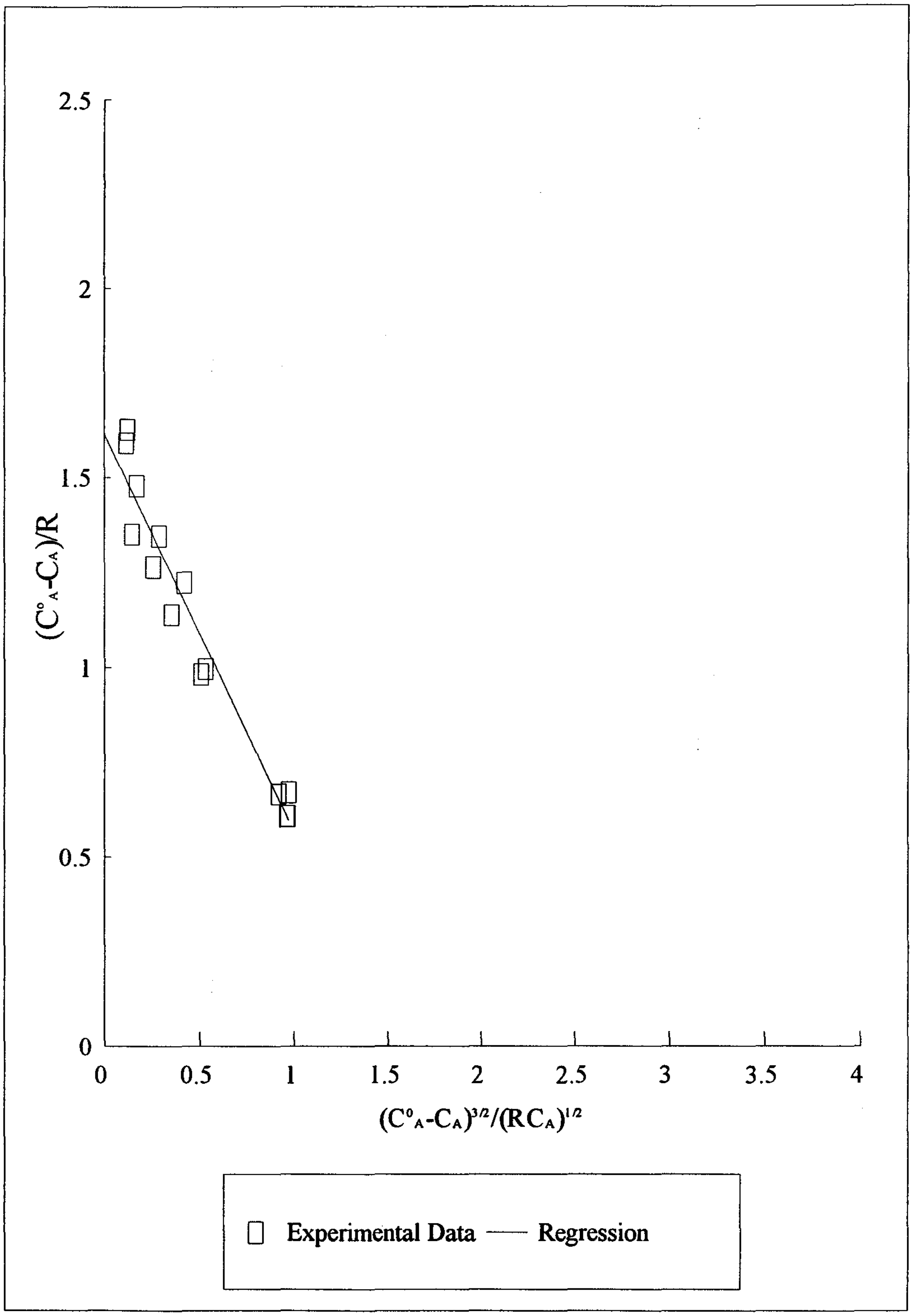


Figure 4.5: Determination of binary parameters for Zn^{2+}-Na^{+} system.

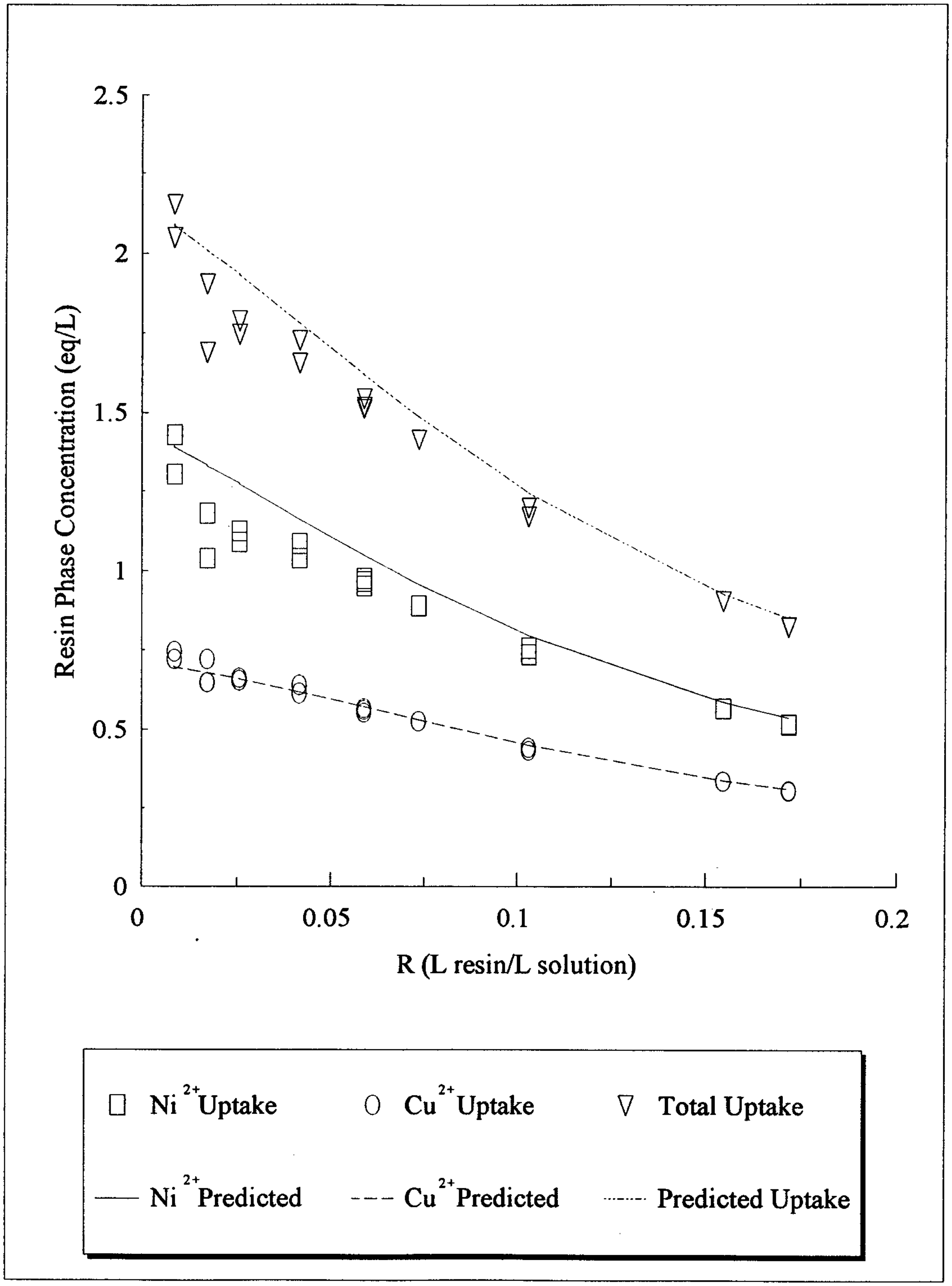


Figure 4.6: Resin phase concentration vs. resin/solution ratio R for the system Ni^{2+}-Cu^{2+}-Na^{+}. Initial solution concentrations: Ni^{2+} 0.1N; Cu^{2+} 0.05N.

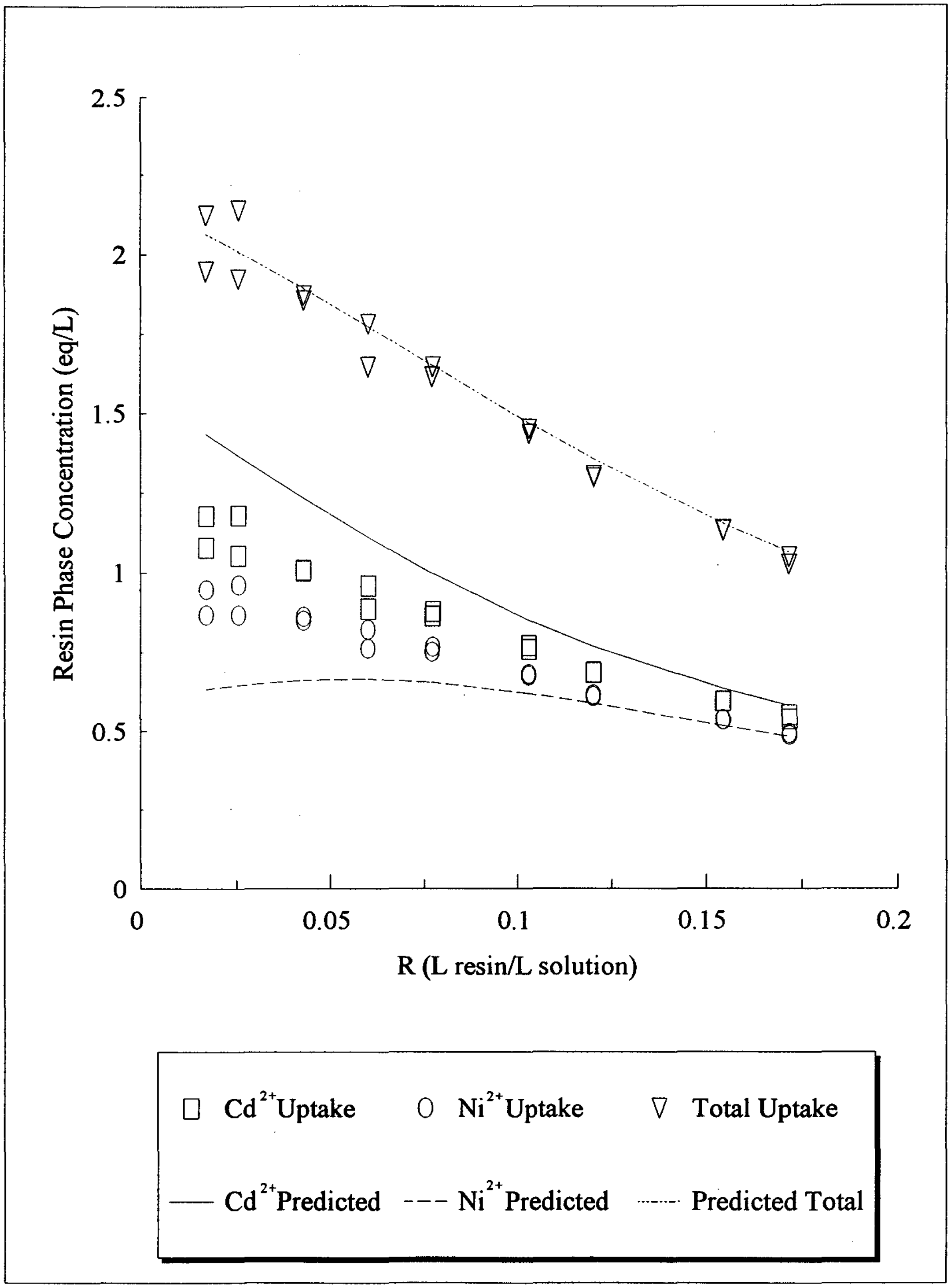


Figure 4.7: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Ni^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.1N; Ni^{2+}, 0.1N.

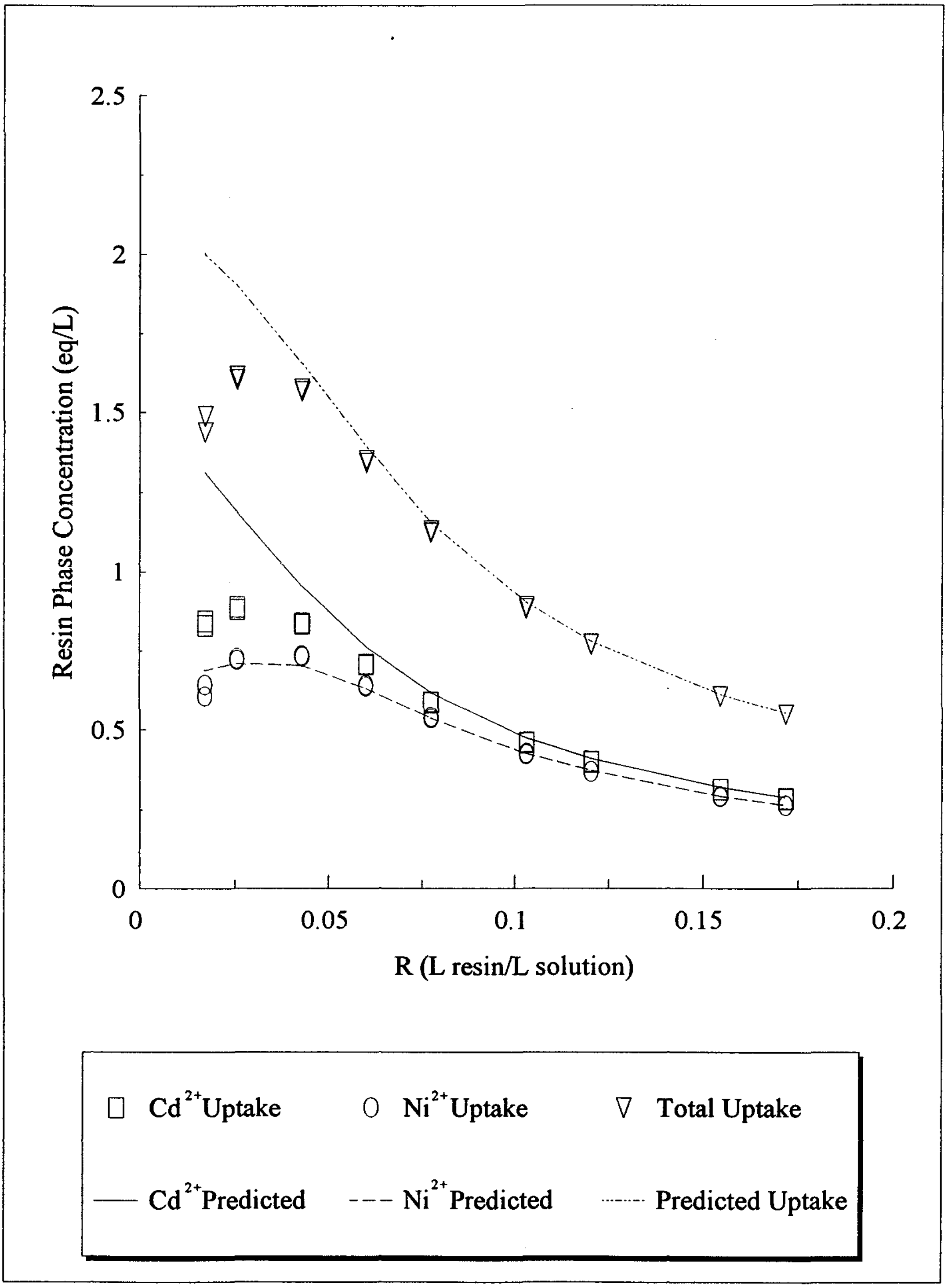


Figure 4.8: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Ni^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.05N; Ni^{2+}, 0.05N.

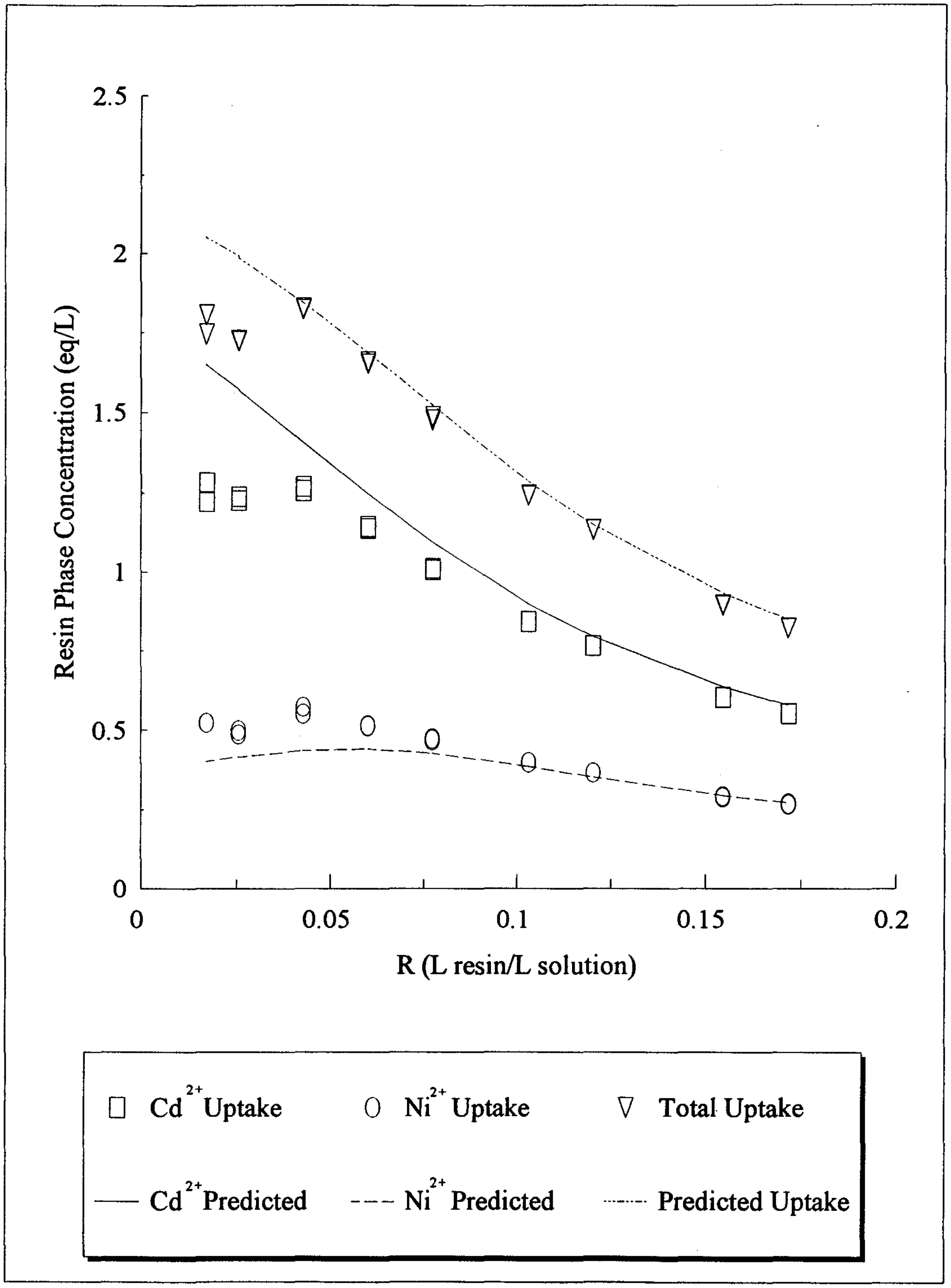


Figure 4.9: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Ni^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.1N; Ni^{2+}, 0.05N.

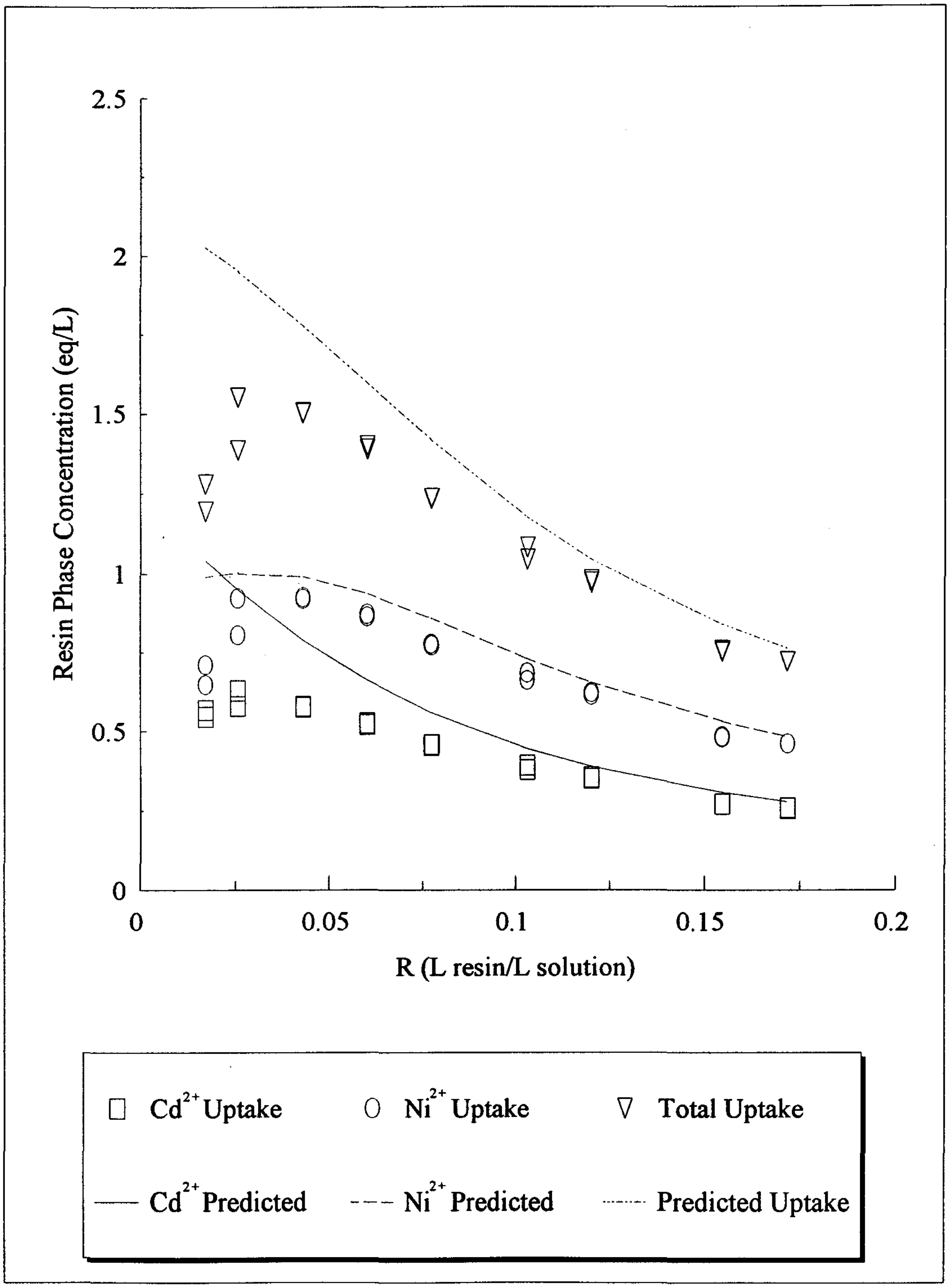


Figure 4.10: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Ni^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.05N; Ni^{2+}, 0.1N.

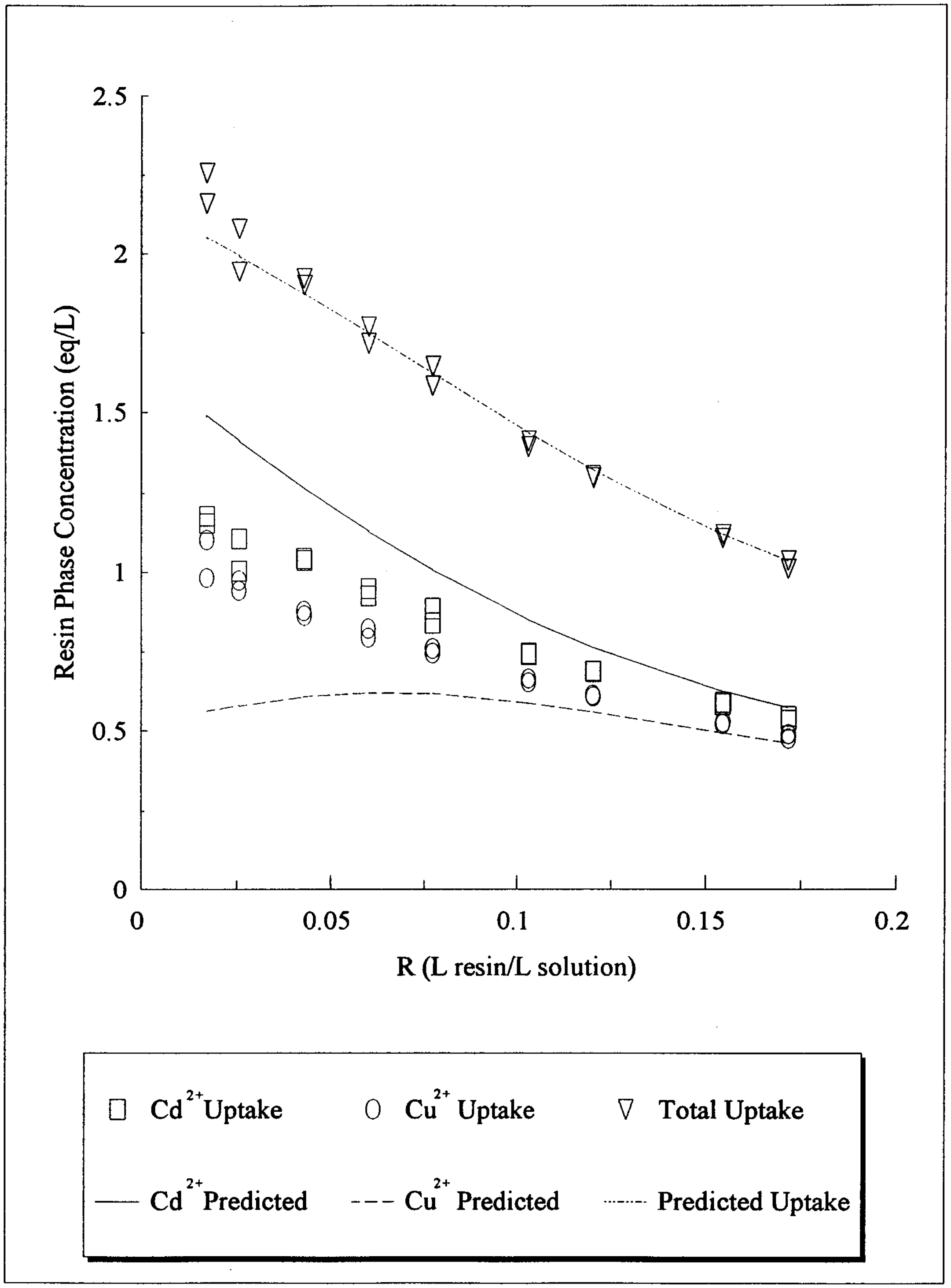


Figure 4.11: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Cu^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.1N; Cu^{2+}, 0.1N.

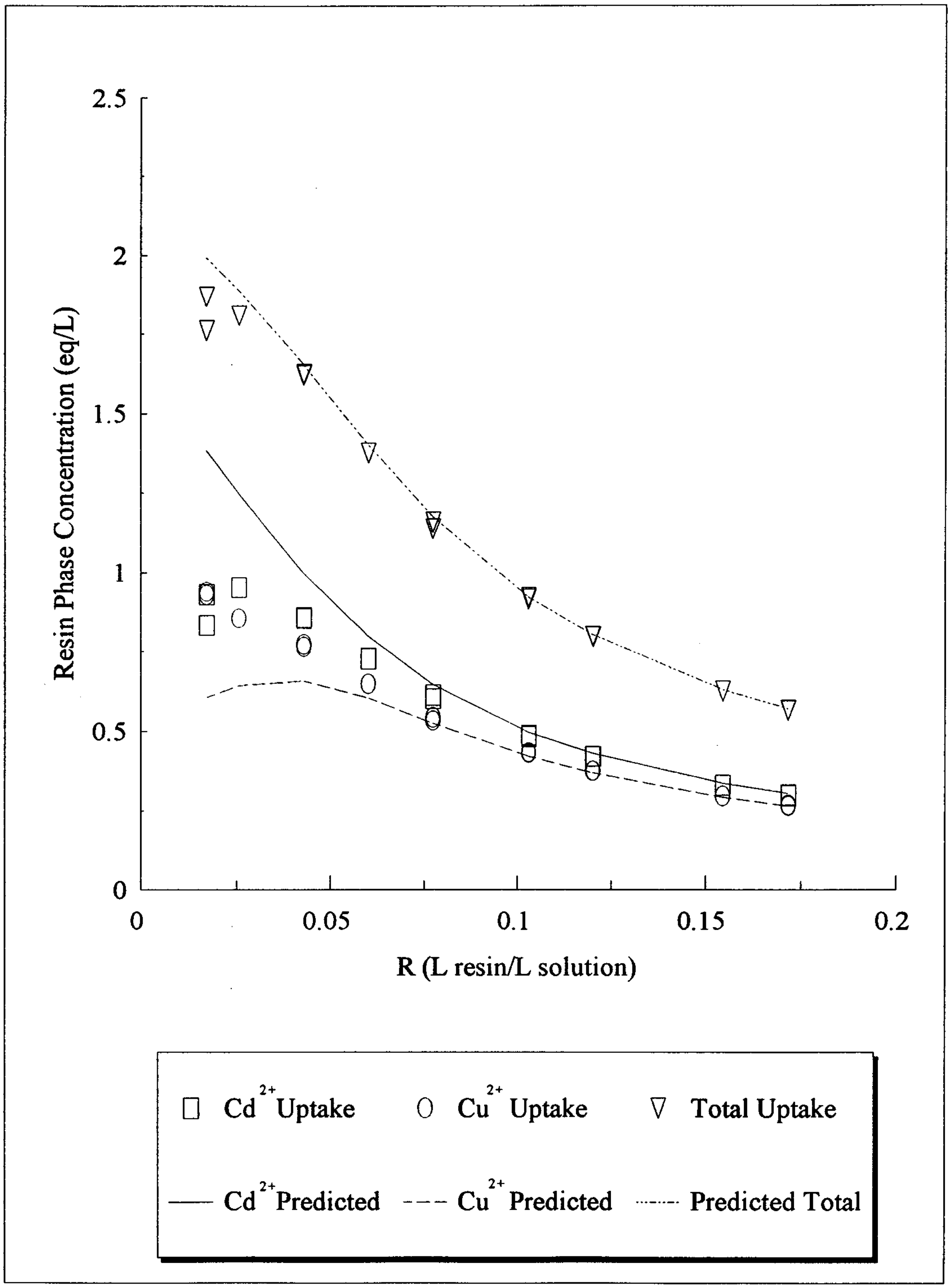


Figure 4.12: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Cu^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.05N; Cu^{2+}, 0.05N.

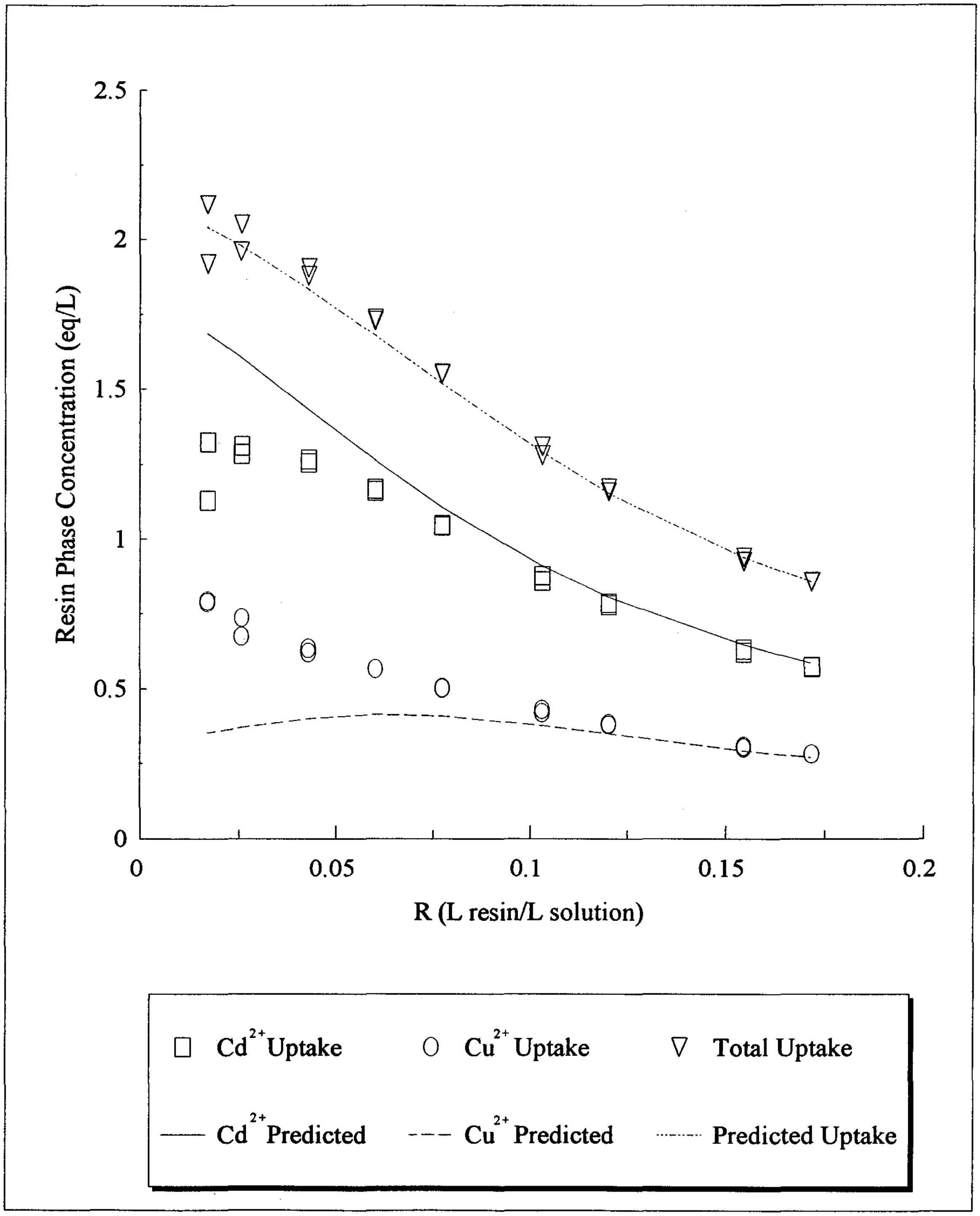


Figure 4.13: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Cu^{2+}-Na^+. Initial solution concentrations: Cd^{2+}, 0.1N; Cu^{2+}, 0.05N.

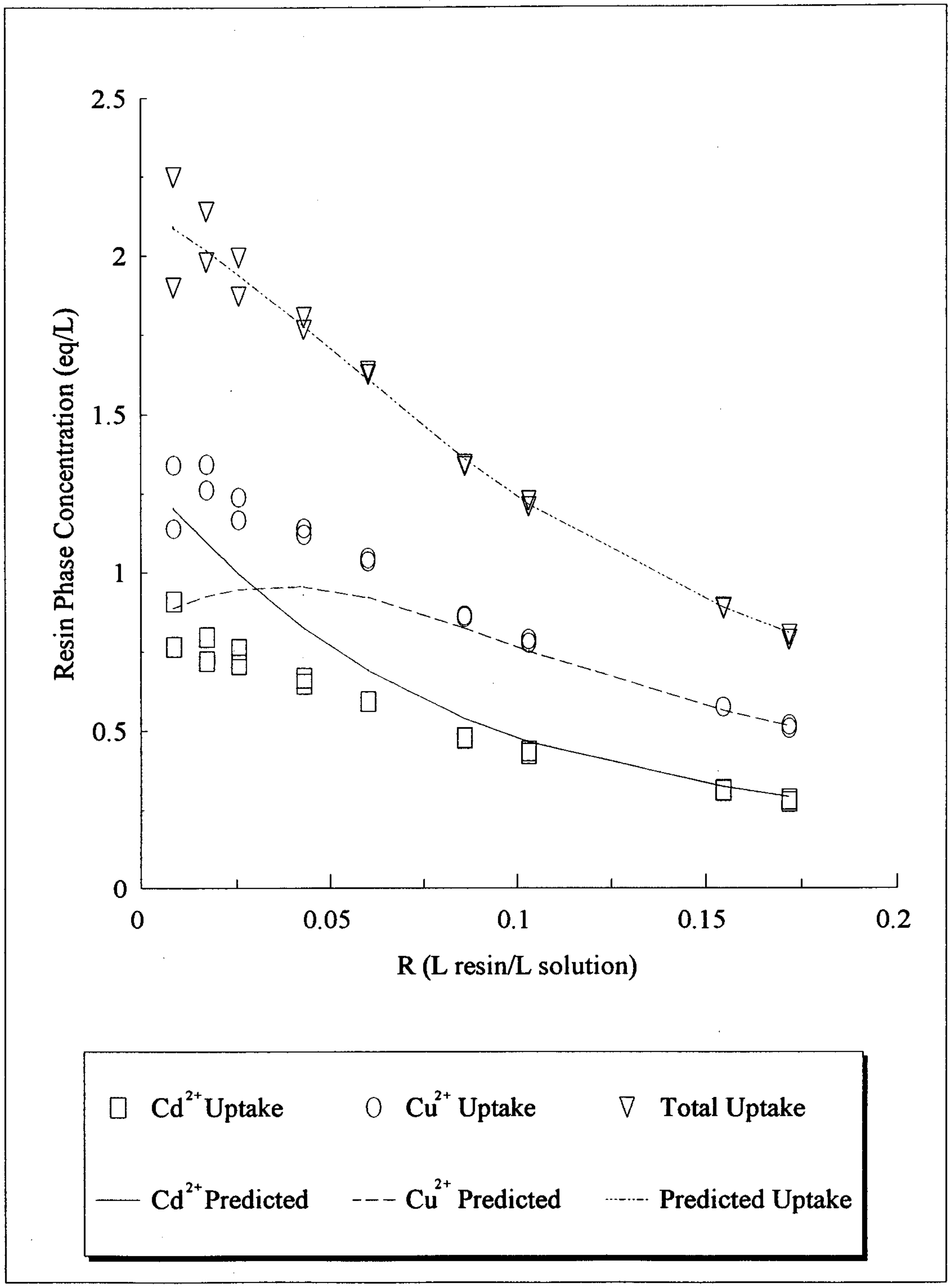


Figure 4.14: Resin phase concentration vs. resin/solution ratio R for the system Cd^{2+}-Cu^{2+}-Na^{+}. Initial solution concentrations: Cd^{2+}, 0.05N; Cu^{2+}, 0.1N.

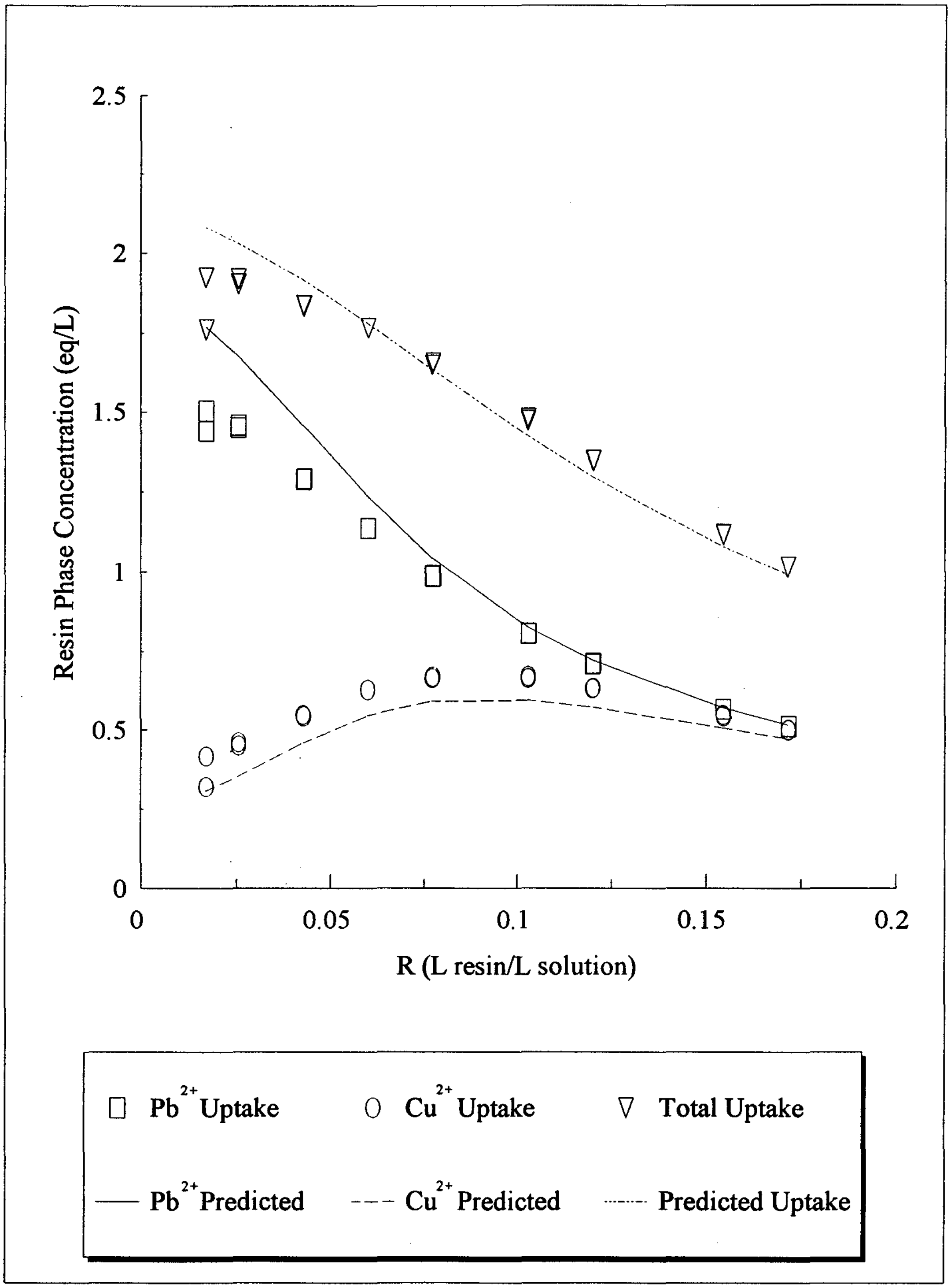


Figure 4.15: Resin phase concentration vs. resin/solution ratio R for the system Pb^{2+}-Cu^{2+}-Na^{+}. Initial solution phase concentrations: Pb^{2+}, 0.1N; Cu^{2+}, 0.1N.

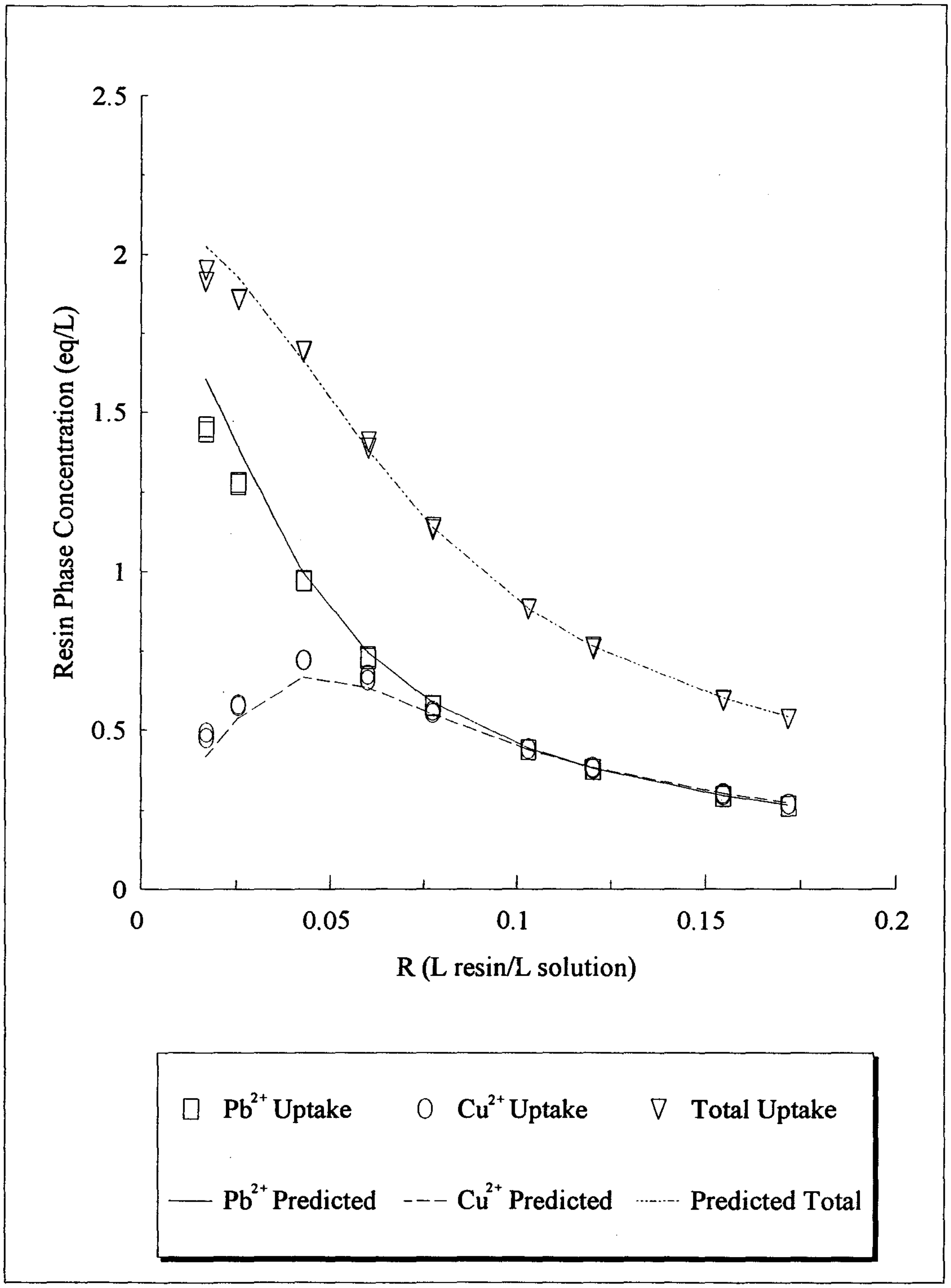


Figure 4.16: Resin phase concentration vs. resin/solution ratio R for the system Pb^{2+}-Cu^{2+}-Na^{+}. Initial solution concentrations: Pb^{2+}, 0.05N; Cu^{2+}, 0.05N.

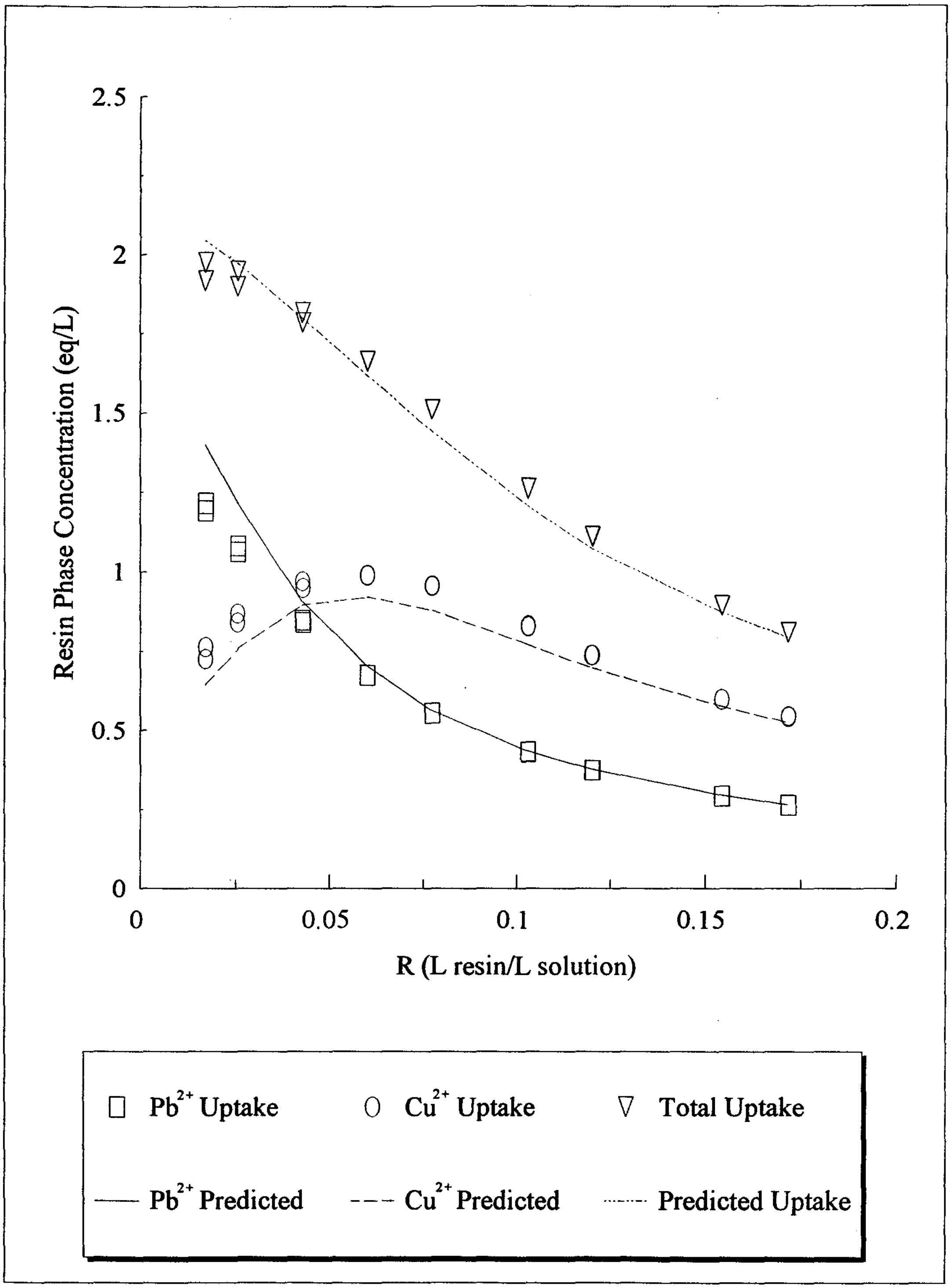


Figure 4.17: Resin phase concentrations vs. resin/solution ratio R for the system Pb^{2+}-Cu^{2+}-Na^{+}. Initial solution concentrations: Pb^{2+}, 0.05N; Cu^{2+}, 0.1N.

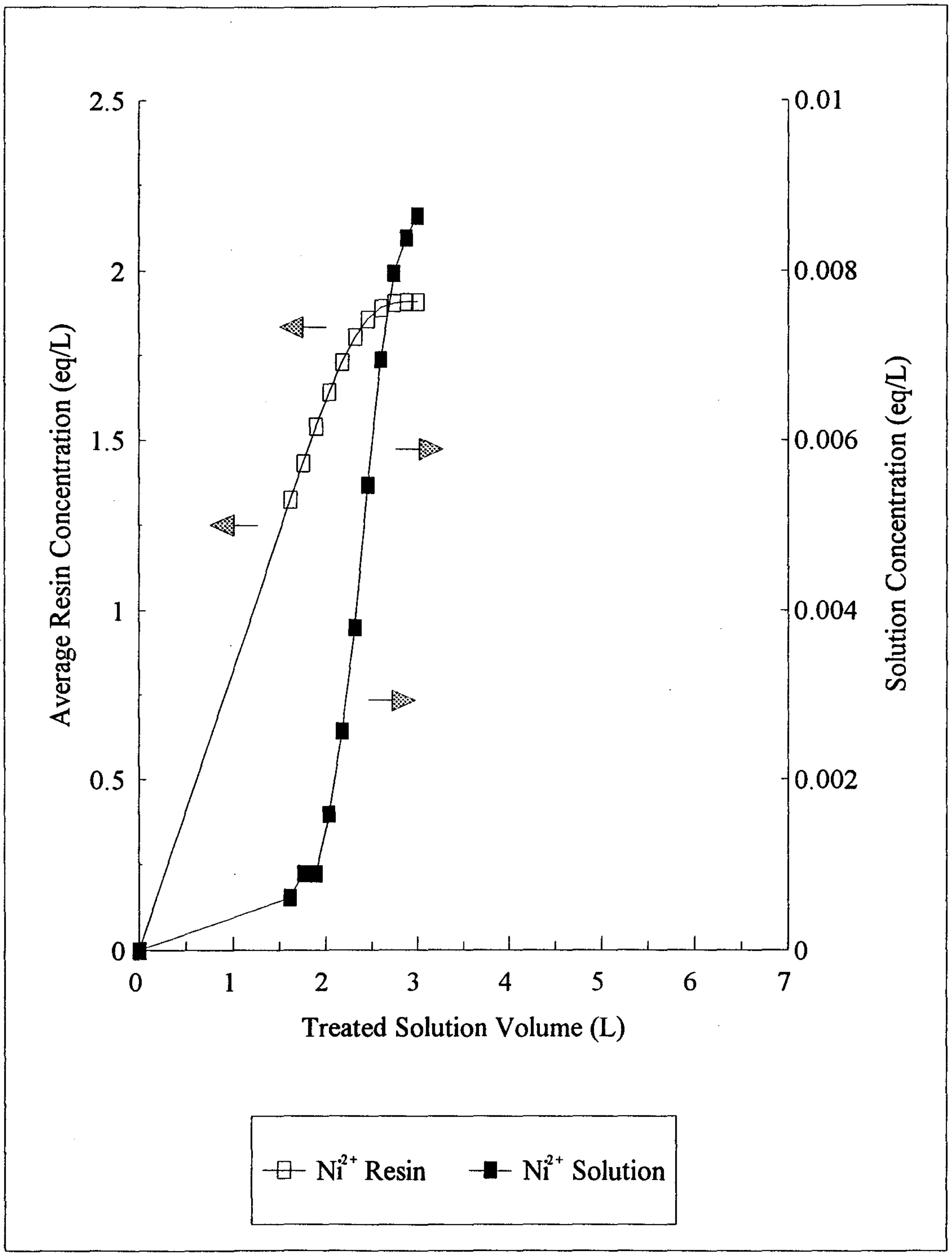


Figure 4.18: Resin concentration vs. treated solution volume and breakthrough curve for a packed bed with initial solution concentration: Ni^{2+}, 0.0085N, and flow rate, 9.3 mL/min.

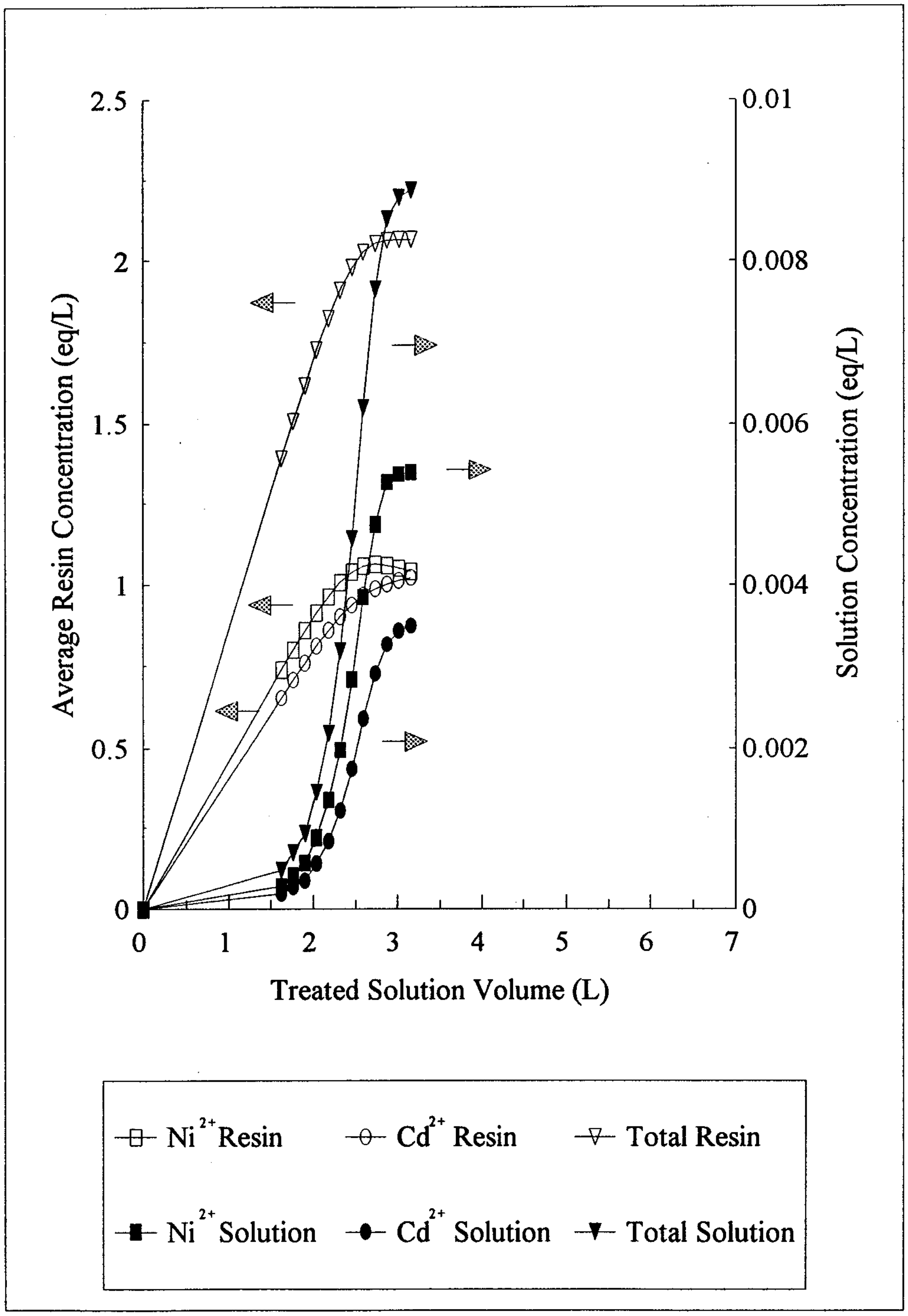


Figure 4.19: Resin concentration vs. treated solution volume and breakthrough curve for a packed bed with initial solution concentrations: Ni^{2+}, 0.0047N; Cd^{2+}, 0.0041N, and flow rate, 9.5 mL/min.

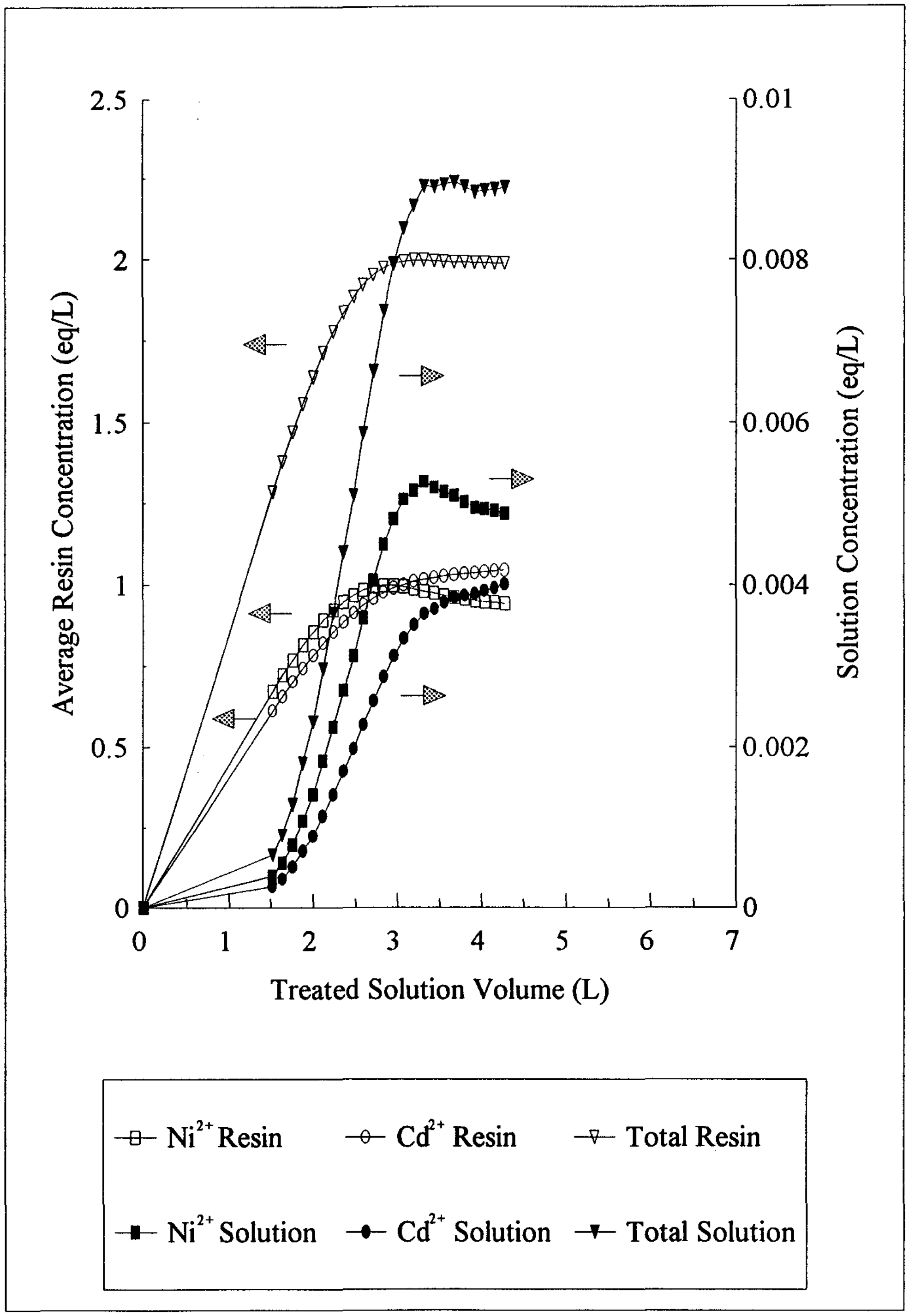


Figure 4.20: Resin concentration vs. treated solution volume and breakthrough curve for a packed bed with initial solution concentrations: Ni^{2+}, 0.0046N; Cd^{2+}, 0.0042N, and flow rate, 5.8 mL/min.

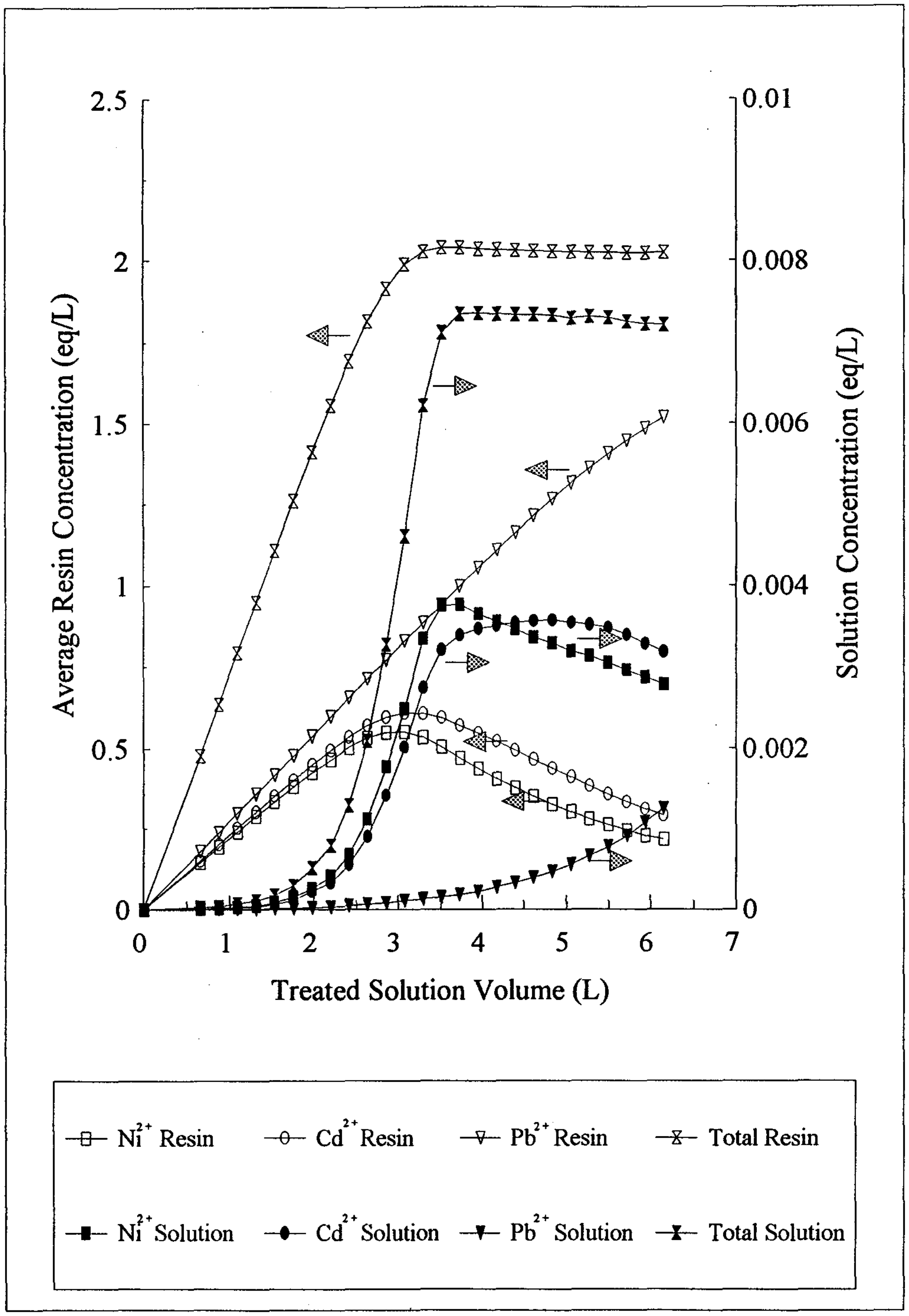


Figure 4.21: Resin concentration vs. treated solution volume and breakthrough curve for a packed bed with initial solution concentrations: Ni^{2+}, 0.0022N; Cd^{2+}, 0.0023N; Pb^{2+}, 0.0027N, and flow rate, 8.5 mL/min.

CHAPTER 5: DISCUSSION

5.1 Binary Equilibrium

The determination of binary selectivity coefficients and resin capacities was accomplished by plotting $(C^o_A-C_A)/R$ vs. $(C^o_A-C_A)^{3/2}/(RC_A)^{1/2}$ according to Equation 2.9 as developed in Section 2.2. Figures 4.1-4.5 show the experimental data and the best fit linear regression lines. The data for these systems are summarized in Table 4.1 and the raw data are presented in Appendix B. All graphs follow the predicted linear behaviour as proposed in Section 2.2, with limited experimental scatter. The largest confidence interval for the calculated selectivity coefficients was 36% for Zn^{2+}, and the smallest was 16% for Ni^{2+}.

Vasquez et al. (1986) studied both the Na^+-Ni^{2+} and the Na^+-Cu^{2+} systems on Lewatit resins, which are similar to the resins studied here in that both resins are of the strong acid type. The equilibrium constants as defined in Equation 1.2 (not the selectivity coefficients as defined by Equation 2.2) determined for the Na^+-Ni^{2+} system ranged from 3.0-4.3 and the Na^+-Cu^{2+} constants ranged from 2.2-3.8 for a total solution concentration of 0.1 N. To compare the values obtained in this study, it is necessary to first convert the selectivity coefficients to the same units used by Vasquez et al. (1986), who calculated the equilibrium coefficients using resin phase equivalent fraction instead of concentration. Performing this conversion, it is found that the selectivity coefficient for the Na^+-Ni^{2+} system is 3.5 and that for the Na^+-Cu^{2+} system is 3.3, both giving excellent agreement with the values reported by Vasquez et al. (1986).

Allen et al. (1989) have tabulated equilibrium constant data from several sources, including the study by Vasquez et al. (1986). The only additional equilibrium constant of interest is that for the Na^+-Zn^{2+} system, with a value of 4.5, which does not agree well with the calculated value of 3.0 determined for these experiments (after conversion to resin phase equivalent fractions). It should be noted that although the data for the Na^+-Zn^{2+} system do follow the prediction of a straight line, the calculated capacity is almost 25% lower than the average for the other four systems, indicating a possible inconsistency. There is also a fair amount of scatter in the individually calculated values for K when the units of Allen et al. (1988) are used.

The capacities calculated from the data for this resin show a fair amount of discrepancy, with the highest being 1.5 times the lowest. The possible reason for the difference in the capacity in relation to the Zn^{2+} ion has already been noted. The Ni^{2+} ion has the smallest ionic radius (see Appendix D for a list of ionic radii) of the five ions. This could make more sites available to that particular ion, increasing the apparent capacity for Ni^{2+}. It could also affect the selectivity for Ni^{2+}, explaining why it appears to be out of order with the other ions, which all show an increase in selectivity corresponding to an increase in ionic radius. The Na^+ ion has a larger radius that the Ni^{2+} ion, which may mean that there are some sites on the resin still in the hydrogen form for the original production of the resin which are inaccessible to the Na^+ ions, but accessible to the Ni^{2+} ions. This would allow the Ni^{2+} ions to exchange with the hydrogen ions, affecting the equilibrium between Na^+ and Ni^{2+}, without being accounted for. This results because the Na^+ ions that are displaced from the resin are being determined by difference, and not by measurement.

Another possible source of error in the apparent capacity is the presence of the diffuse double layer. This diffuse layer is of greater concentration than the bulk solution, but of lower concentration than the Stern layer which is the layer of ions directly next to the resin particle (even within the pores) which are considered to have exchanged onto the resin. The diffuse layer would account for more uptake of ions by the resin than were actually exchanged. Because of the experimental procedures employed for separating the solution from the resin, the diffuse layer would not have been included in the solution separated from the resin. This may account for the fact that the average capacity value obtained of 2.17 eq/L differs by 10% from the value of 2.0 eq/L reported by the Dow Chemical Company (1996).

According to Kennedy (1980), there is the possibility that anionic complexes may form (speciation) between the metal ions and the co-ions (sulphate and nitrate). Of the five metal ions studied, the only ion that may show this speciation effect is the Cu^{2+} ion when the concentration of sulphate exceeds 0.05M. The binary equilibrium experiment for Cu^{2+} had an initial concentration of 0.076N, which equates to 0.038M, below the specified limit for speciation. In all batch experiments conducted (including ternary), it was assumed that no anionic complexes were formed and all cationic species were of the 2+ form.

5.2 Ternary Equilibrium

5.2.1 Copper-Nickel

Only one batch experiment was carried out for the Cu^{2+}-Ni^{2+} system because the two ions are very close in both selectivity and size (see Appendix D for ionic radii). The primary goal of this single experiment was to determine if using the capacity value of 2.17 eq/L as opposed to the experimentally determined value of 2.41 eq/L for Ni^{2+} would cause significant errors in the prediction of the final equilibrium conditions. As mentioned previously, it was assumed that no speciation effects occurred.

Figure 4.6 shows that there appear to be no problems associated with using the lower value of the capacity, as the predicted concentrations (based on the theory developed in Section 2.3) are in excellent agreement with the experimental values except for a few cases around the R values of 0.02-0.03 L resin/L solution for the Ni^{2+} values. These experimental points seem to be in conflict with the trend of the other data surrounding them, indicating possible experimental error.

5.2.2 Cadmium-Nickel

Four batch experiments were performed for the Cd^{2+}-Ni^{2+} system, with initial solution concentrations set at either approximately 0.1 N or 0.05 N for both metals and the four experiments covering all possible combinations.

The first to be examined will be the experiment where both metals have an initial concentration of approximately 0.1 N. Given the difference in selectivity coefficients between the two ions (0.826 vs. 1.98) and the assumption that there is no third ion interaction, the predicted equilibrium concentrations should show a definite separation, as indicated by the lines on Figure 4.7. This is obviously not what occurs though, as the two experimentally determined concentrations remain fairly close together, indicating the presence of third ion interactions.

For this case, it is found that the Ni^{2+} has been taken up in greater amounts than predicted and the Cd^{2+} in lesser amounts. One possible explanation, based solely on thermodynamic principles is that the high concentrations reached in the resin phase have large effects on the activity coefficients of the ionic species, causing a shift in the equilibrium position. Were this the only cause however, it should also be present at the higher resin ratios, as the total and individual ionic concentrations decrease by less than 50%, which should not be enough to cause large changes in the activity coefficient. The counter to this reasoning is that the predicted concentrations converge to within 0.1N of each other, leaving only a narrow range for the experimental concentrations to lie within. This point will be addressed later.

Another possible explanation for the experimental behaviour is based on a kinetic influence. Given that the Ni^{2+} is the smaller of the two ions, it would be natural to expect it to have a greater rate of diffusion both within the resin particle and in the bulk solution when all other factors are equal. This means that the Ni^{2+} ions will reach the exchange sites before the Cd^{2+} ions and exchange with the Na^+ ions. When the Cd^{2+} ions reach these sites, they then exchange for some of the Ni^{2+} ions, but not as many as would be predicted by the binary selectivity coefficient. This preference of an ion exchange resin for an ion already on the resin has been noted by both Nachod (1949) and Helfferich (1962).

Gregory (1976) points out that the resin, upon first coming into contact with the solution, will be devoid of both new competing species. The initial stages of the exchange will occur for each ion as though the other were not present, as only a small portion of the exchange sites are in use. As the exchange proceeds and the uptake on the resin increases, the competition for the sites between the two competing species will also increase, slowing the uptake of the less preferred ion, but as previously mentioned here, not necessarily displacing all the ions to the predicted equilibrium concentrations.

At higher resin ratios (corresponding to lower ionic uptake), the experimentally determined pseudo-binary selectivity coefficient for Ni^{2+} appears to be converging toward the binary selectivity coefficient previously determined. This would limit the amount of Ni^{2+} exchanged by the resin in the early stages of the experiment, allowing more Cd^{2+} to be exchanged. This occurs as the predicted Ni^{2+} represents a greater percentage (45% vs. 31%) of the predicted total uptake, meaning that as the Ni^{2+} ion is exchanged first, it will not overshoot its predicted concentration by as much before it reaches its maximum value and is subsequently partially displaced by the incoming Cd^{2+} ion. At lower resin ratios, the predicted Ni^{2+} represents only 31% of the total ionic uptake and the Ni^{2+} will overshoot this percentage significantly before it reaches its own temporary equilibrium and partial displacement by the Cd^{2+} begins.

For the case where both Cd^{2+} and Ni^{2+} have a low initial solution concentration (see Figure 4.8), again the predictions for both species show excellent agreement at the higher resin ratios. The Ni^{2+} predictions continue to show excellent agreement even at lower resin ratios, but the Cd^{2+} predictions and consequently the total predicted uptake show significant error.

The most likely explanation for the decrease in the experimental uptake of the Cd^{2+} would seem to be a steric hindrance effect. The Ni^{2+} enters the resin first as in the previous case and exchanges for the Na^+. As the Cd^{2+} diffuses into the resin, it displaces some of the Ni^{2+}, but the remaining Ni^{2+} and the Cd^{2+} now on the resin act to prevent access to some of the exchange sites, effectively reducing the capacity of the resin. The thermodynamic driving force is not strong enough to overcome this effect, resulting in the observed decrease in the Cd^{2+} uptake. Experimental error can be discounted because if it were present, then there should be a more marked drop in the Ni^{2+} uptake as well, which does not occur.

For the case of an initial Cd^{2+} concentration of approximately 0.1N and Ni^{2+} of 0.05N (see Figure 4.9), again there is excellent agreement at the higher levels of resin ratios. As the ratio decreases below 0.08, the experimental points start to diverge slightly from the predicted values, but not as severely as in the first case and again there is excellent agreement with the overall predicted uptake, except at low values of R (see below).

The fact that the departure of the experimentally observed values from the predicted values is less severe than the first case would appear to support the statement that there is a diffusional kinetic effect influencing the measured uptake. For this case, the Cd^{2+} has a higher solution concentration than the Ni^{2+}, which would give it a corresponding increase in its diffusional characteristics over the first case where the initial solution concentrations are almost equal.

The two sets of data for the $0.01<R<0.03$ range again appear to show the decrease in uptake noted for the previous case. Closer examination of the data indicates that they follow the trend of increasing uptake present with the previous data, but are shifted down by approximately 15%. This apparent discontinuity happens to coincide with a change in the dilution factor of the analyzed samples, indicating a possibility that the apparent errors in these data are due to experimental error.

The final case for the Cd^{2+}-Ni^{2+} solution has an initial concentration for Cd^{2+} of approximately 0.05N and for Ni^{2+} approximately 0.1N (see Figure 4.10). Taking into account the initial concentrations and the hypothesis that there is a diffusional kinetic effect occurring, it is to be expected that the predicted concentrations for this case would show the greatest error. However, this is not the case, as the error is almost the same as that observed for the first case (Figure 4.7).

The Ni^{2+} data in Figure 4.10 show reasonable agreement until the same effect that was observed in Figure 4.8 occurs again below the resin ratio of 0.03. The Cd^{2+} data show good agreement until R drops below 0.1, where the experimental Cd^{2+} uptake begins to fall away from the predicted value. This should be due to the hypothesis already presented.

Another interesting feature of Figure 4.10 is that both the experimental uptakes are below their respective predicted values. This has occurred in only a few isolated instances in the previous three cases, indicating the possibility of experimental error. The experimental error here appears to be most likely in the calibration of the analyzer.

Another possibility to be noted is the previously mentioned diffuse layer. As was the case for the binary experiments, the diffuse layer was not separated from the resin after the systems had equilibrated. As the concentrations of the individual ions in the diffuse layer cannot be predicted, this adds another possible source of error to the experiments.

5.2.3 Cadmium-Copper

The same four experiments were performed for Cd^{2+}-Cu^{2+} as for Cd^{2+}-Ni^{2+} (see Figures 4.11-4.14) and they will be discussed in the same order. If the assumption is made that ionic radius is the only contributing factor to the diffusion of an ion other than concentration, it would be expected that the Cd^{2+}-Cu^{2+} experiments would show less error than the Cd^{2+}-Ni^{2+} case because of the larger radius of the Cu^{2+} ion in comparison to the Ni^{2+} ion. As will be seen, this does not occur, indicating the possibility of other effects being present.

For the first case (Figure 4.11), the same trends occur in the experimental data that occurred in the Cd^{2+}-Ni^{2+} case (Figure 4.7). For this experiment, although the binary data predict even greater separation of the two uptakes over the Cd^{2+}-Ni^{2+}, the opposite is found to occur. At low resin ratios, the experimental uptake of the two ions is within 5% at one point, despite the prediction of a 60% difference. The experimental total uptake of ions is again in excellent agreement with the predicted value.

For the second case (Figure 4.12), again there is excellent agreement between the experimental observations and the predicted values at resin ratios above 0.06. These data do not show the same severe drop in overall uptake, nor the drop in Ni^{2+} uptake that occurs in Figure 4.8. The same decrease in uptake is also predicted for the Cu^{2+} by the binary data. It does show the same drop in Cd^{2+} uptake seen in Figure 4.8 and likely for the same reasons as stated previously.

The third case (Figure 4.13) also shows good agreement for R values above 0.06. Below this value the trend is the same as that observed in the corresponding experiment (Figure 4.9) for Cd^{2+}-Ni^{2+} if the apparent experimental error were accounted for. As in the first case, the error is greater than that found in the Cd^{2+}-Ni^{2+} system.

The final Cd^{2+}-Cu^{2+} case (Figure 4.14) has the same good agreement for the higher values of R and also shows the larger discrepancies for the lower values of R.

The uptake of Cu^{2+} does appear to be leveling, although it does not appear to be decreasing as predicted.

For three of the four cases (Figures 4.11-4.14), the total uptake did not show the same drop off that was observed at lower values of R for the Cd^{2+}-Ni^{2+} system and in the fourth, the drop off was very slight. This may indicate that the Cd^{2+}-Ni^{2+} system (Figures 4.7-4.10) has some other non-ideal effect disturbing the thermodynamic equilibrium.

5.2.4 Lead-Copper

The final ternary system studied was Pb^{2+}-Cu^{2+}. Only three runs (Figures 4.15-4.17) were performed for this system due to resin constraints. The experiment omitted was with initial concentrations of approximately 0.1N for Pb^{2+} and 0.05N for Cu^{2+}. The large difference in the ionic radii would seem to indicate that there should be a much greater error in the predictions than in any of the previous cases.

For the first run (Figure 4.15), there is reasonable agreement between all experimental and predicted uptakes, except for the Pb^{2+} uptake at low levels of R. This is the same trend as observed earlier in Figure 4.8 and can likely be attributed to the same cause.

The second run (Figure 4.16) shows the best overall agreement between the experimental and predicted uptakes of any of the runs. There appears to be only a slight decrease in the Pb^{2+} uptake at low levels of R. This is the most dilute system in both Pb^{2+} and Cu^{2+}, and of the three runs for this system (Figures 4.15-4.17) would be expected to behave the most ideally.

The final case (Figure 4.17) also shows good agreement except for the slight drop off of Pb^{2+} uptake at low R values.

The errors between the experimental and predicted uptakes, expected from the size difference of the ions obviously do not occur for this system. The primary reason that this system was chosen for the ternary runs was the large difference between the values of the previously determined binary selectivity coefficients. The most likely explanation for the excellent agreement observed for this system lies in this difference.

As previously mentioned, the hypothesis for the observed errors in the previous systems is that the resin tends to favour ions that have *already* exchanged onto the resin over those trying to exchange. The smaller ions (assumed to be the more mobile ions) are able to reach the exchange sites more quickly than the large ions. Once these smaller ions have reached the active sites and exchanged with the Na^+ ions initially there, the selectivity coefficient for these new ions effectively increases, making it more difficult for them to be dislodged by the incoming larger ions than would be suggested by the difference in the binary selectivity coefficients. This appears to have been the predominant effect occurring in the Cd^{2+}-Ni^{2+} and the Cd^{2+}-Cu^{2+} systems.

In the Pb^{2+}-Cu^{2+} system, the difference in the binary selectivity coefficients is significantly higher than in the other two systems. This difference means that the resin much prefers the Pb^{2+} ions over the Cu^{2+} ions. In this case, this preference appears strong enough to overcome the kinetic effects due to ionic radii so that the Pb^{2+} can exchange for the Cu^{2+} ions and reach uptake levels very close to those predicted from the binary selectivity coefficients.

Table 5.1: Summary of Ternary System Discussion

System	Summary
Cu^{2+}-Ni^{2+}	Good agreement, possible experimental error.
Cd^{2+}-Ni^{2+}	Significant errors in predictions at low values of R, indicative of third ion interactions. These interactions are assumed to be kinetic in nature. The smaller ion (Ni^{2+}) has a higher uptake than predicted and the larger (Cd^{2+}) has a lower uptake than predicted. This is assumed to be due to the fact that the Ni^{2+} ions can reach the exchange sites faster and once exchanged, are harder to dislodge.
Cd^{2+}-Cu^{2+}	Same trends as previous system.
Pb^{2+}-Cu^{2+}	Good agreement, large difference in selectivity coefficients appears to overcome kinetic effects of previous two systems.

5.3 Packed Bed

5.3.1 Basis for Showing Results

The results for the packed bed experiments are presented in Figures 4.18-4.21. Each graph contains two sets of data, one for the average resin phase concentration, represented by the open symbols and the left axis, and one for the outlet solution phase concentration, represented by the filled symbols and the right axis. The average resin phase concentration is calculated as the total uptake/resin bed volume. It is displayed in this manner for easier comparison to the results from the batch experiments. The solution phase concentration is displayed for the purpose of demonstrating breakthrough curves and exchange/reaction zones.

The average resin phase concentration is used to simplify the calculation and presentation of the results. The entire bed is not at the concentration level depicted. Instead, the top part of the bed is completely loaded, while the bottom part of the bed is almost entirely still in the Na^+ form. Somewhere along the length of the bed is the exchange zone, where the ion exchange reaction is occurring. A narrow exchange zone is preferable for operation because more of the bed can be used before the concentration in the effluent reaches a critical point and the column must be taken off line for regeneration. For research work, the experiment is continued past this point until the entire column is completely loaded so that certain effects can be observed.

5.3.2 Discussion of Packed Bed Results

Four exploratory experimental runs were conducted with packed beds. The operating conditions for all four runs are presented in Table 4.2 and the graphs for each run are given in Figures 4.18-4.21. The experiments were conducted so that the initial total solution concentrations were approximately equal in all runs and the concentrations of the individual ions were approximately the same within each run. For all four experiments, the measured final capacity of the resin was approximately 2.0 eq/L, which is within 10% of the capacity determined from the batch experiments.

The first experiment (Figure 4.18) was conducted with only Ni^{2+} in solution at an initial concentration of 0.0085 eq/L. The rate of change of the resin phase concentration is almost constant until the resin is within 15% of its maximum uptake, indicating almost complete uptake of Ni^{2+} from the feed solution, which is supported by the solution phase concentration which remains low until this point is reached. At this point the concentration begins to level off until it reaches a value of about 2.0 eq/L, the solution phase concentration increases rapidly or 'breaks through' and the resin is fully loaded or converted to the Ni^{2+} form. The fact that the rate of change of the concentration is almost constant for the entire run indicates that the flow rate is low enough to give a narrow, well defined reaction zone where the ion exchange is occurring, as opposed to a reaction zone that is stretched out over a broader volume of the bed. This narrow zone gives the sharp breakthrough curve observed, which is operationally preferable over a gradual breakthrough curve which would be observed with a high flow rate.

The second experiment (Figure 4.19) had both Ni^{2+} and Cd^{2+} in solution with respective initial concentrations of 0.0047 eq/L and 0.0041 eq/L. The data representing the total ionic concentration show the same characteristics as for the first experiment. This is to be expected because both the total solution concentration and the flow rate are close to those in the first experiment. The rate of change of the concentration of both ionic species is almost constant again until about 85% of the total capacity of the resin is used and the solution phase concentration remains almost at zero. At this point, the Cd^{2+} uptake starts to level off and the Ni^{2+} uptake goes through a maximum before decreasing. The initial part of the experiment (before the concentrations start to level off) follows the explanation of Gregory (1976) presented in Section 5.2.2, where the initial exchange will occur for both species as though the other were not present. This means that the Ni^{2+}, which has a higher solution concentration, will be exchanged in greater amounts than the Cd^{2+}. As the resin becomes exhausted (all the Na^+ has been exchanged for Ni^{2+} and Cd^{2+}), the preference of the resin for Cd^{2+} over Ni^{2+} begins to take effect and some of the Ni^{2+} is displaced from the resin. The experiment was terminated before an equilibrium position was reached because of time constraints and a lack of online analysis, so no comments can be made regarding that aspect.

The third experiment (Figure 4.20) had essentially the same initial solution concentrations as the second experiment, but with a much lower flow rate to determine if it would have any effect. The same trends are seen as in the previous experiment. Beyond the point where the Cd^{2+} curve crosses over the Ni^{2+} curve, the concentration of Cd^{2+} appears to be very slowly increasing while the concentration of the Ni^{2+} appears to be slowly decreasing. This is confirmed by the solution phase concentrations, neither of which have reached their respective initial concentrations, which is the requirement for the column to be at equilibrium with the feed.

The binary selectivities determined experimentally for these two ions (see Table 4.1) differ by a factor of 2.4, indicating a stronger preference for Cd^{2+} than is observed in the column. The ternary experiments involving the Cd^{2+}-Ni^{2+} system, in particular the runs in Figures 4.7 and 4.8 where the initial solution concentrations of the two ions are approximately equal, would seem to indicate that the final equilibrium concentrations in the resin would differ only slightly, with Cd^{2+} being slightly favoured. This is consistent with the column data in Figure 4.20. The change in flow rate appeared to have no significant effect on the experiment besides increasing the run time.

The final experiment (Figure 4.21) involved all three ionic species used in the packed bed experiments, with Pb^{2+} having a slightly higher initial concentration than the other ions and the total solution concentration being slightly lower than the previous three experiments. Here again the total concentration and the concentrations of the individual ionic species change at an almost constant rate until the resin is about 85% exhausted. At this point, the total concentration begins to level off to a value of about 2.0 eq/L. The concentrations of Cd^{2+} and Ni^{2+} go through maxima and begin to decrease and the concentration of Pb^{2+} continues to increase. The overall solution phase concentration shows a very sharp breakthrough point, and the Ni^{2+} and Cd^{2+} show fairly sharp breakthroughs, but the Pb^{2+} appears to be breaking through very gradually, indicating a broad reaction zone for the loading of the resin with Pb^{2+} and a much higher affinity of the resin for Pb^{2+}. This would seem to indicate that the Pb^{2+} is not exchanging as quickly as the other ions, possibly due to slower diffusion, supporting the hypothesis made in Section 5.2.2 that the larger the ion, the lower the rate of diffusion to the exchange sites.

The significantly higher binary selectivity coefficient for Pb^{2+} (over seven times higher than for Ni^{2+} and over three times higher than that for Cd^{2+}) indicates that the resin should strongly prefer Pb^{2+} over the other two ions and this preference is observed as the Pb^{2+} displaces the Cd^{2+} and Ni^{2+} from the resin. The difference in selectivities between Ni^{2+} and Cd^{2+} can be seen as the Ni^{2+} is displaced more quickly from the resin than the Cd^{2+} (the resin concentration of the Ni^{2+} decreases more rapidly initially). The rate of change of the concentration of the Pb^{2+} appears to be decreasing only slightly, and based on the ternary equilibrium runs (Figures 4.15 and 4.16) between Pb^{2+} and Cu^{2+} (which is close to Ni^{2+} in selectivity) it would be expected that a large difference between the final equilibrium concentrations of the three heavy metal ions would result. This difference was still increasing at the end of the experiment shown in Figure 4.21.

The diffuse layer mentioned in section 5.1 may also account for some of the discrepancies observed in the packed bed experiments. Because of the difference in total solution volume (several litres for the packed bed as opposed to only 50 mL for the batch experiments), the diffuse layer may have a more noticeable effect on the concentrations determined in the batch experiments. Also, in the packed bed experiments, the concentration of heavy metal ions in the bulk solution remained high at the end of the experiment, whereas it was correspondingly lower for the batch experiments, providing another difference in conditions affecting the diffuse layer.

CHAPTER 6: CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

The major conclusions of this research are presented as follows:

1. The binary selectivity coefficients and resin capacities were determined and summarized in Table 4.1 for the five ions under consideration. Capacities are approximately the same for each ion, with an average value of 2.17 for the ions used in the ternary systems. The selectivity coefficients vary from 0.694 for Cu^{2+} to 5.95 for Pb^{2+}.
2. The ternary systems were examined and it was found that the binary data could be used for calculating the ternary system equilibria when the selectivity coefficients of the two ion involved were either almost equal (as for Cu^{2+}-Ni^{2+}) or differed by a factor of 5 or more (as for Pb^{2+} - Cu^{2+}).
3. For ternary systems where the selectivity coefficients did not fit the above criteria, the presence of third ion interactions was noted and these interactions were hypothesized to be kinetic in nature, but it was also noted that the diffuse layer may have had an effect.
4. The proposed method of data analysis is very simple compared to that used in modern literature and provided comparable results except for the case of Zn^{2+}.
5. The capacity of the resin determined in the packed bed experiments agreed to

within 10% of the capacity determined in the batch experiments.

6. The order of selectivity between the five heavy metals and the trends for equilibrium positions observed in the ternary systems were consistent with results from the packed bed experiments.

6.2 Recommendations

The following recommendations are made for continuing the research in this area:

1. Binary parameters for other heavy metals should be determined to provide a better range of values for ternary systems.
2. Kinetic data should be obtained for the heavy metals of interest so rates of diffusion can be calculated.
3. Ternary system with a range of selectivity coefficients should be examined to determine if there is a correlation between rates of diffusion, selectivity coefficients and equilibrium position.
4. The same binary and ternary systems should be tested with other types of resin to determine effects of resin type.
5. Packed bed experiments with the present systems and other systems with different total solution concentration and individual ion concentrations should be run for industrial interests.

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APPENDIX A: COMPUTER CODE FOR TERNARY SYSTEMS

```
60 REM Output string for equilibria conditions
65 A$= ' #.##### #.##### #.#####  #.####   #.###   #.###   #.###'
110 CCO=0.10801; REM Initial concentration for ion C
115 CPO=.09915; REM Initial concentration for ion P
117 print 'BATCH ION EXCHANGE OF ION C AND ION P WITH
        SODIUM RESIN'
118 print 'INITIAL CONCS.';CCO;' AND ';CPO;' eq/L RESPECTIVELY'
120 print 'FINAL CONCS GIVEN BELOW IN eq/L'
124 print ' R     Aq.C    Aq.P    Aq.Na    Res.C  Res.P  Res.Na'
126 KC=1.98; REM Selectivity coefficient for ion C
128 KP=0.826; REM Selectivity coefficient for ion P
130 CRNO=2.17; REM Initial concentration of sodium on resin (capacity of resin)
200 for R=0.01 to .18 step .01; REM For/next loop for range of R  (resin/solution
        ratio)
 205 f=0; REM Flag for determining convergence
 210 X=.001; REM Equivalent fraction of sodium remaining on resin
  215 REM Begin iteration for calculating equilibrium concentrations
  220 CC=CCO/(1+KC*X^2/(R*(1-X)^2)); REM Equilibrium concentration of C
  230 CP=CPO/(1+KP*X^2/(R*(1-X)^2)); REM Equilibrium concentration of P
  240 CN=CCO+CPO-(CC+CP); REM First calculation of sodium concentration
  250 CNB=R*CRNO*(1-X); REM Second calculation of sodium concentration
  260 if CN<(CNB*1.0001) and CN>(CNB/1.0001) then f=1; REM Comparison
        of calculated sodium concentrations to determine convergence
  270 if f=1 then print using A;R,CC,CP,CN,(CCO-CC)/R,(CPO-CP)/R,
        CRNO-CN/R; REM Output of equilibrium concentrations
  275 if CN<CNB then X=X*1.01; REM Adjustment of parameter X
  277 if CN>CNB then X=X*.999; REM Adjustment of parameter X
 280 if f=0 then goto 220; REM End of iteration loop
310 next R; REM End of for/next loop
```

The initial concentrations (lines 110&115) and selectivity coefficients (lines 126&128) are entered by the user before each case is calculated. The capacity of the resin can be adjusted by changing the value in line 130. The range of R values calculated can be changed in line 200. The convergence criteria can be set by changing the values in line 260.

APPENDIX B: RAW DATA FOR BINARY AND TERNARY SYSTEMS

Raw data for binary system Ni^{2+}-Na^{+}.

Eq. Wt= 29.35 Dens. Res= 815 g/L Vol Soln= 0.05 L C(0) (ppm) 3643

C(0) (eq/L) 0.124123

Mass Res (g)	Equ Conc (ppm)	R L res/L sol	C (eq/L)	(C(0)-C)/R	(C(0)-C)^1.5/(RC)^.5	Regression
				0		2.4109
7.02	124.3	0.1723	0.0042	0.6959	1.5368	1.6421
7.021	122.2	0.1723	0.0042	0.6962	1.5513	1.6417
7.02	111.9	0.1723	0.0038	0.6984	1.6283	1.6394
6.319	145.3	0.1551	0.0050	0.7685	1.4848	1.5619
6.317	142.6	0.1550	0.0049	0.7694	1.5008	1.5609
6.318	137	0.1550	0.0047	0.7705	1.5347	1.5597
4.204	333.8	0.1032	0.0114	1.0929	1.1053	1.2035
4.206	310.5	0.1032	0.0106	1.1001	1.1578	1.1956
2.8	676.4	0.0687	0.0230	1.4710	0.8075	0.7857
2.801	672.5	0.0687	0.0229	1.4724	0.8113	0.7842
0.707	2593	0.0173	0.0883	2.0620	0.1728	0.1328
0.709	2530	0.0174	0.0862	2.1796	0.1907	0.0030
0.356	3062	0.0087	0.1043	2.2659	0.0923	-
0.356	3037	0.0087	0.1035	2.3634	0.0987	-
0.355	2996	0.0087	0.1021	2.5304	0.1098	-

Regression Output:

Constant	2.410922
Std Err of Y Est	0.093856
R Squared	0.983336
No. of Observations	15
Degrees of Freedom	13

X Coefficient(s)	-1.10479
Std Err of Coef.	0.0398882

Raw data for binary system Cu^{2+}-Na^{+}.

Eq. Wt=	31.75	Dens. Res=	815 g/L	Vol Soln=	0.05 L	C(0) (ppm)	2427
						C(0) (eq/L)	0.076441

Mass Res (g)	Equ Conc (ppm)	R L res/L sol	C (eq/L)	(C(0)-C)/R	(C(0)-C)^1.5/(RC)^.5	Regression
7.004	33.1	0.1719	0.0010	0.4387	1.5466	0.3287
7.005	35.22	0.1719	0.0011	0.4382	1.4973	0.3879
6.3	39.64	0.1546	0.0012	0.4864	1.4841	0.4037
6.298	46.27	0.1546	0.0015	0.4852	1.3682	0.5425
7.003	44.42	0.1719	0.0014	0.4367	1.3257	0.5933
4.198	72.67	0.1030	0.0023	0.7198	1.3150	0.6062
6.301	53.52	0.1546	0.0017	0.4835	1.2660	0.6648
4.2	91.56	0.1031	0.0029	0.7137	1.1572	0.7952
2.799	170.5	0.0687	0.0054	1.0347	0.9865	0.9995
2.798	170.7	0.0687	0.0054	1.0350	0.9860	1.0002
0.698	1356	0.0171	0.0427	1.9693	0.2291	1.9066
0.698	1367	0.0171	0.0431	1.9491	0.2246	1.9120
0.697	1374	0.0171	0.0433	1.9390	0.2220	1.9151
0.351	1839	0.0086	0.0579	2.1501	0.1128	2.0458
0.351	1866	0.0086	0.0588	2.0513	0.1044	2.0559
0.351	1908	0.0086	0.0601	1.8978	0.0919	2.0710
					0	2.1810

Regression Output:

Constant	2.18096
Std Err of Y Est	0.103833
R Squared	0.980015
No. of Observations	16
Degrees of Freedom	14

X Coefficient(s)	-1.197569
Std Err of Coef.	0.0457063

Raw data for binary system Cd^{2+}-Na^{+}.

Eq. Wt= 56.2		Dens. Res= 815 g/L		Vol Soln= 0.05 L		C(0) (ppm)	5910
						C(0) (eq/L)	0.10516
Mass Res (g)	Equ Conc (ppm)	R L res/L sol	C (eq/L)	(C(0)-C)/R	(C(0)-C)^1.5/(RC)^.5	Regression	
6.3	123.5	0.1546	0.0022	0.6660	1.7925	0.6574	
7.199	114.6	0.1767	0.0020	0.5837	1.7447	0.6913	
6.299	141.2	0.1546	0.0025	0.6641	1.6688	0.7452	
4.201	258.6	0.1031	0.0046	0.9754	1.4641	0.8906	
4.2	260	0.1031	0.0046	0.9754	1.4598	0.8936	
2.999	648.5	0.0736	0.0115	1.2721	0.9830	1.2322	
2.999	655.2	0.0736	0.0117	1.2705	0.9761	1.2371	
2.399	1152	0.0589	0.0205	1.4381	0.7091	1.4267	
2.401	1193	0.0589	0.0212	1.4245	0.6876	1.4420	
1.7	2087	0.0417	0.0371	1.6306	0.4508	1.6101	
1.699	2097	0.0417	0.0373	1.6273	0.4481	1.6121	
1	3526	0.0245	0.0627	1.7286	0.2227	1.7721	
0.999	3531	0.0245	0.0628	1.7267	0.2219	1.7726	
					0	1.9302	

Regression Output:		
Constant		1.93023
Std Err of Y Est		0.060242
R Squared		0.980844
No. of Observations		13
Degrees of Freedom		11
X Coefficient(s)	-0.710109	
Std Err of Coef.	0.0299216	

Raw data for binary system Pb^{2+}-Na^{+}.

Eq. Wt= 103.6 Dens. Res 815 g/L Vol Soln= 0.05 L C(0) (ppm 10287
C(0) (eq/L 0.0993

Mass Res (g)	Equ Con (ppm)	R L res/L sol	C (eq/L)	(C(0)-C)/R	(C(0)-C)^1.5/(RC)^.5	Regression
4.899	55.74	0.1202	0.0005	0.8215	3.8589	0.6004
4.9	65.19	0.1202	0.0006	0.8205	3.5629	0.7227
6.999	49.06	0.1718	0.0005	0.5754	3.4446	0.7716
6.3	54.52	0.1546	0.0005	0.6389	3.4413	0.7730
4.201	89.1	0.1031	0.0009	0.9548	3.2799	0.8397
6.3	61.55	0.1546	0.0006	0.6384	3.2355	0.8581
6.999	57.1	0.1718	0.0006	0.5749	3.1892	0.8772
4.201	97	0.1031	0.0009	0.9541	3.1398	0.8976
3.15	159.1	0.0773	0.0015	1.2647	2.8054	1.0359
3.151	198.3	0.0773	0.0019	1.2594	2.4979	1.1630
2.45	527.3	0.0601	0.0051	1.5669	1.6529	1.5123
2.449	552.1	0.0601	0.0053	1.5635	1.6095	1.5303
1.749	1875.8	0.0429	0.0181	1.8916	0.8299	1.8526
1.75	1899.8	0.0429	0.0183	1.8852	0.8208	1.8563
1.05	4815	0.0258	0.0465	2.0499	0.3508	2.0507
1.049	4857.5	0.0257	0.0469	2.0359	0.3453	2.0529
0.7	6557.5	0.0172	0.0633	2.0957	0.2071	2.1100
0.7	6677.5	0.0172	0.0645	2.0282	0.1954	2.1149
					0	2.1957

Regression Output:

Constant	2.19567
Std Err of Y Est	0.14729
R Squared	0.93936
No. of Observations	18
Degrees of Freedom	16
X Coefficient(s)	-0.41341
Std Err of Coef.	0.02626

Raw data for binary system Zn^{2+}-Na^{+}.

Eq. Wt= 32.7		Dens. Res 815 g/L		Vol Soln= 0.05 L		C(0) (ppm	3650
						C(0) (eq/L	0.11162
Mass Res (g)	Equ Con (ppm)	R L res/L sol	C (eq/L)	(C(0)-C)/R	(C(0)-C)^1.5/(RC)^.5	Regression	
6.3	251.1	0.1546	0.0077	0.6723	0.9726	0.5987	
6.999	230.5	0.1718	0.0070	0.6088	0.9719	0.5995	
7	234.2	0.1718	0.0072	0.6081	0.9625	0.6092	
6.299	275.6	0.1546	0.0084	0.6676	0.9184	0.6553	
3.501	847.1	0.0859	0.0259	0.9977	0.5319	1.0592	
3.5	885.9	0.0859	0.0271	0.9842	0.5095	1.0827	
2.451	1239	0.0601	0.0379	1.2258	0.4194	1.1769	
2.45	1406	0.0601	0.0430	1.1414	0.3536	1.2456	
1.751	1759	0.0430	0.0538	1.3458	0.2893	1.3129	
1.751	1873	0.0430	0.0573	1.2647	0.2553	1.3483	
1.05	2404	0.0258	0.0735	1.4788	0.1709	1.4365	
1.049	2513	0.0257	0.0769	1.3507	0.1458	1.4628	
0.7	2736	0.0172	0.0837	1.6272	0.1233	1.4863	
0.699	2757	0.0172	0.0843	1.5920	0.1187	1.4911	
					0	1.6151	

Regression Output:

Constant		1.61515
Std Err of Y Est		0.08409
R Squared		0.95027
No. of Observations		14
Degrees of Freedom		12
X Coefficient(s)	-1.045079	
Std Err of Coef.	0.069014	

Raw data for ternary system with initial concentrations: Ni^{2+}, 0.1N; Cu^{2+}, 0.05N.

Eq. Wt Ni	29.35	Dens. Res	815 g/L	Ni(0) (ppm)	2944	Cu(0) (ppm	1866
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Ni(0) (eq/L	0.100307	Cu(0) (eq/L	0.058772
X(0)=	2.17 eq/L	K(Ni)=	0.826	K(Cu)=	0.694		

Mass Res (g)	Conc Ni (ppm)	Conc Cu (ppm)	R L res/L sol	C(Ni) (eq/L)	C(Cu) (eq/L)	Pred(Ni) (eq/L)	Pred(Cu) (eq/L)	%Dif(Ni)	%Dif(Cu)	Ni Uptak (eq/L res)	Cu Uptak (eq/L res)	Ni Predic (eq/L res)	Cu Predi (eq/L res)	%er Ni	%er Cu	Total Upta (eq/L res)	Predicted (eq/L res)
0.35	2583	1669	0.0086	0.0880	0.0526	0.0883	0.0528	-0.3659	-0.3659	1.4321	0.7224	1.3944	0.6999	2.6985	3.2116	2.1545	2.0944
0.351	2614	1662	0.0086	0.0891	0.0523	0.0883	0.0528	0.8299	-0.7838	1.3053	0.7459	1.3905	0.6979	-6.1205	6.8790	2.0513	2.0884
0.7	2419	1512	0.0172	0.0824	0.0476	0.0774	0.0471	6.4433	1.1513	1.0413	0.6491	1.3317	0.6806	-21.8086	-4.6362	1.6904	2.0124
0.701	2347	1472	0.0172	0.0800	0.0464	0.0774	0.0471	3.2751	-1.5246	1.1824	0.7214	1.3298	0.6797	-11.0852	6.1394	1.9038	2.0095
1.049	2093	1323	0.0257	0.0713	0.0417	0.0675	0.0417	5.6314	-0.1694	1.1264	0.6644	1.2740	0.6616	-11.5919	0.4152	1.7907	1.9357
1.051	2118	1329	0.0258	0.0722	0.0419	0.0675	0.0417	6.8931	0.2833	1.0912	0.6558	1.2716	0.6604	-14.1891	-0.6944	1.7470	1.9320
1.7	1669	1048	0.0417	0.0569	0.0330	0.0518	0.0329	9.7364	0.3279	1.0413	0.6176	1.1623	0.6202	-10.4058	-0.4170	1.6589	1.7824
1.7	1613	1015	0.0417	0.0550	0.0320	0.0518	0.0329	6.0544	-2.8313	1.0870	0.6425	1.1623	0.6202	-6.4707	3.6005	1.7295	1.7824
2.399	1257	801.3	0.0589	0.0428	0.0252	0.0386	0.0251	11.0971	0.7497	0.9763	0.5696	1.0490	0.5728	-6.9271	-0.5569	1.5460	1.6218
2.399	1301	814.6	0.0589	0.0443	0.0257	0.0386	0.0251	14.9860	2.4219	0.9509	0.5625	1.0490	0.5728	-9.3546	-1.7991	1.5134	1.6218
2.401	1275	829.3	0.0589	0.0434	0.0261	0.0386	0.0251	12.6880	4.2702	0.9651	0.5542	1.0481	0.5723	-7.9202	-3.1721	1.5193	1.6205
3.001	1022	636.3	0.0736	0.0348	0.0200	0.0298	0.0197	16.6928	1.7824	0.8892	0.5259	0.9569	0.5307	-7.0688	-0.8980	1.4151	1.4875
4.199	715.2	451.6	0.1030	0.0244	0.0142	0.0184	0.0124	32.2191	14.5219	0.7370	0.4323	0.7946	0.4498	-7.2523	-3.8912	1.1693	1.2444
4.2	656.9	418.6	0.1031	0.0224	0.0132	0.0184	0.0124	21.4411	6.1534	0.7561	0.4423	0.7944	0.4497	-4.8263	-1.6488	1.1984	1.2441
6.301	357.7	223.7	0.1546	0.0122	0.0070	0.0094	0.0065	29.2407	9.0661	0.5699	0.3345	0.5877	0.3383	-3.0342	-1.1196	0.9044	0.9260
6.999	325.6	205.8	0.1718	0.0111	0.0065	0.0079	0.0054	40.0719	19.1524	0.5194	0.3044	0.5379	0.3105	-3.4352	-1.9536	0.8239	0.8484
7.001	339.1	211	0.1718	0.0116	0.0066	0.0079	0.0054	45.8796	22.1630	0.5166	0.3034	0.5377	0.3104	-3.9331	-2.2607	0.8200	0.8482
								15.4597	4.4923					-7.8074	-0.1648		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.1N; Ni^{2+}, 0.1N.

Eq. Wt Cd	56.2	Dens. Res=	815 g/L	Cd(0) (ppm)	6070	Ni(0) (ppm	2910
Eq. Wt Ni	29.35	Vol Soln=	0.05 L	Cd(0) (eq/L)	0.108007	Ni(0) (eq/L	0.09915
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Ni)=	0.826		

Mass Res (g)	Conc Cd (ppm)	Conc Ni (ppm)	R L res/L sol	C(Cd) (eq/L)	C(Ni) (eq/L)	Pred(Cd) (eq/L)	Pred(Ni) (eq/L)	%Dif(Cd)	%Dif(Ni)	Cd Uptak (eq/L res)	Ni Uptak (eq/L res)	Cd Predi (eq/L res)	Ni Predic (eq/L res)	%er Cd	%er Ni	Total Upta (eq/L res)	Predicted (eq/L res)
0.7	4933	2433	0.0172	0.0878	0.0829	0.0834	0.0883	5.2594	-6.0987	1.1778	0.9461	1.4331	0.6327	-17.8161	49.5382	2.1239	2.0658
0.7	5028	2472	0.0172	0.0895	0.0842	0.0834	0.0883	7.2865	-4.5935	1.0793	0.8688	1.4331	0.6327	-24.6828	37.3118	1.9481	2.0658
1.049	4543	2253	0.0257	0.0808	0.0768	0.0729	0.0825	10.9627	-6.9875	1.0555	0.8696	1.3657	0.6456	-22.7160	34.7017	1.9251	2.0113
1.05	4363	2183	0.0258	0.0776	0.0744	0.0729	0.0825	6.5662	-9.8774	1.1788	0.9613	1.3644	0.6449	-13.6059	49.0534	2.1401	2.0094
1.75	3643	1836	0.0429	0.0648	0.0626	0.0550	0.0707	17.8583	-11.5450	1.0056	0.8521	1.2343	0.6620	-18.5297	28.7202	1.8577	1.8963
1.751	3628	1821	0.0430	0.0646	0.0620	0.0550	0.0707	17.3730	-12.2677	1.0112	0.8635	1.2336	0.6616	-18.0262	30.5179	1.8747	1.8952
2.449	2828	1457	0.0601	0.0503	0.0496	0.0412	0.0592	22.0477	-16.1023	0.9599	0.8238	1.1111	0.6652	-13.6129	23.8324	1.7836	1.7763
2.45	3073	1565	0.0601	0.0547	0.0533	0.0412	0.0592	32.6212	-9.8834	0.8870	0.7622	1.1107	0.6649	-20.1412	14.6280	1.6492	1.7756
3.149	2316	1203	0.0773	0.0412	0.0410	0.0309	0.0485	33.5817	-15.5233	0.8644	0.7526	0.9985	0.6552	-13.4271	14.8769	1.6170	1.6536
3.15	2251	1165	0.0773	0.0401	0.0397	0.0309	0.0485	29.8327	-18.1918	0.8791	0.7691	0.9981	0.6550	-11.9281	17.4342	1.6482	1.6531
4.199	1661	867.5	0.1030	0.0296	0.0296	0.0203	0.0353	45.9514	-16.2926	0.7614	0.6754	0.8517	0.6195	-10.6033	9.0117	1.4367	1.4712
4.199	1598	850	0.1030	0.0284	0.0290	0.0203	0.0353	40.4156	-17.9813	0.7722	0.6811	0.8517	0.6195	-9.3259	9.9457	1.4534	1.4712
4.901	1433	748.3	0.1203	0.0255	0.0255	0.0156	0.0285	63.7651	-10.6040	0.6860	0.6124	0.7686	0.5872	-10.7405	4.2819	1.2984	1.3558
4.901	1418	736.5	0.1203	0.0252	0.0251	0.0156	0.0285	62.0508	-12.0137	0.6883	0.6157	0.7686	0.5872	-10.4518	4.8512	1.3040	1.3558
6.299	907	475.5	0.1546	0.0161	0.0162	0.0098	0.0192	64.1789	-15.5317	0.5943	0.5366	0.6351	0.5173	-6.4259	3.7252	1.1309	1.1525
6.3	888	473.3	0.1546	0.0158	0.0161	0.0098	0.0192	60.7397	-15.9225	0.5964	0.5370	0.6350	0.5173	-6.0816	3.8189	1.1334	1.1523
6.999	732	413.5	0.1718	0.0130	0.0141	0.0081	0.0161	61.3991	-12.3844	0.5530	0.4952	0.5819	0.4836	-4.9580	2.3973	1.0483	1.0655
7	858.5	457.3	0.1718	0.0153	0.0156	0.0081	0.0161	89.2912	-3.1037	0.5398	0.4865	0.5818	0.4836	-7.2103	0.6008	1.0263	1.0654
								37.2878	-11.9391					-13.3491	18.8471		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.05N; Ni^{2+}, 0.05N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm	2824	Ni(0) (ppm)	1369
Eq. Wt Ni	29.35	Vol Soln=	0.05 L	Cd(0) (eq/L	0.050249	Ni(0) (eq/L	0.046644
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Ni)=	0.826		

Mass Res (g)	Conc Cd (ppm)	Conc Ni (ppm)	R L res/L s	C(Cd) (eq/L)	C(Ni) (eq/L)	Pred(Cd) (eq/L)	Pred(Ni) (eq/L)	%Dif(Cd)	%Dif(Ni)	Cd Uptak (eq/L res)	Ni Uptak (eq/L res)	Cd Predi (eq/L res)	Ni Predic (eq/L res)	%er Cd	%er Ni	Total Upta (eq/L res)	Predicted (eq/L res)
0.699	2023	1063	0.0172	0.0360	0.0362	0.0277	0.0348	29.9980	4.0450	0.8309	0.6078	1.3151	0.6899	-36.8208	-11.8985	1.4387	2.0050
0.7	2008	1044	0.0172	0.0357	0.0356	0.0277	0.0348	29.0341	2.1853	0.8452	0.6446	1.3133	0.6889	-35.6377	-6.4281	1.4899	2.0022
1.049	1538	819.2	0.0257	0.0274	0.0279	0.0196	0.0283	39.3409	-1.2684	0.8889	0.7277	1.1891	0.7138	-25.2426	1.9516	1.6166	1.9028
1.05	1548	821.1	0.0258	0.0275	0.0280	0.0196	0.0283	40.2469	-1.0394	0.8812	0.7245	1.1879	0.7131	-25.8240	1.5993	1.6056	1.9010
1.749	797.9	441.4	0.0429	0.0142	0.0150	0.0093	0.0164	52.9904	-8.3536	0.8400	0.7364	0.9545	0.7044	-12.0030	4.5340	1.5763	1.6590
1.75	806.9	446.8	0.0429	0.0144	0.0152	0.0093	0.0164	54.7161	-7.2324	0.8358	0.7317	0.9540	0.7040	-12.3939	3.9255	1.5674	1.6580
2.449	428.7	237.6	0.0601	0.0076	0.0081	0.0044	0.0088	71.8044	-8.0068	0.7092	0.6414	0.7622	0.6297	-6.9596	1.8619	1.3506	1.3919
2.449	441.9	246.1	0.0601	0.0079	0.0084	0.0044	0.0088	77.0944	-4.7158	0.7053	0.6366	0.7622	0.6297	-7.4723	1.0966	1.3419	1.3919
3.15	270	148.8	0.0773	0.0048	0.0051	0.0024	0.0051	97.7066	0.1946	0.5879	0.5378	0.6186	0.5380	-4.9651	-0.0237	1.1257	1.1566
3.151	260.9	142.6	0.0773	0.0046	0.0049	0.0024	0.0051	91.0432	-3.9802	0.5898	0.5404	0.6184	0.5378	-4.6265	0.4843	1.1302	1.1562
4.2	143.8	80.97	0.1031	0.0026	0.0028	0.0013	0.0028	99.8999	-0.0444	0.4627	0.4258	0.4751	0.4258	-2.6113	0.0028	0.8885	0.9009
4.201	159	87.97	0.1031	0.0028	0.0030	0.0013	0.0028	121.0298	8.5969	0.4600	0.4234	0.4750	0.4257	-3.1636	-0.5407	0.8834	0.9007
4.9	118.1	65.33	0.1202	0.0021	0.0022	0.0010	0.0021	121.2025	8.5802	0.4004	0.3694	0.4100	0.3709	-2.3356	-0.3944	0.7698	0.7808
4.9	110.1	61.46	0.1202	0.0020	0.0021	0.0010	0.0021	106.2184	2.1482	0.4016	0.3705	0.4100	0.3709	-2.0468	-0.0988	0.7721	0.7808
6.3	78.1	43.26	0.1546	0.0014	0.0015	0.0006	0.0013	131.6133	11.6618	0.3160	0.2922	0.3211	0.2932	-1.5905	-0.3396	0.6082	0.6143
6.301	82.85	46.19	0.1546	0.0015	0.0016	0.0006	0.0013	145.6999	19.2246	0.3154	0.2915	0.3211	0.2931	-1.7608	-0.5599	0.6069	0.6142
6.999	60.75	33.96	0.1718	0.0011	0.0012	0.0005	0.0011	111.9531	3.3098	0.2863	0.2648	0.2896	0.2651	-1.1479	-0.0814	0.5511	0.5546
7	67.32	37.58	0.1718	0.0012	0.0013	0.0005	0.0011	134.8754	14.3222	0.2855	0.2641	0.2896	0.2650	-1.3829	-0.3524	0.5496	0.5546
								86.4704	2.2015					-10.4436	-0.2923		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.1N; Ni^{2+}, 0.05N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm	5783	Ni(0) (ppm	1478
Eq. Wt Ni	29.35	Vol Soln=	0.05 L	Cd(0) (eq/L	0.1029	Ni(0) (eq/L	0.050358
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Ni)=	0.826		

Mass Res (g)	Conc Cd (ppm)	Conc Ni (ppm)	R L res/L so	C(Cd) (eq/L)	C(Ni) (eq/L)	Pred(Cd) (eq/L)	Pred(Ni) (eq/L)	%Dif(Cd)	%Dif(Ni)	Cd Uptak (eq/L res)	Ni Uptak (eq/L res)	Cd Predi (eq/L res)	Ni Predic (eq/L res)	%er Cd	%er Ni	Total Upta (eq/L res)	Predicted (eq/L res)
0.699	4545	1214	0.0172	0.0809	0.0414	0.0745	0.0435	8.4946	-4.8254	1.2842	0.5244	1.6533	0.4021	-22.3265	30.4032	1.8086	2.0555
0.7	4602.5	1213	0.0172	0.0819	0.0413	0.0745	0.0435	9.8672	-4.9038	1.2228	0.5256	1.6510	0.4015	-25.9342	30.8972	1.7484	2.0525
1.049	3990	1111	0.0257	0.0710	0.0379	0.0624	0.0396	13.8128	-4.4586	1.2394	0.4857	1.5741	0.4171	-21.2645	16.4514	1.7251	1.9912
1.051	4003	1099	0.0258	0.0712	0.0374	0.0624	0.0396	14.1836	-5.4906	1.2280	0.5007	1.5711	0.4163	-21.8353	20.2590	1.7287	1.9874
1.749	2750	756.2	0.0429	0.0489	0.0258	0.0425	0.0316	15.2706	-18.4397	1.2574	0.5730	1.4084	0.4373	-10.7235	31.0378	1.8304	1.8457
1.749	2714	781.8	0.0429	0.0483	0.0266	0.0425	0.0316	13.7616	-15.6786	1.2723	0.5527	1.4084	0.4373	-9.6638	26.3903	1.8250	1.8457
2.45	1910	568.1	0.0601	0.0340	0.0194	0.0280	0.0238	21.5079	-18.6037	1.1462	0.5156	1.2463	0.4421	-8.0285	16.6453	1.6619	1.6883
2.45	1935	566.7	0.0601	0.0344	0.0193	0.0280	0.0238	23.0983	-18.8043	1.1388	0.5164	1.2463	0.4421	-8.6221	16.8248	1.6553	1.6883
3.15	1387	399.7	0.0773	0.0247	0.0136	0.0183	0.0172	34.7882	-20.8233	1.0119	0.4753	1.0943	0.4289	-7.5301	10.8017	1.4872	1.5232
3.151	1407	409.3	0.0773	0.0250	0.0139	0.0183	0.0172	36.7318	-18.9216	1.0070	0.4709	1.0940	0.4288	-7.9508	9.8152	1.4779	1.5228
4.2	896.6	268.8	0.1031	0.0160	0.0092	0.0102	0.0105	56.4092	-12.8598	0.8436	0.3997	0.8994	0.3866	-6.2068	3.3918	1.2433	1.2860
4.201	901	267.8	0.1031	0.0160	0.0091	0.0102	0.0105	57.1767	-13.1840	0.8426	0.4000	0.8992	0.3865	-6.2913	3.4773	1.2426	1.2857
4.9	598.8	184	0.1202	0.0107	0.0063	0.0073	0.0078	45.3589	-19.8316	0.7671	0.3667	0.7948	0.3538	-3.4789	3.6458	1.1338	1.1486
4.901	595.2	183.3	0.1203	0.0106	0.0062	0.0073	0.0078	44.4850	-20.1366	0.7675	0.3668	0.7946	0.3537	-3.4119	3.7019	1.1343	1.1483
6.3	523	148.8	0.1546	0.0093	0.0051	0.0044	0.0048	113.4415	4.9658	0.6054	0.2929	0.6374	0.2945	-5.0193	-0.5268	0.8983	0.9319
6.3	541.8	162.3	0.1546	0.0096	0.0055	0.0044	0.0048	121.1140	14.4889	0.6032	0.2900	0.6374	0.2945	-5.3588	-1.5371	0.8932	0.9319
6.999	439.2	128.1	0.1718	0.0078	0.0044	0.0036	0.0040	120.1393	9.9387	0.5536	0.2678	0.5784	0.2701	-4.2928	-0.8506	0.8214	0.8485
7.001	419.7	125.3	0.1718	0.0075	0.0043	0.0036	0.0040	110.3654	7.5356	0.5555	0.2683	0.5783	0.2700	-3.9436	-0.6449	0.8237	0.8483
								47.7782	-8.8907					-10.1046	12.2324		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.05N; Ni^{2+}, 0.1N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm	2767	Ni(0) (ppm	2594
Eq. Wt Ni	29.35	Vol Soln=	0.05 L	Cd(0) (eq/L	0.049235	Ni(0) (eq/L	0.088382
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Ni)=	0.826		

Mass Res (g)	Conc Cd (ppm)	Conc Ni (ppm)	R L res/L sol	C(Cd) (eq/L)	C(Ni) (eq/L)	Pred(Cd) (eq/L)	Pred(Ni) (eq/L)	%Dif(Cd)	%Dif(Ni)	Cd Upta (eq/L res)	Ni Uptak (eq/L res)	Cd Predi (eq/L res)	Ni Predic (eq/L res)	%er Cd	%er Ni	Total Upta (eq/L res)	Predicted (eq/L res)
0.7	2239	2267	0.0172	0.0398	0.0772	0.0314	0.0714	27.0404	8.1644	0.5469	0.6486	1.0406	0.9880	-47.4401	-34.3527	1.1955	2.0286
0.7	2218	2235	0.0172	0.0395	0.0761	0.0314	0.0714	25.8488	6.6376	0.5687	0.7121	1.0406	0.9880	-45.3496	-27.9285	1.2807	2.0286
1.049	1856	1896	0.0257	0.0330	0.0646	0.0248	0.0626	33.3801	3.2273	0.6297	0.9238	0.9508	1.0023	-33.7690	-7.8277	1.5535	1.9531
1.051	1926	1983	0.0258	0.0343	0.0676	0.0248	0.0626	38.4106	7.9640	0.5802	0.8072	0.9490	1.0004	-38.8581	-19.3162	1.3874	1.9493
1.751	1373	1424	0.0430	0.0244	0.0485	0.0153	0.0459	59.8862	5.7726	0.5773	0.9277	0.7902	0.9893	-26.9493	-6.2286	1.5050	1.7796
1.751	1362	1432	0.0430	0.0242	0.0488	0.0153	0.0459	58.6052	6.3668	0.5818	0.9214	0.7902	0.9893	-26.3729	-6.8698	1.5032	1.7796
2.449	988.5	1052	0.0601	0.0176	0.0358	0.0095	0.0321	86.1266	11.8006	0.5266	0.8742	0.6620	0.9372	-20.4574	-6.7173	1.4008	1.5992
2.45	1001	1067	0.0601	0.0178	0.0364	0.0095	0.0321	88.4803	13.3947	0.5227	0.8654	0.6617	0.9368	-21.0165	-7.6247	1.3880	1.5985
3.149	775.5	829.5	0.0773	0.0138	0.0283	0.0060	0.0220	130.3661	28.2903	0.4586	0.7780	0.5596	0.8586	-18.0575	-9.3929	1.2365	1.4182
3.15	766.3	834.6	0.0773	0.0136	0.0284	0.0060	0.0220	127.6332	29.0791	0.4605	0.7755	0.5594	0.8584	-17.6789	-9.6548	1.2360	1.4178
4.199	471.1	516.9	0.1030	0.0084	0.0176	0.0033	0.0131	150.9749	34.2346	0.3965	0.6868	0.4454	0.7304	-10.9872	-5.9680	1.0833	1.1758
4.2	553	590.7	0.1031	0.0098	0.0201	0.0033	0.0131	194.6065	53.3999	0.3822	0.6622	0.4453	0.7302	-14.1625	-9.3089	1.0445	1.1755
4.899	354.5	395.5	0.1202	0.0063	0.0135	0.0024	0.0098	159.5814	37.6435	0.3571	0.6231	0.3893	0.6537	-8.2851	-4.6892	0.9801	1.0431
4.899	383.6	411.9	0.1202	0.0068	0.0140	0.0024	0.0098	180.8898	43.3511	0.3528	0.6184	0.3893	0.6537	-9.3914	-5.4002	0.9712	1.0431
6.3	391.5	391.7	0.1546	0.0070	0.0133	0.0015	0.0062	367.5297	117.0053	0.2734	0.4854	0.3088	0.5319	-11.4697	-8.7507	0.7588	0.8407
6.301	403.2	402.8	0.1546	0.0072	0.0137	0.0015	0.0062	381.5018	123.1548	0.2720	0.4828	0.3088	0.5318	-11.9057	-9.2106	0.7548	0.8406
6.999	259.4	263	0.1718	0.0046	0.0090	0.0012	0.0051	275.2568	75.3585	0.2598	0.4624	0.2795	0.4848	-7.0527	-4.6244	0.7222	0.7643
7	254.2	264.7	0.1718	0.0045	0.0090	0.0012	0.0051	267.7343	76.4920	0.2603	0.4620	0.2795	0.4848	-6.8600	-4.6940	0.7223	0.7642
								147.4363	37.8521					-20.8924	-10.4755		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.1N; Cu^{2+}, 0.1N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm)	5930	Cu(0) (ppm	3050
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Cd(0) (eq/L	0.105516	Cu(0) (eq/L	0.096063
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Cu)=	0.694		

Mass Res (g)	Conc Cd (ppm)	Conc Cu (ppm)	R L res/L so	C(Cd) (eq/L)	C(Cu) (eq/L)	Pred(Cd) (eq/L)	Pred(Cu) (eq/L)	% Dif(A)	% Dif(B)	Cd Uptak (eq/L res)	Cu Upta (eq/L res)	Cd Predi (eq/L res)	Cu Predi (eq/L res)	%er Cd	%er Cu	Total Upta (eq/L res)	Predicted (eq/L res)
0.699	4793	2515	0.0172	0.0853	0.0792	0.0800	0.0864	6.6059	-8.3188	1.1794	0.9823	1.4875	0.5633	-20.7113	74.3807	2.1618	2.0509
0.7	4813	2449	0.0172	0.0856	0.0771	0.0799	0.0864	7.1847	-10.7247	1.1570	1.1019	1.4912	0.5625	-22.4101	95.8931	2.2590	2.0537
1.049	4478	2281	0.0257	0.0797	0.0718	0.0691	0.0811	15.3107	-11.4149	1.0037	0.9409	1.4146	0.5813	-29.0524	61.8692	1.9445	1.9959
1.051	4325	2252	0.0258	0.0770	0.0709	0.0691	0.0811	11.3709	-12.5411	1.1073	0.9745	1.4119	0.5802	-21.5765	67.9735	2.0818	1.9921
1.749	3410	1854	0.0429	0.0607	0.0584	0.0511	0.0700	18.7400	-16.5804	1.0447	0.8777	1.2678	0.6072	-17.5980	44.5317	1.9224	1.8751
1.751	3420	1872	0.0430	0.0609	0.0590	0.0511	0.0699	19.0882	-15.6500	1.0394	0.8635	1.2664	0.6089	-17.9250	41.8124	1.9029	1.8753
2.448	2805	1536	0.0601	0.0499	0.0484	0.0376	0.0588	32.7421	-17.7246	0.9256	0.7938	1.1305	0.6203	-18.1268	27.9689	1.7194	1.7508
2.449	2728	1478	0.0601	0.0485	0.0466	0.0376	0.0588	29.0982	-20.8313	0.9480	0.8238	1.1301	0.6200	-16.1095	32.8713	1.7719	1.7501
3.148	2085	1184	0.0773	0.0371	0.0373	0.0277	0.0484	33.9337	-22.9518	0.8856	0.7608	1.0073	0.6170	-12.0793	23.3067	1.6464	1.6243
3.149	2280	1219	0.0773	0.0406	0.0384	0.0277	0.0484	46.4599	-20.6742	0.8404	0.7463	1.0070	0.6168	-16.5382	20.9939	1.5867	1.6238
4.199	1609	869.8	0.1030	0.0286	0.0274	0.0180	0.0355	59.0550	-22.8302	0.7462	0.6664	0.8493	0.5877	-12.1462	13.3823	1.4126	1.4371
4.199	1628.5	914.5	0.1030	0.0290	0.0288	0.0180	0.0355	60.9826	-18.8644	0.7428	0.6527	0.8493	0.5877	-12.5427	11.0577	1.3955	1.4371
4.899	1267	709	0.1202	0.0225	0.0223	0.0138	0.0289	63.3658	-22.7311	0.6902	0.6133	0.7629	0.5587	-9.5343	9.7811	1.3035	1.3216
4.901	1277	722.5	0.1203	0.0227	0.0228	0.0138	0.0289	64.6552	-21.2598	0.6884	0.6095	0.7626	0.5584	-9.7283	9.1480	1.2979	1.3210
6.299	841.3	484.5	0.1546	0.0150	0.0153	0.0088	0.0197	70.1108	-22.5389	0.5858	0.5227	0.6257	0.4940	-6.3792	5.8145	1.1085	1.1197
6.3	791.3	451.3	0.1546	0.0141	0.0142	0.0088	0.0197	60.0008	-27.8468	0.5914	0.5294	0.6256	0.4939	-5.4594	7.1839	1.1208	1.1195
6.998	660.5	377.3	0.1717	0.0118	0.0119	0.0072	0.0166	63.2315	-28.4129	0.5460	0.4902	0.5725	0.4627	-4.6306	5.9355	1.0362	1.0352
6.999	776	449.5	0.1718	0.0138	0.0142	0.0072	0.0166	91.7754	-14.7140	0.5339	0.4769	0.5724	0.4627	-6.7210	3.0738	1.0108	1.0351
								41.8729	-18.7005					-14.4038	30.9432		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.05N; Cu^{2+}, 0.05N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm)	2972	Cu(0) (ppm)	1497
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Cd(0) (eq/L	0.052883	Cu(0) (eq/L	0.04715
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Cu)=	0.694		

Mass Res (g)	Conc Cd (ppm)	Conc Cu (ppm)	R L res/L sol	C(Cd) (eq/L)	C(Cu) (eq/L)	Pred(Cd) (eq/L)	Pred(Cu) (eq/L)	% Dif(Cd)	% Dif(Cu)	Cd Upta (eq/L res)	Cu Upta (eq/L res)	Cd Predi (eq/L res)	Cu Predi (eq/L res)	%er Cd	%er Cu	Total Upt (eq/L res)	Predicted (eq/L res)
0.7	2073	984.3	0.0172	0.0369	0.0310	0.0291	0.0367	26.7564	-15.5270	0.9312	0.9400	1.3845	0.6083	-32.7388	54.5324	1.8713	1.9928
0.7	2167	989.8	0.0172	0.0386	0.0312	0.0291	0.0367	32.5042	-15.0550	0.8339	0.9300	1.3845	0.6083	-39.7717	52.8747	1.7638	1.9928
1.049	1591	797.3	0.0257	0.0283	0.0251	0.0208	0.0306	36.1039	-17.9353	0.9546	0.8561	1.2463	0.6429	-23.4071	33.1621	1.8107	1.8892
1.75	909	443.3	0.0429	0.0162	0.0140	0.0100	0.0189	61.7438	-26.1259	0.8548	0.7728	0.9986	0.6578	-14.3983	17.4792	1.6276	1.6564
1.751	899.7	452.7	0.0430	0.0160	0.0143	0.0100	0.0189	60.0890	-24.5594	0.8581	0.7655	0.9980	0.6574	-14.0124	16.4311	1.6236	1.6554
2.45	511.5	257.8	0.0601	0.0091	0.0081	0.0050	0.0108	82.0285	-24.8177	0.7282	0.6492	0.7964	0.6046	-8.5656	7.3737	1.3774	1.4010
3.15	352.2	183.2	0.0773	0.0063	0.0058	0.0028	0.0064	123.8180	-9.8425	0.6030	0.5353	0.6479	0.5272	-6.9224	1.5458	1.1384	1.1751
3.151	299.7	161.4	0.0773	0.0053	0.0051	0.0028	0.0064	90.4550	-20.5709	0.6149	0.5440	0.6477	0.5270	-5.0571	3.2308	1.1589	1.1747
4.199	147.9	77.94	0.1030	0.0026	0.0025	0.0015	0.0036	75.4448	-31.8110	0.4877	0.4337	0.4987	0.4226	-2.2024	2.6296	0.9214	0.9213
4.2	166.1	84.61	0.1031	0.0030	0.0027	0.0015	0.0036	97.0344	-25.9755	0.4844	0.4316	0.4985	0.4225	-2.8327	2.1472	0.9160	0.9211
4.899	123.7	60.59	0.1202	0.0022	0.0019	0.0011	0.0027	100.0971	-29.3205	0.4216	0.3763	0.4307	0.3697	-2.1263	1.7810	0.7979	0.8005
4.9	122.7	62.44	0.1202	0.0022	0.0020	0.0011	0.0027	98.4795	-27.1624	0.4216	0.3758	0.4306	0.3697	-2.0920	1.6499	0.7974	0.8003
6.301	86.8	43.01	0.1546	0.0015	0.0014	0.0007	0.0017	120.6406	-20.3150	0.3320	0.2962	0.3375	0.2939	-1.6183	0.7599	0.6282	0.6314
7	77.55	40.49	0.1718	0.0014	0.0013	0.0006	0.0015	129.9822	-14.9816	0.2998	0.2671	0.3044	0.2657	-1.4917	0.4923	0.5669	0.5701
7	72.06	34.21	0.1718	0.0013	0.0011	0.0006	0.0015	113.7011	-28.1680	0.3004	0.2682	0.3044	0.2657	-1.3048	0.9256	0.5686	0.5701
								83.2586	-22.1445								

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.1N; Cu^{2+}, 0.05N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm)	5870	Cu(0) (ppm)	1635
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Cd(0) (eq/L)	0.104448	Cu(0) (eq/L	0.051496
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Cu)=	0.694		

Mass Res (g)	Conc Cd (ppm)	Conc Cu (ppm)	R L res/L sol	C(Cd) (eq/L)	C(Cd) (eq/L)	Pred(Cd) (eq/L)	Pred(Cu) (eq/L)	% Dif(Cd)	%Dif(Cu)	Cd Upta (eq/L res)	Cu Upta (eq/L res)	Cd Predi (eq/L res)	Cu Predi (eq/L res)	%er Cd	%er Cu	Total Upta (eq/L res)	Predicted (eq/L res)
0.699	4593	1203	0.0172	0.0817	0.0379	0.0755	0.0454	8.2463	-16.5424	1.3247	0.7932	1.6876	0.3554	-21.5072	123.1981	2.1179	2.0430
0.7	4778	1205	0.0172	0.0850	0.0380	0.0755	0.0454	12.6063	-16.4036	1.1311	0.7884	1.6852	0.3549	-32.8785	122.1648	1.9196	2.0401
1.049	4010	1084	0.0257	0.0714	0.0341	0.0631	0.0419	13.0782	-18.5162	1.2857	0.6742	1.6062	0.3728	-19.9580	80.8484	1.9598	1.9790
1.05	3970	1031	0.0258	0.0706	0.0325	0.0631	0.0419	11.9502	-22.5001	1.3121	0.7383	1.6047	0.3724	-18.2367	98.2440	2.0504	1.9771
1.749	2810	767.4	0.0429	0.0500	0.0242	0.0429	0.0343	16.5501	-29.5333	1.2686	0.6367	1.4340	0.4007	-11.5356	58.9084	1.9053	1.8347
1.75	2838	786	0.0429	0.0505	0.0248	0.0429	0.0343	17.7115	-27.8253	1.2563	0.6227	1.4332	0.4004	-12.3451	55.5016	1.8789	1.8336
2.449	1949	550.8	0.0601	0.0347	0.0173	0.0284	0.0266	22.1117	-34.7818	1.1609	0.5682	1.2654	0.4143	-8.2575	37.1624	1.7291	1.6797
2.45	1919	551.6	0.0601	0.0341	0.0174	0.0284	0.0266	20.2321	-34.6871	1.1693	0.5676	1.2649	0.4141	-7.5556	37.0612	1.7369	1.6790
3.149	1321	396.1	0.0773	0.0235	0.0125	0.0188	0.0198	25.0284	-36.9920	1.0475	0.5049	1.1083	0.4102	-5.4938	23.1083	1.5524	1.5185
3.15	1322	397.7	0.0773	0.0235	0.0125	0.0188	0.0198	25.1230	-36.7375	1.0469	0.5041	1.1080	0.4100	-5.5146	22.9493	1.5510	1.5180
4.199	886.8	261.2	0.1030	0.0158	0.0082	0.0106	0.0126	48.8619	-34.7082	0.8605	0.4199	0.9108	0.3775	-5.5189	11.2434	1.2804	1.2882
4.2	782.5	225	0.1031	0.0139	0.0071	0.0106	0.0126	31.3537	-43.7570	0.8783	0.4309	0.9106	0.3774	-3.5413	14.1747	1.3092	1.2879
4.899	605.2	180.9	0.1202	0.0108	0.0057	0.0077	0.0095	39.8530	-40.0249	0.7792	0.3810	0.8048	0.3493	-3.1718	9.0541	1.1602	1.1541
4.9	557	168.2	0.1202	0.0099	0.0053	0.0077	0.0095	28.7147	-44.2354	0.7862	0.3842	0.8046	0.3493	-2.2853	10.0066	1.1704	1.1538
6.299	383.1	111.5	0.1546	0.0068	0.0035	0.0046	0.0060	48.1897	-41.4698	0.6316	0.3104	0.6459	0.2943	-2.2201	5.4690	0.9420	0.9403
6.3	461.4	144	0.1546	0.0082	0.0045	0.0046	0.0060	78.4775	-24.4094	0.6225	0.3038	0.6458	0.2943	-3.6154	3.2191	0.9262	0.9401
7	326.3	93.37	0.1718	0.0058	0.0029	0.0038	0.0050	52.7908	-41.1843	0.5742	0.2827	0.5859	0.2707	-1.9931	4.4288	0.8569	0.8566
7	311.1	90.4	0.1718	0.0055	0.0028	0.0038	0.0050	45.6733	-43.0551	0.5758	0.2832	0.5859	0.2707	-1.7244	4.6300	0.8590	0.8566
								30.3640	-32.6313					-9.2974	40.0762		

Raw data for ternary system with initial concentrations: Cd^{2+}, 0.05N; Cu^{2+}, 0.1N.

Eq. Wt Cd	56.2	Dens. Res	815 g/L	Cd(0) (ppm)	2929	Cu(0) (ppm)	3058
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Cd(0) (eq/L)	0.052117	Cu(0) (eq/L)	0.096315
X(0)=	2.17 eq/L	K(Cd)=	1.98	K(Cu)=	0.694		

Mass Res (g)	Conc Cd (ppm)	Conc Cu (ppm)	R L res/L sol	C(Cd) (eq/L)	C(Cu) (eq/L)	Pred(Cd) (eq/L)	Pred(Cu) (eq/L)	% Dif(Cd)	%Dif(Cu)	Cd Upta (eq/L res)	Cu Upta (eq/L res)	Cd Predi (eq/L res)	Cu Predi (eq/L res)	%er Cd	%er Cu	Total Upta (eq/L res)	Predicted (eq/L res)
0.349	2560	2749	0.0086	0.0456	0.0866	0.0418	0.0887	8.9751	-2.3871	0.7666	1.1364	1.2047	0.8891	-36.3618	27.8048	1.9030	2.0938
0.35	2490	2692	0.0086	0.0443	0.0848	0.0418	0.0887	5.9953	-4.4110	0.9095	1.3421	1.2012	0.8866	-24.2895	51.3804	2.2516	2.0878
0.701	2159	2324	0.0172	0.0384	0.0732	0.0333	0.0804	15.3645	-8.9591	0.7965	1.3439	1.0939	0.9252	-27.1895	45.2602	2.1403	2.0190
0.701	2233	2369	0.0172	0.0397	0.0746	0.0333	0.0804	19.3186	-7.1963	0.7199	1.2615	1.0939	0.9252	-34.1869	36.3546	1.9814	2.0190
1.051	1831	2045	0.0258	0.0326	0.0644	0.0265	0.0719	22.9437	-10.4180	0.7575	1.2371	0.9933	0.9466	-23.7341	30.6802	1.9946	1.9399
1.051	1900	2104	0.0258	0.0338	0.0663	0.0265	0.0719	27.5767	-7.8335	0.7099	1.1650	0.9933	0.9466	-28.5268	23.0690	1.8749	1.9399
1.75	1366	1532	0.0429	0.0243	0.0483	0.0167	0.0553	45.5452	-12.7451	0.6476	1.1192	0.8247	0.9551	-21.4754	17.1841	1.7668	1.7798
1.751	1315	1503	0.0430	0.0234	0.0473	0.0167	0.0553	40.1112	-14.3968	0.6684	1.1398	0.8242	0.9545	-18.9132	19.4110	1.8082	1.7788
2.449	926.1	1087	0.0601	0.0165	0.0342	0.0107	0.0410	54.0061	-16.4970	0.5930	1.0330	0.6892	0.9204	-13.9522	12.2278	1.6260	1.6096
2.451	925.4	1065	0.0601	0.0165	0.0335	0.0107	0.0409	53.8896	-17.9870	0.5927	1.0436	0.6886	0.9213	-13.9221	13.2756	1.6364	1.6099
3.5	620.4	714.1	0.0859	0.0110	0.0225	0.0059	0.0256	87.1042	-12.1432	0.4783	0.8595	0.5381	0.8233	-11.1195	4.3960	1.3378	1.3614
3.5	608.9	701.8	0.0859	0.0108	0.0221	0.0059	0.0256	83.6359	-13.6565	0.4807	0.8640	0.5381	0.8233	-10.6767	4.9439	1.3447	1.3614
4.199	435.2	517.3	0.1030	0.0077	0.0163	0.0041	0.0190	88.8725	-14.2478	0.4306	0.7766	0.4660	0.7503	-7.5884	3.5014	1.2072	1.2163
4.201	387.3	473.8	0.1031	0.0069	0.0149	0.0041	0.0190	68.0844	-21.4588	0.4387	0.7895	0.4658	0.7500	-5.8134	5.2734	1.2282	1.2157
6.3	182.3	240.6	0.1546	0.0032	0.0076	0.0019	0.0094	70.7249	-19.3835	0.3161	0.5740	0.3248	0.5622	-2.6759	2.0964	0.8901	0.8870
6.3	204.1	249.3	0.1546	0.0036	0.0079	0.0019	0.0094	91.1407	-16.4684	0.3136	0.5722	0.3248	0.5622	-3.4483	1.7811	0.8858	0.8870
7	247.7	285.7	0.1718	0.0044	0.0090	0.0016	0.0079	175.4671	13.9041	0.2777	0.5083	0.2941	0.5147	-5.5574	-1.2424	0.7860	0.8088
7	181.4	233.7	0.1718	0.0032	0.0074	0.0016	0.0079	101.7349	-6.8275	0.2846	0.5178	0.2941	0.5147	-3.2222	0.6100	0.8024	0.8088
								58.9161	-10.7285					-16.2585	16.5560		

Raw data for ternary system with initial concentrations: Pb^{2+}, 0.1N; Cu^{2+}, 0.1N.

Eq. Wt Pb 103.6 Dens. Res 815 g/L Pb(0) (ppm) 9395 Cu(0) (ppm) 3033
Eq. Wt Cu 31.75 Vol Soln= 0.05 L Pb(0) (eq/L) 0.090685 Cu(0) (eq/L 0.095528
X(0)= 2.17 eq/L K(Pb)= 5.95 K(Cu)= 0.694

Mass Res (g)	Conc Pb (ppm)	Conc Cu (ppm)	R Lres /L sol	C(Pb) (eq/L)	C(Cu) (eq/L)	Pred(Pb) (eq/L)	Pred(Cu) (eq/L)	% Dif(Pb)	% Dif(Cu)	Pb Uptake (eq/L res)	Cu Upta (eq/L res)	Pb Predi (eq/L res)	Cu Predi (eq/L res)	%er Pb	%er Cu	Total Upt (eq/L res)	Predicted (eq/L res)
0.699	6833	2858	0.0172	0.0660	0.0900	0.0603	0.0902	9.3791	-0.2043	1.4417	0.3213	1.7714	0.3106	-18.6129	3.4585	1.7630	2.0820
0.701	6710	2805	0.0172	0.0648	0.0883	0.0602	0.0902	7.5886	-2.0549	1.5066	0.4174	1.7721	0.3097	-14.9854	34.7916	1.9240	2.0818
1.049	5525	2663	0.0257	0.0533	0.0839	0.0475	0.0864	12.2739	-2.9236	1.4511	0.4527	1.6776	0.3546	-13.5002	27.6743	1.9038	2.0322
1.049	5505	2655	0.0257	0.0531	0.0836	0.0475	0.0864	11.8675	-3.2152	1.4586	0.4625	1.6776	0.3546	-13.0532	30.4348	1.9211	2.0322
1.749	3660	2285	0.0429	0.0353	0.0720	0.0281	0.0758	25.7231	-5.0547	1.2898	0.5489	1.4582	0.4596	-11.5493	19.4220	1.8387	1.9178
1.75	3648	2290	0.0429	0.0352	0.0721	0.0281	0.0758	25.3109	-4.8470	1.2917	0.5449	1.4573	0.4594	-11.3643	18.6238	1.8367	1.9167
2.449	2315	1831	0.0601	0.0223	0.0577	0.0165	0.0627	35.4276	-8.0235	1.1371	0.6299	1.2344	0.5462	-7.8797	15.3247	1.7671	1.7806
2.45	2311	1830	0.0601	0.0223	0.0576	0.0165	0.0627	35.1936	-8.0737	1.1373	0.6302	1.2339	0.5460	-7.8276	15.4206	1.7675	1.7799
3.149	1508	1397.3	0.0773	0.0146	0.0440	0.0102	0.0497	42.7057	-11.4498	0.9852	0.6667	1.0415	0.5930	-5.4121	12.4173	1.6518	1.6346
3.152	1471	1388	0.0773	0.0142	0.0437	0.0101	0.0496	40.5826	-11.8618	0.9888	0.6698	1.0418	0.5938	-5.0863	12.8103	1.6587	1.6356
4.199	750.8	836.5	0.1030	0.0072	0.0263	0.0055	0.0341	31.7655	-22.7377	0.8097	0.6714	0.8267	0.5961	-2.0509	12.6223	1.4811	1.4228
4.201	767.3	853	0.1031	0.0074	0.0269	0.0055	0.0340	34.6613	-20.9819	0.8078	0.6660	0.8263	0.5968	-2.2379	11.5946	1.4738	1.4231
4.899	514.8	611.8	0.1202	0.0050	0.0193	0.0039	0.0267	27.4131	-27.8304	0.7130	0.6343	0.7219	0.5725	-1.2319	10.7961	1.3473	1.2944
4.901	507.5	604	0.1203	0.0049	0.0190	0.0039	0.0267	25.6064	-28.7505	0.7133	0.6361	0.7216	0.5723	-1.1507	11.1531	1.3494	1.2939
6.3	290.8	354.3	0.1546	0.0028	0.0112	0.0023	0.0173	22.0413	-35.4968	0.5684	0.5457	0.5717	0.5060	-0.5736	7.8501	1.1141	1.0777
6.301	272.3	342	0.1546	0.0026	0.0108	0.0023	0.0173	14.2773	-37.7361	0.5695	0.5481	0.5716	0.5059	-0.3715	8.3453	1.1176	1.0775
7	246.4	304.9	0.1718	0.0024	0.0096	0.0018	0.0144	32.1321	-33.3115	0.5141	0.5002	0.5174	0.4723	-0.6507	5.9127	1.0143	0.9897
7.001	270.5	293	0.1718	0.0026	0.0092	0.0018	0.0144	45.0558	-35.9143	0.5126	0.5023	0.5174	0.4722	-0.9124	6.3747	1.0150	0.9896
								26.6114	-16.6926					-6.5806	14.7237		

Raw data for ternary system with initial concentrations: Pb^{2+}, 0.05N; Cu^{2+}, 0.05N.

Eq. Wt Pb	103.6	Dens. Res=	815 g/L	Pb(0) (ppm)	4780	Cu(0) (ppm)	1540
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Pb(0) (eq/L)	0.046139	Cu(0) (eq/L)	0.048504
X(0)=	2.17 eq/L	K(Pb)=	5.95	K(Cu)=	0.694		

Mass Res (g)	Conc Pb (ppm)	Conc Cu (ppm)	R L res/L sol	C(Pb) (eq/L)	C(Cu) (eq/L)	Pred(Pb) (eq/L)	Pred(Cu) (eq/L)	%Dif(Pb)	%Dif(Cu)	Pb Uptak (eq/L res)	Cu Uptak (eq/L res)	Pb Predic (eq/L res)	Cu Predi (eq/L res)	%er Pb	%er Cu	Total Upta (eq/L res)	Predicted (eq/L res)
0.7	2187	1270	0.0172	0.0211	0.0400	0.0185	0.0413	14.1083	-3.1477	1.4570	0.4951	1.6090	0.4194	-9.4433	18.0457	1.9521	2.0284
0.701	2212	1280	0.0172	0.0214	0.0403	0.0185	0.0413	15.4127	-2.3851	1.4409	0.4760	1.6067	0.4188	-10.3164	13.6736	1.9170	2.0255
1.049	1363	1068	0.0257	0.0132	0.0336	0.0104	0.0346	26.5036	-2.7809	1.2813	0.5775	1.3883	0.5401	-7.7125	6.9204	1.8588	1.9285
1.05	1372	1063	0.0258	0.0132	0.0335	0.0104	0.0346	27.3389	-3.2361	1.2767	0.5831	1.3870	0.5396	-7.9556	8.0530	1.8597	1.9266
1.749	461.7	554.7	0.0429	0.0045	0.0175	0.0034	0.0198	31.0754	-11.7633	0.9712	0.7230	0.9958	0.6688	-2.4721	8.1143	1.6942	1.6646
1.751	462.9	554.4	0.0430	0.0045	0.0175	0.0034	0.0198	31.4161	-11.8110	0.9698	0.7224	0.9946	0.6680	-2.4992	8.1473	1.6922	1.6626
2.449	214.1	251.3	0.0601	0.0021	0.0079	0.0014	0.0103	47.6145	-23.1557	0.7333	0.6754	0.7444	0.6357	-1.4900	6.2429	1.4087	1.3801
2.449	239.9	281.6	0.0601	0.0023	0.0089	0.0014	0.0103	65.4026	-13.8904	0.7292	0.6595	0.7444	0.6357	-2.0466	3.7449	1.3887	1.3801
3.151	143.3	161.5	0.0773	0.0014	0.0051	0.0007	0.0059	97.6007	-13.7862	0.5788	0.5615	0.5876	0.5510	-1.5036	1.9092	1.1403	1.1386
3.152	148.8	176.2	0.0773	0.0014	0.0055	0.0007	0.0059	105.1848	-5.9389	0.5779	0.5553	0.5874	0.5508	-1.6204	0.8224	1.1333	1.1382
4.2	87.44	94.13	0.1031	0.0008	0.0030	0.0004	0.0032	111.0039	-7.3524	0.4395	0.4418	0.4438	0.4396	-0.9708	0.5193	0.8813	0.8833
4.2	77.69	91.94	0.1031	0.0007	0.0029	0.0004	0.0032	87.4759	-9.5079	0.4404	0.4425	0.4438	0.4396	-0.7650	0.6716	0.8829	0.8833
4.899	71.11	73.82	0.1202	0.0007	0.0023	0.0003	0.0024	128.7967	-3.1234	0.3781	0.3841	0.3813	0.3835	-0.8429	0.1626	0.7622	0.7648
4.9	80.51	89.29	0.1202	0.0008	0.0028	0.0003	0.0024	159.0412	17.1785	0.3772	0.3800	0.3812	0.3834	-1.0409	-0.8942	0.7572	0.7646
6.3	50.3	56.26	0.1546	0.0005	0.0018	0.0002	0.0016	142.7606	10.7480	0.2953	0.3023	0.2971	0.3034	-0.6215	-0.3666	0.5976	0.6005
6.3	65.63	70.83	0.1546	0.0006	0.0022	0.0002	0.0016	216.7471	39.4291	0.2943	0.2993	0.2971	0.3034	-0.9436	-1.3450	0.5936	0.6005
7	67.96	63.94	0.1718	0.0007	0.0020	0.0001	0.0013	555.9846	54.9122	0.2648	0.2706	0.2680	0.2748	-1.2076	-1.5123	0.5354	0.5428
7	66.71	66.4	0.1718	0.0006	0.0021	0.0001	0.0013	543.9189	60.8722	0.2648	0.2702	0.2680	0.2748	-1.1814	-1.6764	0.5350	0.5428
								133.7437	3.9590					-3.0352	3.9574		

Raw data for ternary system with initial concentrations: Pb^{2+}, 0.05N; Cu^{2+}, 0.1N.

Eq. Wt Pb	103.6	Dens. Res	815 g/L	Pb(0) (ppm)	4765	Cu(0) (ppm)	3116
Eq. Wt Cu	31.75	Vol Soln=	0.05 L	Pb(0) (eq/L)	0.045994	Cu(0) (eq/L)	0.098142
X(0)=	2.17 eq/L	Alpha(A)	5.95	Alpha(B)=	0.694		

Mass Res (g)	Conc Pb (ppm)	Conc Cu (ppm)	R Lres/L sol	C(Pb) (eq/L)	C(Cu) (eq/L)	Pred(Pb) (eq/L)	Pred(Cu) (eq/L)	%Dif(Pb)	%Dif(Cu)	Pb Uptak (eq/L res)	Cu Upta (eq/L res)	Pb Predi (eq/L res)	Cu Predi (eq/L res)	%er Pb	%er Cu	Total Upta (eq/L res)	Predicted (eq/L res)
0.699	2649	2720	0.0172	0.0256	0.0857	0.0220	0.0871	16.2250	-1.6426	1.1907	0.7271	1.3988	0.6437	-14.8765	12.9573	1.9178	2.0425
0.7	2603	2700	0.0172	0.0251	0.0850	0.0220	0.0870	14.2067	-2.2536	1.2149	0.7627	1.3968	0.6486	-13.0260	17.5972	1.9776	2.0454
1.049	1875	2408	0.0257	0.0181	0.0758	0.0147	0.0787	23.1187	-3.6309	1.0837	0.8662	1.2157	0.7552	-10.8597	14.6977	1.9499	1.9709
1.05	1927	2430	0.0258	0.0186	0.0765	0.0147	0.0786	26.5332	-2.6267	1.0631	0.8385	1.2145	0.7584	-12.4636	10.5649	1.9017	1.9729
1.749	1001	1793	0.0429	0.0097	0.0565	0.0071	0.0598	36.0868	-5.5645	0.8465	0.9709	0.9062	0.8933	-6.5875	8.6787	1.8174	1.7995
1.75	1026	1825	0.0429	0.0099	0.0575	0.0071	0.0597	39.4856	-3.7181	0.8404	0.9468	0.9057	0.8951	-7.2079	5.7742	1.7872	1.8008
2.449	556	1225	0.0601	0.0054	0.0386	0.0038	0.0430	41.2315	-10.2728	0.6760	0.9910	0.7021	0.9175	-3.7133	8.0109	1.6670	1.6196
2.45	552.2	1229	0.0601	0.0053	0.0387	0.0038	0.0429	40.2662	-9.7700	0.6764	0.9885	0.7018	0.9188	-3.6264	7.5873	1.6649	1.6206
3.15	297.3	772.9	0.0773	0.0029	0.0243	0.0023	0.0304	24.7692	-19.9233	0.5579	0.9547	0.5653	0.8763	-1.3038	8.9409	1.5126	1.4416
3.15	300.6	768.9	0.0773	0.0029	0.0242	0.0023	0.0304	26.1541	-20.3378	0.5575	0.9563	0.5653	0.8763	-1.3767	9.1268	1.5138	1.4416
4.2	140.8	410.9	0.1031	0.0014	0.0129	0.0012	0.0187	13.2561	-30.7929	0.4331	0.8266	0.4346	0.7708	-0.3551	7.2484	1.2597	1.2054
4.2	139.2	403.2	0.1031	0.0013	0.0127	0.0012	0.0187	11.9691	-32.0898	0.4332	0.8290	0.4346	0.7708	-0.3206	7.5537	1.2622	1.2054
4.899	105.1	298.4	0.1202	0.0010	0.0094	0.0009	0.0142	12.7199	-33.8139	0.3741	0.7382	0.3751	0.6982	-0.2539	5.7201	1.1123	1.0733
4.9	107.3	300.1	0.1202	0.0010	0.0095	0.0009	0.0142	15.0794	-33.4368	0.3739	0.7376	0.3750	0.6981	-0.3010	5.6563	1.1115	1.0731
6.299	62.26	174.1	0.1546	0.0006	0.0055	0.0005	0.0090	20.1931	-39.0726	0.2937	0.5994	0.2943	0.5767	-0.2219	3.9449	0.8931	0.8710
6.299	59.01	173.9	0.1546	0.0006	0.0055	0.0005	0.0090	13.9189	-39.1426	0.2939	0.5995	0.2943	0.5767	-0.1530	3.9519	0.8933	0.8710
6.999	54.63	145.5	0.1718	0.0005	0.0046	0.0004	0.0075	31.8292	-38.8976	0.2647	0.5447	0.2655	0.5277	-0.2792	3.2185	0.8094	0.7932
7	47.65	137.1	0.1718	0.0005	0.0043	0.0004	0.0075	14.9855	-42.4252	0.2651	0.5462	0.2654	0.5277	-0.1315	3.5104	0.8113	0.7931
								23.4460	-20.5229					-4.2810	8.0411		

APPENDIX C: RAW DATA FOR PACKED BED EXPERIMENTS

Raw data for packed bed experiment with initial concentration: Ni^{2+}, 0.0085N.

Eq.Wt Ni	29.35	Ni(0) (eq/L	0.0085	
LiqVol (L)	Conc Ni (ppm)	Ni Solutio (eq/L)	Ni Resin (eq/L res)	Tot (eq/L res)
0	0	0	0	0
1.62	18.13	0.0006	1.3260	1.3260
1.76	26.34	0.0009	1.4343	1.4343
1.9	26.32	0.0009	1.5407	1.5407
2.04	46.82	0.0016	1.6421	1.6421
2.18	75.39	0.0026	1.7319	1.7319
2.32	111.7	0.0038	1.8062	1.8062
2.46	160.7	0.0055	1.8602	1.8602
2.6	203.9	0.0069	1.8921	1.8921
2.74	234.1	0.0080	1.9066	1.9066
2.88	246	0.0084	1.9110	1.9110
3	253.6	0.0086	1.9108	1.9108

Raw data for packed bed experiment with initial concentrations: Ni^{2+}, 0.0047N, Cd^{2+}, 0.0041N.

Eq.Wt Cd	56.2	Eq.Wt Ni	29.35	Cd(0) (eq/L)	0.004126	Ni(0) (eq/L)	0.004712

LiqVol (L)	Conc Ni (ppm)	Conc Cd (ppm)	Ni Solutio (eq/L)	Cd Solution (eq/L)	Total Soluti (eq/L)	Ni Resin (eq/L res)	Cd Resin (eq/L res)	Total Resin (eq/L res)
0	0	0	0	0	0	0	0	0
1.62	8.448	10.98	0.0003	0.0002	0.0005	0.7400	0.6526	1.3927
1.76	12.32	15.83	0.0004	0.0003	0.0007	0.8011	0.7071	1.5081
1.9	17	20.36	0.0006	0.0004	0.0009	0.8600	0.7603	1.6204
2.04	26.03	31.77	0.0009	0.0006	0.0015	0.9157	0.8116	1.7274
2.18	39.6	47.23	0.0013	0.0008	0.0022	0.9661	0.8595	1.8256
2.32	58.03	68.51	0.0020	0.0012	0.0032	1.0087	0.9029	1.9116
2.46	83.26	97.99	0.0028	0.0017	0.0046	1.0410	0.9399	1.9809
2.6	113.1	132.7	0.0039	0.0024	0.0062	1.0602	0.9690	2.0291
2.74	139.3	163.6	0.0047	0.0029	0.0077	1.0659	0.9898	2.0557
2.88	154.7	183.3	0.0053	0.0033	0.0085	1.0618	1.0044	2.0662
3.02	157.5	192.9	0.0054	0.0034	0.0088	1.0533	1.0153	2.0686
3.16	158.1	196.8	0.0054	0.0035	0.0089	1.0440	1.0245	2.0685

Raw data for packed bed experiment with initial concentrations: Ni^{2+}, 0.0046N, Cd^{2+}, 0.0042N.

Eq.Wt Cd 56.2 Eq.Wt Ni 29.35 Cd(0) (eq/L) 0.0041512 Ni(0) (eq/L) 0.0046303

LiqVol (L)	Conc Ni (ppm)	Conc Cd (ppm)	Ni Solutio (eq/L)	Cd Solution (eq/L)	Total Soluti (eq/L)	Ni Resin (eq/L res)	Cd Resin (eq/L res)	Total Resin (eq/L res)
0	0	0	0	0	0	0	0	0
1.52	11.68	14.97	0.0004	0.0003	0.0007	0.6736	0.6107	1.2843
1.64	16.4	20	0.0006	0.0004	0.0009	0.7234	0.6568	1.3802
1.76	22.96	28.8	0.0008	0.0005	0.0013	0.7709	0.7014	1.4723
1.88	31.9	40.02	0.0011	0.0007	0.0018	0.8153	0.7439	1.5592
2	41.5	50.28	0.0014	0.0009	0.0023	0.8558	0.7841	1.6399
2.12	53.42	64.54	0.0018	0.0011	0.0030	0.8920	0.8216	1.7136
2.24	65.93	79.63	0.0022	0.0014	0.0037	0.9231	0.8561	1.7792
2.36	79.32	95.5	0.0027	0.0017	0.0044	0.9490	0.8872	1.8362
2.48	91.78	110.9	0.0031	0.0020	0.0051	0.9696	0.9150	1.8845
2.6	105.6	127.7	0.0036	0.0023	0.0059	0.9848	0.9393	1.9241
2.72	119.1	144.5	0.0041	0.0026	0.0066	0.9944	0.9600	1.9545
2.84	131.9	161.4	0.0045	0.0029	0.0074	0.9987	0.9772	1.9759
2.96	141.3	175.9	0.0048	0.0031	0.0079	0.9984	0.9910	1.9894
3.08	148.1	188.1	0.0050	0.0033	0.0084	0.9948	1.0020	1.9968
3.2	151.3	197.6	0.0052	0.0035	0.0087	0.9892	1.0106	1.9998
3.32	154.4	205.2	0.0053	0.0037	0.0089	0.9822	1.0174	1.9996
3.44	152.4	208.5	0.0052	0.0037	0.0089	0.9751	1.0231	1.9981
3.56	151	213	0.0051	0.0038	0.0089	0.9686	1.0279	1.9965
3.68	149.8	216.4	0.0051	0.0039	0.0090	0.9627	1.0318	1.9945
3.8	147.4	217.9	0.0050	0.0039	0.0089	0.9575	1.0353	1.9928
3.92	145.1	218.6	0.0049	0.0039	0.0088	0.9533	1.0385	1.9918
4.04	144.7	221.1	0.0049	0.0039	0.0089	0.9496	1.0414	1.9910
4.16	144	222.7	0.0049	0.0040	0.0089	0.9461	1.0438	1.9899
4.28	143.2	225.4	0.0049	0.0040	0.0089	0.9430	1.0458	1.9888

Raw data for packed bed experiment with initial concentrations: Ni^{2+}, 0.0022N, Cd^{2+}, 0.0023N, Pb^{2+}, 0.0027N.

Eq.Wt Cd	56.2	Eq.Wt Ni	29.35	Cd(0) (eq/L)	0.0023149	Ni(0) (eq/L)	0.0022058
Eq.Wt Pb	103.6	Pb(0) (eq/L)	0.0027259				

LiqVol (L)	Conc Ni (ppm)	Conc Cd (ppm)	Conc Pb (ppm)	Ni Solution (eq/L)	Cd Soluti (eq/L)	Pb Solutio (eq/L)	Total Solut (eq/L)	Ni Resin (eq/L res)	Cd Resin (eq/L res)	Pb Resin (eq/L res)	Total Resi (eq/L res)
0	0	0	0	0	0	0	0	0	0	0	0
0.66	0.3531	0.5429	1.22	0.0000	0.0000	0.0000	0.0000	0.1452	0.1525	0.1795	0.4772
0.88	0.558	0.9009	1.272	0.0000	0.0000	0.0000	0.0000	0.1934	0.2031	0.2392	0.6357
1.1	1.077	1.499	1.361	0.0000	0.0000	0.0000	0.0001	0.2413	0.2536	0.2989	0.7938
1.32	1.634	2.411	1.521	0.0001	0.0000	0.0000	0.0001	0.2888	0.3037	0.3586	0.9511
1.54	2.703	3.865	1.797	0.0001	0.0001	0.0000	0.0002	0.3357	0.3534	0.4182	1.1073
1.76	4.507	6.521	2.361	0.0002	0.0001	0.0000	0.0003	0.3815	0.4023	0.4777	1.2616
1.98	7.665	12.72	3.155	0.0003	0.0002	0.0000	0.0005	0.4255	0.4495	0.5371	1.4121
2.2	12.28	18.94	4.104	0.0004	0.0003	0.0000	0.0008	0.4665	0.4942	0.5963	1.5571
2.42	20.04	31.35	5.175	0.0007	0.0006	0.0000	0.0013	0.5030	0.5353	0.6553	1.6936
2.64	32.85	50.72	6.901	0.0011	0.0009	0.0001	0.0021	0.5317	0.5702	0.7140	1.8158
2.86	52.01	79.78	9.056	0.0018	0.0014	0.0001	0.0033	0.5484	0.5956	0.7722	1.9162
3.08	72.99	112.7	12.28	0.0025	0.0020	0.0001	0.0046	0.5501	0.6088	0.8300	1.9888
3.3	98.38	154.3	13.8	0.0034	0.0027	0.0001	0.0062	0.5344	0.6075	0.8872	2.0290
3.52	110.4	180.6	16.35	0.0038	0.0032	0.0002	0.0071	0.5046	0.5929	0.9439	2.0414
3.74	110.8	190.9	19.31	0.0038	0.0034	0.0002	0.0074	0.4703	0.5711	1.0001	2.0415
3.96	107.5	195.3	23.02	0.0037	0.0035	0.0002	0.0074	0.4370	0.5464	1.0556	2.0390
4.18	104.6	197.7	28.51	0.0036	0.0035	0.0003	0.0074	0.4060	0.5204	1.1101	2.0365
4.4	101.8	199.5	34.36	0.0035	0.0035	0.0003	0.0073	0.3772	0.4936	1.1634	2.0342
4.62	99	200.8	41.16	0.0034	0.0036	0.0004	0.0073	0.3505	0.4662	1.2153	2.0320
4.84	96.68	201	48.48	0.0033	0.0036	0.0005	0.0073	0.3256	0.4385	1.2658	2.0299
5.06	93.77	199.3	57.72	0.0032	0.0035	0.0006	0.0073	0.3028	0.4111	1.3145	2.0283
5.28	91.98	198	69.14	0.0031	0.0035	0.0007	0.0073	0.2817	0.3842	1.3610	2.0269
5.5	89.47	195.7	80.43	0.0030	0.0035	0.0008	0.0073	0.2622	0.3581	1.4051	2.0254
5.72	86.69	190.6	94.86	0.0030	0.0034	0.0009	0.0073	0.2447	0.3334	1.4464	2.0245
5.94	84.14	184.8	111.2	0.0029	0.0033	0.0011	0.0072	0.2292	0.3109	1.4845	2.0246
6.16	81.55	179.1	130.1	0.0028	0.0032	0.0013	0.0072	0.2157	0.2906	1.5188	2.0251

APPENDIX D: IONIC RADII

Ion	Radius (nm)
Ni^{2+}	70
Cu^{2+}	73
Zn^{2+}	75
Cd^{2+}	97
Pb^{2+}	120