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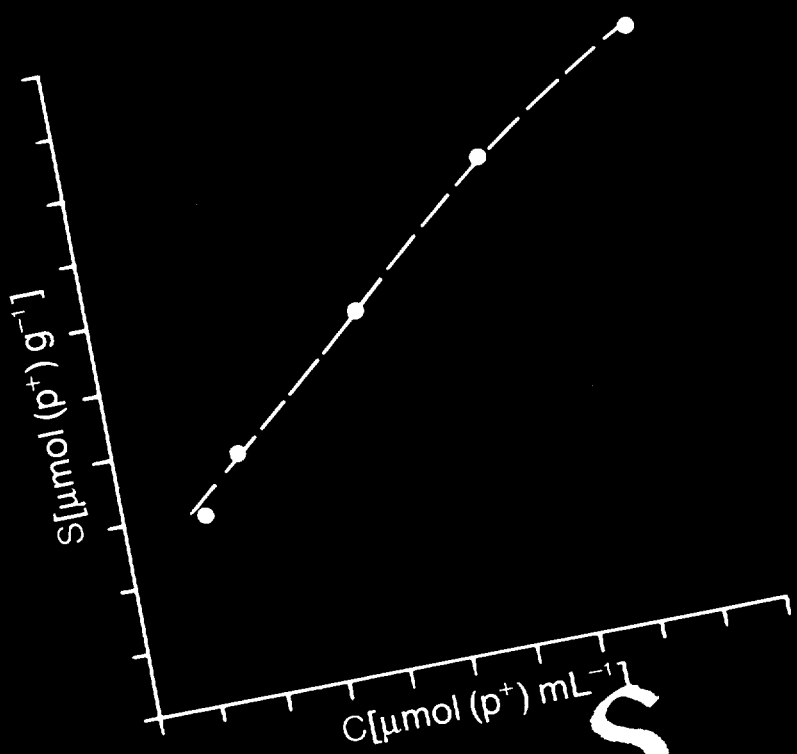
Preliminary Report on Sorption Modeling



$$S = \frac{S_{max} K_D^{\beta} C^{\beta}}{1 + K_D^{\beta} C^{\beta}}$$

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Preliminary Report on Sorption Modeling

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PRELIMINARY REPORT ON SORPTION MODELING

by
H. R. Fuentes, W. L. Polzer, J. Gruber, B. Lauctes,
and E. H. Essington

ABSTRACT

The generic objective of this study is to inventory and model batch sorption data obtained for the Nevada Nuclear Waste Storage Investigations Project by the Los Alamos National Laboratory. This report addresses three main topics: the modeling by various isotherms of data sets inventoried from about 1500 data entries, potential occurrence of precipitation in the sorption experiments, and the evaluation of a computer code to study changes in chemical isolation caused by changes in the chemistry of the porous media.

In general the sorption data for strontium, cesium, barium, and europium were found to be modeled best by the Freundlich and Modified Freundlich isotherms, followed by the linear isotherm; the poorest fits were usually observed with the Langmuir isotherm. The effect of particle size of tuff material on modeling was found to be relatively insignificant for the available size ranges and data sets. Thus, in general, modeling of combined data for different fractions of the same tuff sample remained as effective as before combining data of different sizes. Modeling combined data from samples within the same stratigraphic unit of Yucca Mountain indicates that simple models having acceptable statistical correlation may be found. Best modeling results were obtained for the Topopah Spring and Calico Hills units; poorest results were obtained for the Tram, Prow Pass, and Bullfrog units. In every case, however, at least one isotherm modeled the data from each stratigraphic unit with acceptable statistical correlation.

The analysis of sorption data for the potential precipitation of strontium and barium indicates that the precipitation of $SrSO_4$ may have occurred in experiments with the YM-22 and G1-2840 tuff samples at the high initial concentrations of strontium. The precipitation of BaSO also potentially occurred in experiments with the YM-22 tuff samples at the high initial concentrations of barium. Because of the large CEC of the YM-38 tuff sample, both strontium and barium were probably removed from solution by the cation exchange process rather than by precipitation.

The modeling of microscopic processes on metal oxide surfaces suggests that the intrusion into the isolated environment of a contaminant by a water of different chemical composition can mobilize that contaminant. The intrusion of that water causes the release of protons from oxide surfaces together with the adsorption or desorption of electrolyte ions. As a result the contaminant may be desorbed and mobilized; thus the isolation of the contaminant is breached.

I. INTRODUCTION

This report is a compilation of partial efforts made on the Sorption and Precipitation Subtask, Nevada Nuclear Waste Storage Investigation (NNWSI) Project, by Los Alamos National Laboratory during FY85-86. The report addresses the evaluation of adsorption data obtained in laboratory batch tests for strontium, cesium, barium, europium, and cerium.

The report is divided into three main sections, which address modeling by various isotherms of data sets inventoried from about 1500 entries (Sec. II), potential precipitation during adsorption experiments for the test water chemistries (Sec. III), and the development of a chromatographic model to evaluate the changes in chemical isolation caused by changes in the chemistry of the porous media (Sec. IV).

II. ADSORPTION MODELING

A. Introduction

The scope of this subtask from December 1985 to September 1986 was to model adsorption data from experiments with tuff samples from the Yucca Mountain area. Experiments were performed by the Nuclear and Radiochemistry Group (INC-11) of the Los Alamos National Laboratory.[1] The following radionuclides were studied in this period: ^{85}Sr, ^{137}Cs, ^{133}Ba, ^{152}Eu, and ^{141}Ce.

Five specific objectives were defined in the scope of this subtask (Table I):

1. Selection of well-documented data sets from computer files stored by INC-11.
2. Quantitative and qualitative inventory of the selected data base to identify those data sets, or combinations of data sets, that have a minimum of three different initial concentrations.
3. Modeling of identified data sets and their combinations by at least three different conventional isotherms (a maximum of four isotherms).
4. Comparison of the effectiveness of the models to represent analyzed data sets. The comparison is based on statistical correlation parameters, index of determination, and standard error of the curve fitting.
5. Quality assurance and sensitivity studies. Quality assurance was completed by performing simultaneous analyses by different modelers on some common sets of data. Sensitivity studies focused only on evaluating the effects of different estimates of cation exchange capacities (CEC) on those isotherms that are explicitly a function of this parameter.

It should be understood that the experiments from which the sets of data were generated were not intended to be used for equilibrium or nonequilibrium (kinetics) modeling. Those experiments were intended to provide generic information about the effects of environmental parameters, i.e., pH, temperature, particle size, atmosphere, and sorption time, on adsorption behavior. However, there is a need to obtain as much information as possible from these experiments both to improve present data bases and to plan future experiments.

This report includes only the results from the modeling of equilibrium conditions. The term equilibrium as used here refers to a pseudoequilibrium condition because absolute equilibrium was not verified.

B. Data Bases

About 1500 entries relative to batch equilibrium and kinetic adsorption experiments were retrieved from INC-11 computer files (1,100) and records (400). These entries are documented in a Los Alamos report by K. Thomas.[1] The entries are defined for each core sample and element studied by the following experimental factors: temperature, atmosphere, sampling time, initial element concentration, and particle size range; values for sorption ratios define the results from each experiment. The sorption ratio is defined as

$$Rd = \frac{\text{activity in solid phase per unit mass of solid}}{\text{activity in solution per unit volume of solution}} \qquad (1)$$

The entries retrieved from INC-11 were used to create a data base for further inventory and modeling. The Rd-values and the initial element concentration in solution, along with the mass of sample (1 g) and the solution volume (20 mL) used in the experiments, were used to calculate the amounts of element absorbed on the solid S (μmol(p^+)/g) and the respective solution concentration C (μmol(p^+)/mL) at various equilibration times. These calculations yielded a workable data base with the entries grouped for each sample and element by temperature, atmosphere, equilibration time, initial element concentration in solution, amount adsorbed on the solid, and amount in solution (Appendix A). The data base includes experiments at two temperatures, ambient and 70°C, and at two atmospheres, air and nitrogen. The nitrogen atmosphere, or controlled atmosphere (CA), contained $\leq$0.2 ppm oxygen and $\leq$20 ppm carbon dioxide.

The entries were evaluated in terms of their potential use for equilibrium modeling. The suitability of data sets was based on the criterion that a minimum of three initial concentrations in solution was necessary to perform isotherm analyses when all other variables were constant. About 1% of the grouped data sets met the criterion. These data sets were mostly for ambient temperature in air at 21 days of equilibration time at various particle sizes. The sets of data that met the criterion are listed in Table II. YM-22 was collected from the Topopah Spring formation unit, YM-38 from the Calico Hills unit, and G1-2840 from the Tram unit.[1] Generally, there were not enough data to model cerium; in most cases only strontium, cesium, barium, and europium were modeled. An additional sample, G1-2363, was also analyzed for barium because it met the criterion after combination of various size ranges; this sample corresponds to the Bullfrog unit. The origin and petrologic characterization of these and other samples included in this report are summarized in Tables III-1 and 2.

C. Modeling Strategy

Because of the limited data sets with which to test isotherms, a strategy was devised to get as much information as possible from the workable data base. This strategy considers four cases for modeling (Table IV). In case 1 the data sets include those data for each particle size range where the concentration of solute adsorbed on the solid is less than the CEC. The intention was to model only adsorption; precipitation may be involved in those instances where the amount adsorbed is greater than the CEC. In case 2 the data sets include the data used in case 1 as well as data in which the adsorbed concentrations are greater than the CEC; sorption may involve the process of precipitation in this case (refer to Sec. III). In case 3 the data sets include the combined data for all particle sizes and only one value for

CEC is assumed. The largest CEC was assumed when values for each size fraction were available. In case 4 the data sets include combined data for all particle sizes from the same stratigraphic unit (Table IV). In this last case only those isotherms that do not include CEC as a parameter were used in modeling because a large variability of CEC may occur within the same stratigraphic unit.

The expressions tested were the linear, the Langmuir, the Freundlich, and a Modified Freundlich; only the Modified Freundlich expression depends on the CEC of the samples.

A Fortran 77 computer program (Appendix B), named SOSCOCO (Solute Sorption Computer Code), was devised to test the various isotherms. The program operates in three sequential steps:

1. Data are sorted from the workable data base in accordance with desired combinations, e.g., by size (subroutine GET).
2. The isotherms are fitted to the same data sets by linear regressional analysis; empirical constants, correlation coefficients and standard errors are estimated by using subroutine AN.
3. The raw data sets and those predicted from isotherms are graphed by the subroutine MAP. Also included in this subroutine is the plotting of the predicted versus the observed amounts adsorbed.

Thus the output from SOSCOCO for each data set is composed of a graph of S versus C of the raw data and of those predicted by each isotherm, a graph of S-calculated versus S-observed (to qualitatively judge the effectiveness of the models), and tabulated information on constants and regressional parameters for each isotherm.

D. Models

The simplest and most widely used of the equilibrium sorption isotherms is that given by the linear relationship

$$S = K_d C \tag{2}$$

where S = mass of solute sorbed by the soil,

C = concentration of solute in the soil solution, and

K_d = distribution coefficient.

This expression has been frequently used in transport models to describe the sorption of radioactive and nonradioactive solutes by soils. One limitation is that it does not imply a maximum quantity of adsorption.

The distribution coefficient K_d is a measure of the retention of solute by the soil and is assumed to be independent of concentration. This is not necessarily the case, and thus conclusions from analyses based on assumptions of linear behavior may not be valid.

Langmuir developed a quantitative model that has also been widely applied to describe experimental data.[2] The Langmuir equation was derived for the sorption of gases on a solid surface. Nevertheless, it has been extended to include the sorption of solutes to solids. The basic equation takes the form

$$S = \frac{k\,b\,C}{1 + kC}\ , \tag{3}$$

where k, b = empirical constants.

In this equation k is the Langmuir adsorption constant, which can be related to the binding energy of the adsorbate, and b is the maximum adsorption capacity of the solid.

By rearranging Equation (3) as described below, a plot of C/S versus C results in a linear representation of adsorption data with a slope of 1/b and an intercept of 1/kb.

$$C/S = (1/b)C + 1/kb. \tag{4}$$

Greater accuracy is obtained in estimating the slope of the curve than in estimating the intercept for reasonably low adsorbate concentrations used in most adsorption experiments. Thus, a more accurate estimate of b can be obtained from adsorption data using Equation (4) than other possible

linearizations of Equation (3) for which the intercept is equal to b or 1/b. This isotherm is based on the theoretical assumption that the sorption sites are homogeneously distributed relative to energy potentials.[2] This assumption does not apply to most sorbent surfaces, e.g., soil and geologic material.

The Freundlich isotherm has the form

$$S = KC^N, \tag{5}$$

where K,N = empirical constants.

Estimation of the constants is possible by the simple transformation to the equation

$$\log S = N \log C + \log K. \tag{6}$$

This equation is also very popular in the literature because that log-log equations are easy to use and are relatively insensitive to errors in the data. However, the Freundlich is limited in that it only shows linearity over a relatively narrow range of concentrations.

Solute exchange on soil adsorption sites is known to be heterogeneous, that is, not monoenergetic. Sips[3] derived the general Langmuir equation to accommodate sorption to a surface exhibiting heterogeneous sorption surfaces.

Crickmore and Wojciechowski derived rate models for adsorption and desorption from a Langmuir-type isotherm by allowing the adsorption energy to vary with the amount of solute adsorbed.[4] Their equations, as given by Murali and Aylmore[5] in the case of equilibrium conditions (Modified Freundlich isotherm), may be expressed as

$$S = \frac{S_{max} K_D^{\beta} C^{\beta}}{1+K_D^{\beta} C^{\beta}}. \tag{7}$$

Crickmore and Wojciechowski have described the parameter β as a measure of the coefficient of variation of the distribution of rate constants.[4]

Under those conditions a parameter A as given by Sposito[6] can be related to the parameter K_D as

$$A = S_{max} K_D^{\beta} \tag{8}$$

The parameter A is a measure of a weighted average distribution coefficient for which the parameter β describes the spread (coefficient of variation) of many distribution coefficients about an average distribution coefficient K_D (Ref. 7).

When the adsorbing solute is in trace quantities [$K_D^{\beta} C_1^{\beta} \ll 1$ in Equation (7)], Equation 7 becomes the Freundlich isotherm and A is equivalent to the distribution coefficient K in the Freundlich isotherm.

E. Results and Discussion

Results from modeling cases 1 through 4 are detailed for each data set in Appendices C through F. A typical set of results has a summary table with isotherm constants and statistical parameters, a curve of adsorbed concentration S [μmol(p+)/g] versus solution concentration C [μmol(p+)/mL] with both measured and predicted values, and a figure depicting the relationship between observed S-values and calculated S-values for each isotherm. Figures 1 and 2 are examples of the plots presented in the appendices. Figure 2 characterizes the effectiveness of each model in predicting a data set, either overestimating or underestimating the observed values (respectively above or below the 45° bisecting slope) throughout the range of experimental concentrations. Because experimental ranges cover various orders of magnitude, all the figures are drawn in log-log scale.

In case 1 (Appendix C), four isotherms are evaluated with data sets in which the amount adsorbed is less than the CEC of the sample. Tables V and VI summarize the statistical parameters and the isotherm constants from

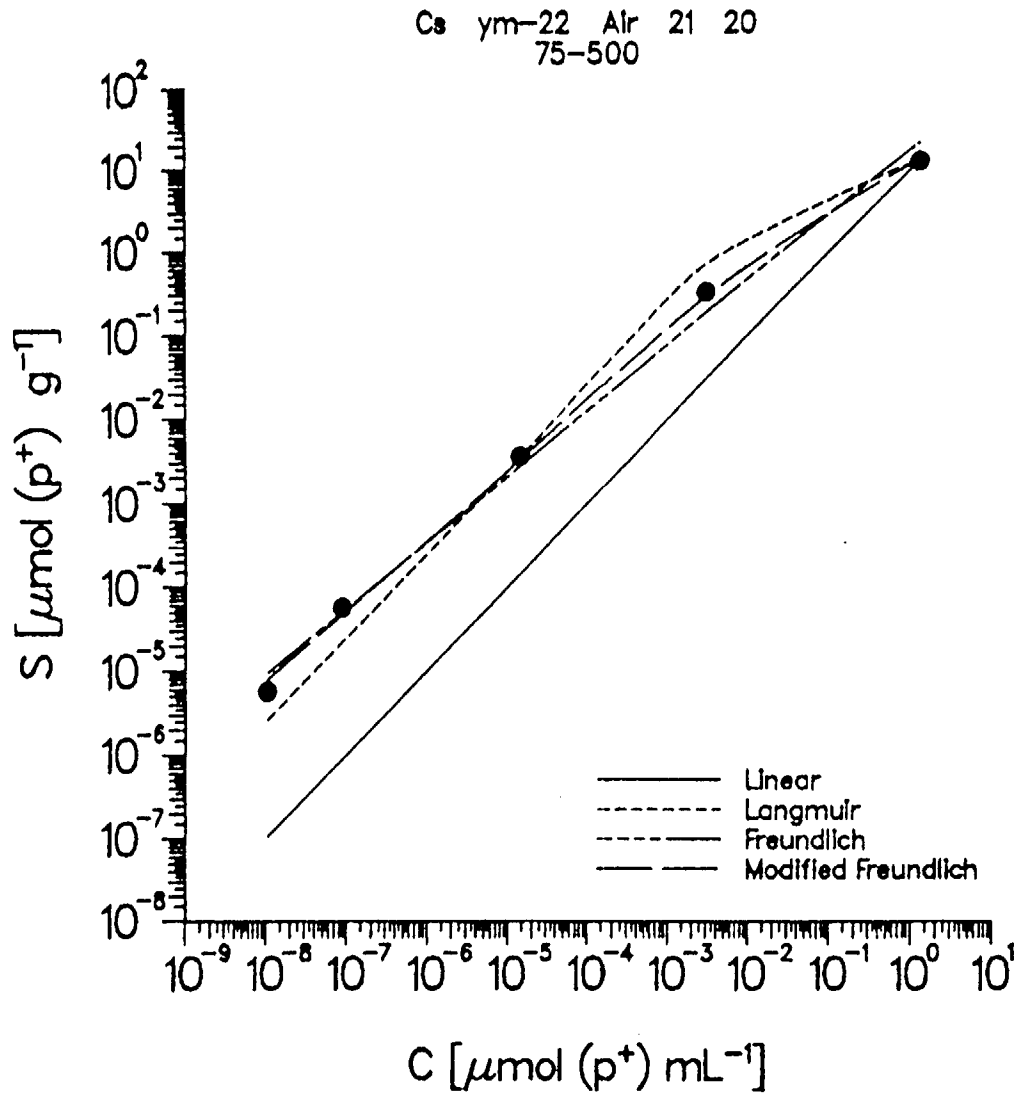

Figure 1. Typical results from the regressional analyses of isotherms for the adsorption of cesium on sample YM-22 (particle size with cation exchange capacity 20 μmol(p+) mL^{-1} at 21 days of equilibration time).

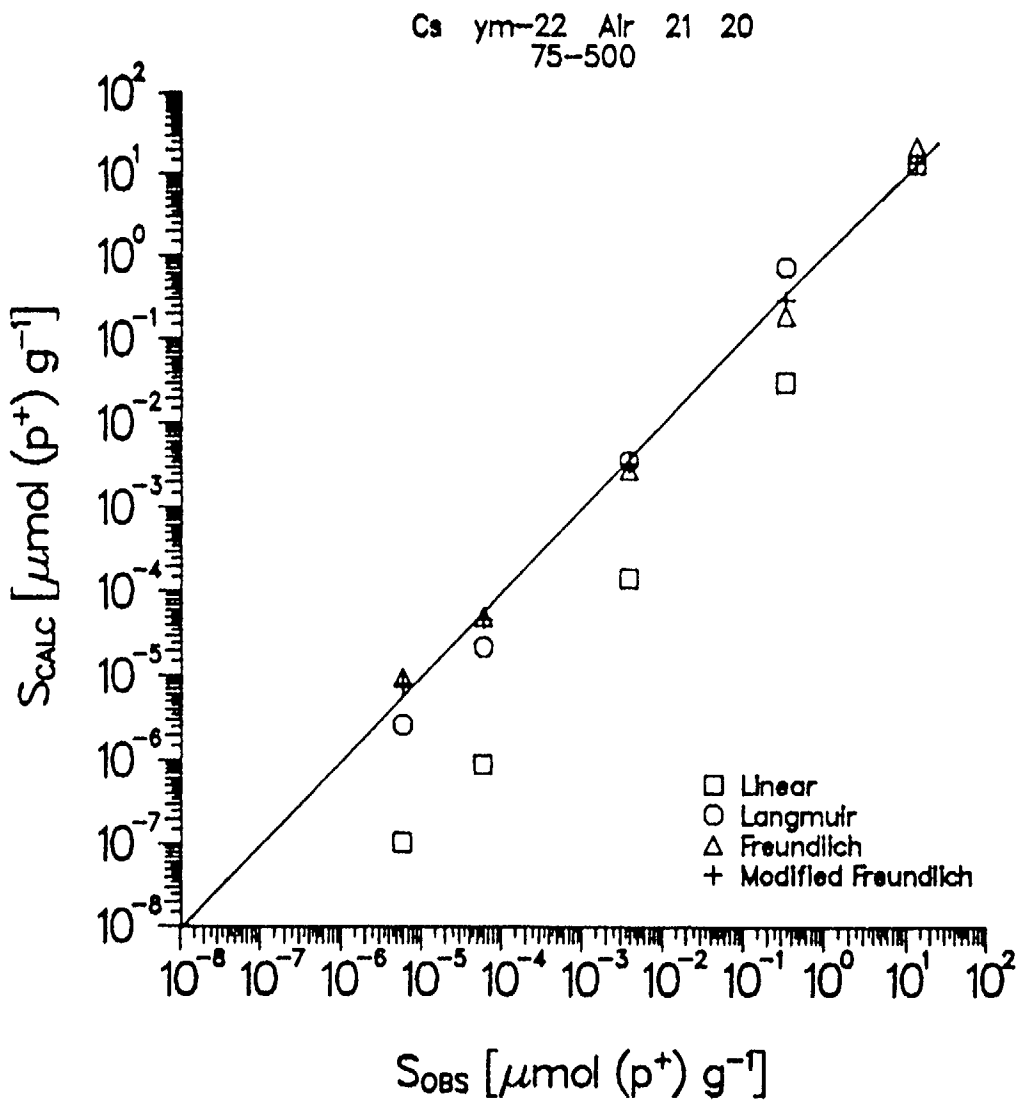

Figure 2. Typical results from the evaluation of the effectiveness of each isotherm in modeling the data set of Figure 1. Points above and below the 45°-slope are respectively overestimated or underestimated. The closer the points to this slope, the higher the effectiveness of the isotherm.

regressional analysis. Table VII qualitatively evaluates the effectiveness of each model as either excellent ($R^2 \geq 0.90$), good ($0.80 \leq R^2 < 0.90$), acceptable ($0.65 \leq R^2 < 0.80$), or poor ($R^2 \leq 0.65$). These criteria are based only on the judgment of the modelers. Overall, the best model is the Freundlich isotherm, followed very closely by the Modified Freundlich isotherm and the linear isotherm. The linear shows highest correlation in most cases except for europium, whose representation is acceptable in some cases and poor in others. The Langmuir isotherm appears to be the poorest model, although it presents good correlation coefficients for strontium and cesium in some samples. For the three best isotherms, no obvious differences are observed among the standard errors. The advantage of the Modified Freundlich isotherm over the empirical Freundlich expression is the wider range of concentrations over which it applies. However, it should be noted that the Freundlich isotherm is a special case of the Modified Freundlich isotherm and thus its constants can be related to those of the Modified Freundlich isotherm.

Values of N in the Freundlich isotherm and β in the Modified Freundlich isotherm for case 1 vary in the 0.7 to 1.0 range, with most values being about 1.0 and only two values for the G1-2840 sample being slightly over 0.7. This high range for β-values indicates very low heterogeneity of adsorption for strontium, cesium, barium, and europium on samples YM-22 and YM-38. On the other hand, the K_D-values from the Modified Freundlich isotherm increase from about 1.1 to 112 for strontium, cesium, europium, and barium. These K_D-values indicate the extent of adsorptivity of the solute. The statistics of correlation between isotherm constants from the <75-μm size range and those from the 75- to 500-μm size range were evaluated for YM-22 and YM-38 samples. No significant effect of particle size on the constants N and β was observed. However, the constants K, A, and K_D were affected by particle size.

Differences in these constants for the two ranges in particle size were as much as a factor of 3 in some cases.

Because previous studies[1] reported several values of CEC for the same sample but for different particle sizes, analyses for the Modified Freundlich isotherm were performed by using two values of CEC to define the sensitivity of CEC to the isotherm prediction. Details of the results are also documented in Appendix C. The statistical parameters, coefficients of determination and standard errors, and isotherm constants determined for each CEC are tabulated in Tables VIII and IX. The CEC ranged from 8 to 20 μmol(p+)/g for sample YM-22, and from 1,220 to 1,520 μmol(p+)/g for sample YM-38. The results indicate that the coefficients of determination, standard errors, and isotherm constants were not significantly affected by the values of the CEC used in the isotherm equation. However, significant changes in the statistical parameters and the isotherm constants did occur with sample G1-2840. The CEC ranged from 3 to 430 μmol(p+)/g, a range of over 2 orders of magnitude. Although statistics were slightly sensitive to a change in CEC (0.996 to 0.969 for the coefficient of determination R^2 and 0.187 to 0.120 for the standard error), the use of the lower CEC increased the constants A and K_D by about 3 orders of magnitude. On the other hand, the use of the lower CEC only increased the β-value by about 30% for strontium and by about 5% for cesium. The use of a lower CEC in the Modified Freundlich isotherm equation is reflected by higher adsorptivities (higher A- and K_d-values). Also, a lower degree of heterogeneity in adsorption (higher β-values) is reflected with the use of a lower CEC.

Sorption of a solute in excess of the CEC suggests that precipitation may be a significant process in the removal of a solute from solution. In case 2 the feasibility of representing experimental sorption data resulting from both adsorption and precipitation processes by the isotherm equations is explored.[8]

Only the linear, Langmuir, and Freundlich expressions were used in this evaluation because the Modified Freundlich isotherm expression breaks down when the amount adsorbed exceeds the CEC. Two samples contained sorbed concentrations in excess of the CEC: YM-22 for strontium at sizes <75 μm and 75 to 500 μm. Comparisons of data in which the CEC is not exceeded (case 1) with data in which the CEC is also exceeded (case 2) are given in Tables X, XI, and XII. The inclusion of the adsorption data when the amount adsorbed exceeds the CEC resulted in slightly higher standard errors with negligible effects on the coefficients of determination, with the exception of the Langmuir isotherm. The coefficients of determination for the Langmuir isotherm were much better when all the data were used in the regression analyses. Thus the results indicate that sorption can still be modeled by simple isotherms when sorption is influenced by precipitation.

In case 3 the possibility of modeling the combination of all particle sizes is explored by all four isotherms. Tabulated and graphed data are compiled in Appendix E. Tables XIII, XIV, and XV summarize those results. By combining data from all sizes, a set of data for barium adsorption on sample G1-2363 could be analyzed. The comparison of the statistical parameters and isotherm constants for cases 1 and 3 (individual particle size ranges and combined particle size ranges) indicates a general minor decrease in the values of the statistical parameters for case 3 compared with that for case 1, but that decrease does not impact the effectiveness of each of the models. The best expressions continue to be the Freundlich, closely followed by the linear isotherm, which surprisingly improved its poor representation for europium. The Langmuir isotherm remains a poor model for either set. The highest estimates of CEC were used in the Modified Freundlich analyses. Combining sizes did not affect isotherm constants, with the exception of those

from the Modified Freundlich expression. Combining data for the two particle size ranges, <75 μm and 75 to 500 μm, resulted in values of the Modified Freundlich isotherm constants that were between those estimated for the data from individual size ranges of <75 μm and 75 to 500 μm, but closer to the estimates for the data from the <75-μm range. The fact that the estimates are closer to those for data from the <75-μm range can be explained by the greater amount of data available for the <75-μm range. The greater amount of data outweighs the effects of regression. Another explanation is that the CEC used in the estimates more closely approximated the CEC of the <75-μm size range than that of the 75- to 500-μm size range.

In case 4 an attempt is made to explore the feasibility of using simple isotherms in modeling the retardation of contaminant according to stratigraphic units at Yucca Mountain.[1] The sorption data of samples belonging to the same stratigraphic units (Table IV) were combined for each element. Data for all ranges in particle size were combined to ensure at least three different concentrations as a minimum requirement for modeling. Detailed results are documented in Appendix F. Summaries of statistical parameters and isotherm constants for the linear, Langmuir, and Freundlich isotherms are compiled in Tables XVI through XXV for strontium, barium, cesium, europium, and cerium, respectively. It should be noted that this approach yielded enough points to study cerium. Because CEC estimates are quite different for samples within the same unit, the Modified Freundlich isotherm was excluded from the analyses in this study. Tables XVI, XVIII, XX, XXII, and XXIV include for each data set a qualitative description of the effectiveness of a model by ranking it as either poor, acceptable, good, or excellent, according to arbitrary ranges of coefficients of determination. Those models classified as acceptable could be used in retardation studies. In almost all trials, it is possible to find a model that is at least

acceptable. The more successful expressions are the Freundlich and linear isotherms. Best results are obtained for all the elements for Tpt (Topopah Spring) and Tht (Calico Hills) units. Poorest results were obtained for the Tct (Tram), Tcp (Prow Pass), and Tcb (Bullfrog) stratigraphic units. Unacceptable results occurred for barium in Tct and Tcb, cesium in Tcb, and europium in Tcp.

F. Conclusions

Results from modeling efforts for batch adsorption data can be summarized as follows:

1. Of nearly 1500 batch data sets, about 1% of the sets have three different concentrations to perform isotherm evaluations. This 1% corresponds to samples YM-22 and YM-38 for strontium, cesium, barium, and europium and to sample G1-2840 for strontium and cesium in particle size ranges <75 μm and 75 to 500 μm.
2. Regressional analyses show that the best isotherms are the Freundlich and Modified Freundlich, followed by the linear; the poorest general fit is by the Langmuir isotherm. Some data sets in a particular size range have groups of data which cluster around two concentration values; as it is expected a good correlation is found for all models in this situation, since almost any function can connect two points or two groups of points well. Future experiments should spread concentrations throughout the range of concern if the results are used for isotherm modeling.
3. Differences within the same order of magnitude of CEC's do not significantly affect the statistics and constants for all four isotherms, with the exception of the constants for the Modified Freundlich. Among these constants, those indicating the extent of

adsorption (A and K_D) are much more sensitive than that related to the degree of heterogeneity (β). Differences of several orders of magnitude in CEC's do significantly alter both statistics and model constants.

4. Equilibrium conditions above CEC estimates can effectively be represented by the linear and Freundlich isotherms without significant changes with respect to the case when values above CEC are not included.

5. Combination of all sizes for modeling by some isotherms allowed analysis for barium in sample G1-2363. Although decreases in statistical correlation occur, the models remain as effective as before any size mixtures.

6. Attempts to model data from different samples in the stratigraphic unit indicate that simple models may be found with acceptable statistical correlation. Best results were obtained for the Topopah Spring and Calico Hills stratigraphic units. Poorest results were for the Tram, Prow Pass, and Bullfrog units for barium, europium, and cesium, respectively. Only linear, Langmuir, and Freundlich expressions were evaluated for stratigraphic units.

III. PRECIPITATION ANALYSES

A. Introduction

Precipitation reactions may influence the sorption process. For example, the solubility of barium was found to be near saturation with respect to the mineral barite ($BaSO_4$) for the J-13 well water.[9] This water was used in determining sorption of the tracers barium, strontium, cesium, europium, and cerium on various tuff samples from Yucca Mountain. The near saturation of barium suggests that any additional barium may result in precipitation. The

strontium concentration of the original J-13 well water was below that for the solubility of strontianite ($SrCO_3$), the strontium mineral most likely to precipitate. However, precipitation could occur with the addition of the strontium tracer to the J-13 well water/tuff systems. The solubility of cesium was found to be large;[9] therefore, precipitation of cesium under the conditions of the sorption experiments would not occur. Europium and cerium solubilities were not evaluated.[9]

The objective of the analyses is to evaluate the potential influence of precipitation on the sorption isotherms of barium and strontium when the J-13 well water is contacted with YM-22, YM-38, and G1-2840 tuff samples. The concentrations of barium and strontium used in the sorption experiments ranged from 2×10^{-7} to 2×10^{-3} moles/L.

The potential for removal from solution of a tracer by the precipitation process was evaluated from the solubility of the tracer in equilibrium with an assumed precipitated solid. The solubility was calculated from equilibrium constants of reactions involving the tracer of interest and other chemical constitutents in the water in contact with the tuff sample. Although the concentration of the tracer was measured at the completion of the water/tuff contact, the other constituents were not analyzed at that time. Those analyses were performed at the time the tuff was in contact with the water for 21 days, but before the tracer was added. The calculations of solubility were performed with the computer code MINEQL and those data in its software program. Some additional data were obtained from the computer code EQ3/6.

B. Data Bases

The chemical compositions of the original J-13 well water[10] and J-13 Well water in contact with YM-22, YM-38,[1] and G1-2840[11] tuff samples are given in Table XXVI. More constituents were analyzed in the original water than in the other waters. The concentrations of those constituents not analyzed were

assumed to be the same as those of the original water and are designated with parentheses. The tracer solubilities were calculated for the water compositions of barium and strontium added to the J-13 well water/tuff systems, and their concentrations after equilibrium are given in Tables XXVII, XXVIII, and XXIX.

C. Results and Discussion

The results of the solubility calculations indicate that the minerals most likely to control tracer concentrations are the sulfate minerals, $SrSO_4$ and $BaSO_4$. The carbonate minerals have a higher solubility than do the sulfate minerals (Table XXX). In the case of strontium, the solubilities are not greatly different (e.g., 7.9×10^{-4} moles/L for $SrCO_3$ compared with 4.7×10^{-4} moles/L for $SrSO_4$). However, in the case of barium, the solubilities are over 3 orders of magnitude different (e.g., 1.4×10^{-4} moles/L for $BaCO_3$ compared with 5.9×10^{-8} moles/L for $BaSO_4$). It should also be noted that differences in solubilities among the four waters (Table XXX) are relatively insignificant. For example, the barium concentrations ranged from 4.3×10^{-8} to 6.0×10^{-8} moles/L.

The original concentrations of strontium added to the water/tuff system were all below the solubility of strontium with a few exceptions. Concentrations of 3×10^{-3} moles/L (YM-22) and 2×10^{-3} moles/L (YM-38) were above the solubility of strontium. The equilibrium concentrations 1.5×10^{-3} and 2.0×10^{-3} moles/L (YM-22) are also greater than the solubility of strontium, indicating the potential for precipitation of $SrSO_4$. The amount of strontium removed from solution 1.5×10^{-3} moles/L (Table XXIX) is equal to or exceeds the CEC of the YM-22 tuff. The CEC is approximately 20 μmol(p+)/g, whereas the strontium removed from solution ranged from 20 μmol(p+)/g to 60 μmol(p+)/g. That difference suggests that precipitation probably occurred

under those conditions. In the case of the YM-38 tuff system (Table XXVIII), the concentration of strontium after equilibration was below that of strontium solubility. YM-38 tuff has a much higher CEC (1220 μeq/g), and thus strontium is expected to be removed from solution by the cation adsorption process.

The data for the G1-2840 tuff system are more difficult to interpret (Table XXIX). Three original concentrations (six samples) were above the solubility of strontium (6.0×10^{-4}, 8.5×10^{-4}, and 1.4×10^{-3} moles/L). The two higher concentrations decreased such that the equilibrium concentrations were equal to or greater than the calculated solubility. Those equilibrated concentrations ranged from 4.74×10^{-4} to 9.60×10^{-4} moles/L. The solubility of strontium for the G1-2840 system was calculated to be 4.75×10^{-4} moles/L. The equilibrated concentrations are less than a factor of 2 higher than the calculated solubility. The solubility was calculated by using the SO_4 concentration before equilibration. Precipitation should result in a decrease in SO_4 concentrations from its original concentration of 1.9×10^{-4} moles/L. The CEC of G1-2840 tuff is approximately 480 μmol(p+)/g (Ref. 1), and the maximum amount of strontium removed from solution was only 18 μmol(p+). Thus the small difference between the calculated solubility and measured strontium and relatively large CEC compared with the strontium "sorbed" suggests that precipitation of $SrSO_4$ probably results in a relatively small amount of strontium being "sorbed." However, precipitation effects cannot be ruled out completely.

The original concentration of barium added to the YM-22 and YM-38 system (Tables XXVII and XXVIII) ranged from 3×10^{-7} to 1×10^{-4} moles/L. In every case, the concentration added was greater than the calculated solubility of barium. However, after equilibration only the two highest concentrations (1×10^{-5} and 1×10^{-6} moles/L) remained greater than the calculated solubility for the YM-22 system. All of the YM-38 equilibrated concentrations were below the

calculated concentration. The amount of barium added was 1% (or less) of the CEC of YM-22 and YM-38. The SO_4 concentration after equilibration was not measured. Thus for the lower concentration of barium added (3×10^{-7} and 4×10^{-7} moles/L) to the YM-22 system, precipitation reactions should not be a factor in sorption. However, for the higher concentrations added (1×10^{-5} and 1×10^{-4} moles/L), precipitation could be a factor.

Another factor could be involved for barium in the YM-22 tuff system. For the two highest concentrations added (1×10^{-5} and 1×10^{-4} moles/L), barium decreased to 2.6×10^{-7} and 4.8×10^{-6} moles/L, respectively, for <75-μm tuff size fraction and 4.1×10^{-7} and 8.7×10^{-6}, respectively, for 75- to 500-μm tuff size fraction. If precipitation occurs, then SO_4 should be removed mole per mole of barium. The concentration of SO_4 should then be lowered from 1.9×10^{-4} moles by the amount of barium originally added (1×10^{-5} and 1×10^{-4} moles/L). Thus at equilibrium the SO_4 concentration should be 1.8×10^{-4} and 0.9×10^{-4} moles/L, respectively. At those concentrations and the measured concentrations of barium after equilibration, the solubility of barium would be exceeded. This supersaturation suggests that colloidal forms of $BaSO_4$ may be present in the water after equilibration. The solution was filtered through a 0.45-μm-diam filter. Other work with these systems supports this contention by the fact that finer filters reduce the concentration of barium in solution.[11] In the case of the YM-38 system, precipitation is not a part of the sorption process because all of the equilibrated concentrations are below that of the calculated solubility. That conclusion assumes equilibrium conditions. Initial precipitation of $BaSO_4$ with a very slow dissolution could, however, affect the sorption process.

D. Conclusions

Various conclusions may be reached from solubility calculations:

1. Sulfate minerals are more likely to control tracer concentrations for strontium and barium.
2. Differences in the solubilities among the waters treated with either YM-22, YM-38, and G1-2840 are relatively insignificant.
3. For sample YM-22 the equilibrium concentrations indicate potential for precipitation of $SrSO_4$. The large CEC for YM-38 suggests that strontium is removed by the cation adsorption process. In the case of G1-2840, it is difficult to determine whether the strontium adsorbed or precipitated or both.
4. Analyses of barium in sample YM-22 suggest that it adsorbed at low concentrations and precipitated at high concentrations, where colloidal forms of $BaSO_4$ might have been present in the water after equilibration. In the case of sample YM-38, all the equilibrated concentrations were well below the calculated solubilities.

IV. TIME-DEPENDENT ENVIRONMENTS

A. Objectives

At the present time, design of isolation has focused on maximizing contaminant travel time to the biota access location. There are two common assumptions: (1) partitioning of the contaminant between the solid and solution is constant and (2) the lower limit of expected retardation factors is a conservative criterion. When time-independent (constant) solid solution partitioning (Kd) of the contaminant in the environment is assumed, contaminant travel times T are simple multiples of ground water travel times t($T = R*t$), where R is the retardation factor.

In transport modeling, the geochemistry of contaminants has generally been treated only marginally, implying that it will mainly provide retardation; however, geochemistry alone would not be able to provide

sufficient isolation. This constant retardation approach implicitly assumes that choosing the lower limit of the range of possible retardation factors leads to a conservative estimate of contaminant transport.

During FY85-86, a mainly geochemical transport model was developed with which it could be shown that in certain environments ("chemistry-dominated environments") the first assumption is expected to be unnecessarily conservative; the second one may underestimate the consequences of a leaking repository.

B. Ranking of Geochemical Isolation

In some environments that provide stable ligand concentrations, precipitation of a mineral of the contaminant provides "absolute" chemical isolation by limiting its concentration to values below permissible levels.[12] In other environments the processes that lead to such upper limits are not known. However, empirical evidence suggests chemical isolation; for example, concentration spectrum of the element of interest is nonzero only in a limited concentration range. Examples of the elements that dominate the potential hazard of activated reactor structure are molybdenum, niobium, and nickel. In rock materials the elements appear in the concentration range 1 to 1000 mg per kg of soil or rock matrix. If the environment is relatively resistant to remobilization of those elements (Kd = 100 to 1000 mL/g), then the environment will isolate them sufficiently (criterion: drinking water pathway), even if they have been activated in the high neutron flux region of the reactor (neutron flux: 10^{12} to 10^{14} cm^2/s). In this case the assumption is made that accumulation of the elements does not happen (see below).

Geochemical barriers may fail during the geochemical evolution of the environment isolating the contaminants, just as travel-time barriers may be breached if the physics of water transport changes (e.g., changes may be caused by changes in the physical rock matrix). Whether geohydraulic barriers

are more stable than the geochemical ones during the necessary millennia of isolation is yet unclear.

C. Breach of Geochemical Isolation

As long as absolute chemical isolation does not exist, a breach of geochemical isolation can be brought about by geochemical reconcentration of the contaminant above permissible levels.

Geochemical models and geochemical scenarios can be used to estimate a range of environmental reconcentrations for waste radionuclides. The geochemical models provide insight into element partitioning, and the geochemical scenarios allow the structuring of information needed to calculate environmental concentrations from the partitioning of the element.

The extremes of the possible natural reconcentration scenarios ("relative" and "absolute" reconcentration) have been given as follows:[13]

1. A contaminant is transported across a spatially stationary, buffered K_d step.
2. A natural K_d step moves through a deposit of contaminant, thereby spatially redistributing the contaminant.

In this report the second accumulation scenario has been investigated. In this scenario the K_d step results from a pH step or pH front; the pH increases with a decrease in hydraulic head.

The pH front is introduced by the intrusion of water into the environment in two ways:

1. The intruding water has a lower pH than that of the environment.
2. The intruding water triggers the release of protons from proton pools (proton buffers) in the environment.

Metal oxide surfaces were chosen as examples of such proton pools.

D. Metal Oxide Surfaces

The charge on metal oxide surfaces varies with the solution composition

in contact with the surfaces. Cations, as well as anions, in solution either adsorb directly on the oxide surface or remain at some distance from the surface (in the "β-plane") as a space charge cloud[14] because of their large radii. The space charge cloud determines the electrostatic potential ψ of the system. It seems possible to interpret adsorption experiments 15-17 on the basis of the hypothesis of mirror charge formation. Each ion in the space charge cloud induces a mirror charge on the surface; that charge is of equal magnitude, but of opposite sign. When the cloud is composed of negative ions, a mirror charge is achieved in two ways: by adsorbing protons from solution and by rearranging the spatial distribution of the surface protons. The mirror image protons are the ones mentioned above in case 2. These protons can lead to the formation of a migrating pH front (see below).

The charge cloud in the β-plane attracts radioactive ions of opposite charge; i.e., a negative space charge accommodates cationic species.

The surface potential ψ determines the balance between the number of positively and negatively charged surface sites, $S\text{-}OH_2$ and S-O, respectively. This balance of positively and negatively charged surface sites determines the polarity of the diffuse layer (located outside the Stern layer). When the negatively charged sites are in the majority, the surface shields itself with a diffuse layer of cations, including cationic radionuclides, such as strontium, cesium, and nickel.

A reduction of a negative space charge in the β-plane, which may result from a change of the composition of the water in contact with the surface, will thus lead to the following consequences:

1. Mirror protons will be released from the surface, thus leading to a decrease in pH and a consequential desorption of contaminant cations.
2. Contaminant cations will be released from the space charge cloud.

3. Contaminant cations will also be released from the diffuse layer.

The chemical equilibrium speciation program MINEQL has been used to model the above-mentioned processes.

An overview of the adequacy of this approach for systems consisting of a single electrolyte and a single oxide has been given by James and Parks.[18] Systems containing two oxides simultaneously have also been investigated.[15]

In FY85-86 some general microscopic processes on modeled metal oxide surfaces were investigated. These processes lead either to accumulation of protons on surfaces or to their release from surfaces; TiO_2 and FeOOH were selected as oxide surfaces, and KNO_3 and $CaSO_4$ were selected as electrolytes. The effect of those processes on the evolution and migration of a pH front was demonstrated. Finally, the remobilization, accumulation, and migration of a radioactive cation in such a pH environment was computed.

E. Results

1. Release of Protons and Contaminant Cations from Oxide Surfaces. The isoelectric point of the α-FeOOH/SO_4 system is strongly dependent on the concentration of sulfate, more so than the isoelectric points of other oxide/electrolyte systems, e.g., TiO_2/KNO_3 (Ref. 13). Thus, the contaminant release modes specified above are of more concern in environments containing that oxide.

The following concentration ranges were used to evaluate the pH dependence of the concentrations of adsorbed species in the system $SO_4/CO_3/Ca/Ni/\alpha$-FeOOH: $SO_{4T} = 10^{-6}$ to 10^{-2} M, $CO_{3T} = 10^{-6}$ M, $Ca_T = 10^{-2}$ to 10^{-6} M, $Ni_T = 10^{-8}$ to 10^{-4} M, α-FeOOH sites (S_T) = 10^{-6} to 10 mole sites per 1000 cm^3 of system volume.

Figure 3 shows the pH dependence of the concentrations of adsorbed species at the highest sulfate concentration. The strong chemical bond between sulfate ions and the surface has two effects:

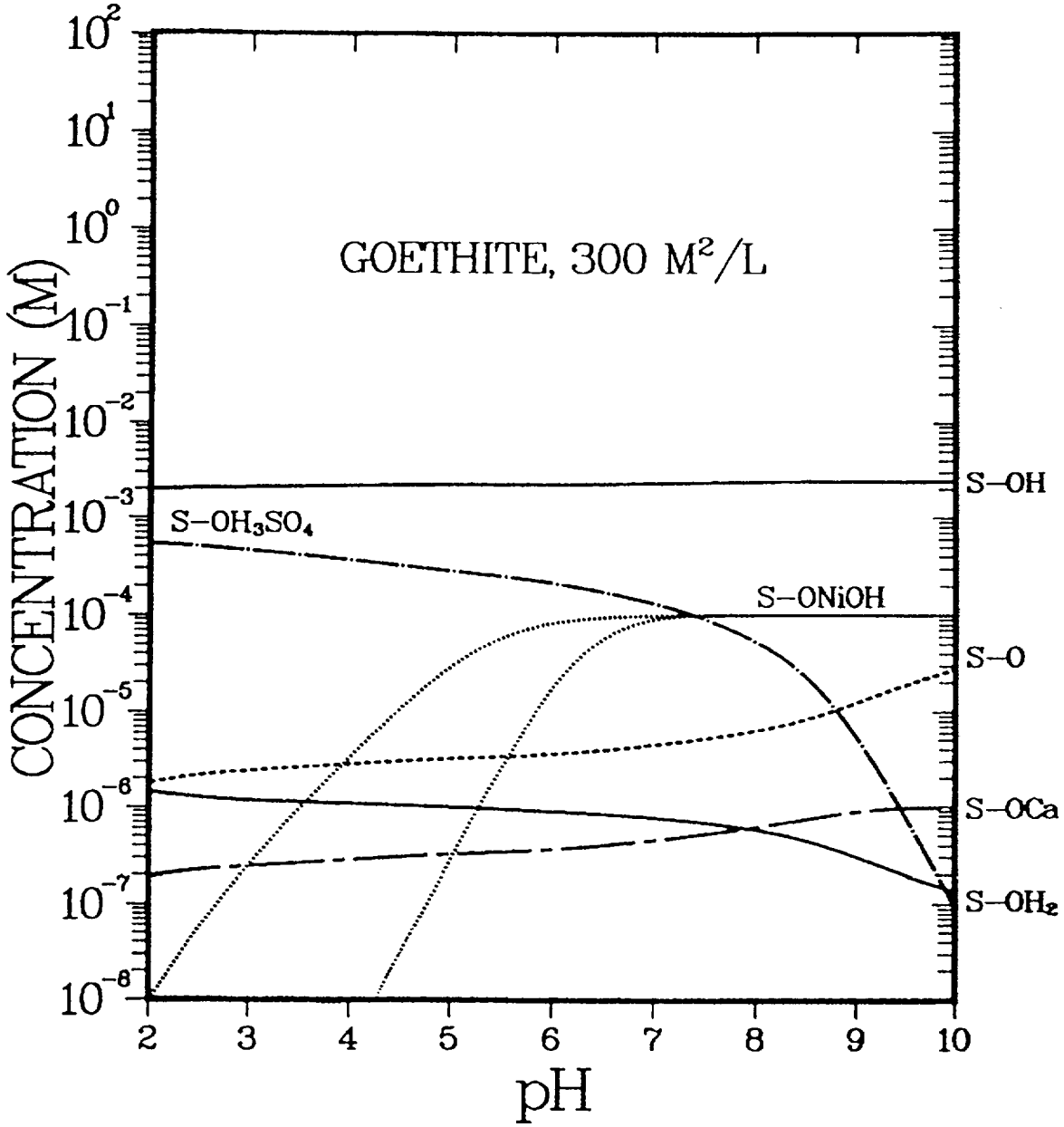

Figure 3. Concentration of surface complexes as a function of pH in an aqueous system containing 2.5 x 10^{-3}M goethite (as adsorbent), 10^{-4}M nickel (example of a radionuclide) and 10^{-2}M sulfate. Sulfate is 10^{-6}M for the lower dotted curve of the S-ONiOH complex. The cation exchange capacity (CEC) of the adsorbent is 1/G [S-O] (dashed curve), where G is the weight of the adsorbent in one liter of system volume. The amount of nickel sorbed on the surface per unit weight of adsorbent is 1/G [S-ONiOH] (dotted curves).

1. A large number of mirror protons is bound onto the surface; proton concentrations are of the order S_T to 10^{-2} S_T.
2. A considerable proton repulsive potential is built up at the surface by the mirror protons. Because the bonds of the S-OH and $S\text{-}OH_2$ complexes are weaker than the $S\text{-}OH_3SO_4$ bond, the surface loses some of those two complexes when sulfate is adsorbed; therefore, the number of proton holes (S-O complexes) is increased. Those losses are overcompensated at pH < 8.5 by the gain in mirror protons. Above pH 8.5, however, the sulfate complex generates more proton holes than can be compensated by the gain in mirror protons.

Consequently, the amount of protons released from the surface upon desorption of sulfate is of the order S_T to $10^{-2}S_T$ for pH < 8.5. At higher pH values, the mirror protons fall into the proton holes on the surface and thus are not released.

As mentioned above, both the release of mirror protons and the decrease of the negative charge in the Stern plane will remobilize adsorbed cationic radionuclides into solution. The amount of cationic radionuclides released is given by the difference of the dashed and corresponding solid curves in Fig. 3. Near the threshold (pH 5.5 to 6.5) about half of the adsorbed radionuclide inventory is released.

The capacity of the diffuse layer, CEC, is about [S-O] - [$S\text{-}OH_2$]. In soil or rock environments with a pH of 7 to 8, CEC is about [S-O] = 10^{-2} to 10^{-3} M at $SO_{4T} = 10^{-2}$ M (see Fig. 3). At $SO_{4T} < 10^{-6}$ M, CEC is approximately zero (the isoelectric point of the system at $SO_{4T} < 10^{-6}$ M is at pH 7.5; note that Figure 3 has been drawn for $SO_{4T} = 10^{-2}$ M). Therefore, the CEC and the concentration of the contaminant in the charge cloud (in the β-plane) are basically unrelated. For example, in the chosen example (Figure 3) the amount of contaminant released from the charge cloud is more than 1 order of

magnitude above the CEC. This quantifies the relative importance of the release of cations from the space charge cloud and the diffuse layer.

2. Redistribution of Contaminants Through Migrating pH Fronts. The protons released from the surface together with the ad- or desorption of electrolyte ions can have a profound influence on the migration of contaminant when the environment of the contaminant is not sufficiently buffered. In a nonbuffered environment, the free-proton activity will then increase. Even if the net increase is negligible when one volume element of the matrix (V^S) releases its protons into the adjacent volume of pore water (V^W), the proton concentration will increase steadily when the pore water is successively brought into contact and equilibrated with new matrix volumes. This increase occurs when water that remobilizes protons intrudes into an environment in which the proton pools are filled.

3. Simulation of Front Formation by Intrusion of Remobilizing Water. Figure 4 is an example of a breach of isolation scenario when the intruding water triggers the release of protons from proton pools. In this scenario the release and accumulation of protons and a cationic radionuclide from goethite surfaces is induced by the intrusion of low-sulfate water ($SO_{4T} = 10^{-6}$ M) into a moderately concentrated sulfate environment ($SO_{4T} = 10^{-2}$ M). A low pH front develops by accumulating the mirror protons released upon desorption of the sulfate. This accumulation continues until the desorption threshold of sulfate (pH 6.6) is reached. Other surface proton pools consume some of the released protons. Therefore, the minimum pH in the front is given by the balance between the protons delivered by the sulfate surface complex and the protons consumed by the other surface complexes, mainly S-OH and $S\text{-}OH_2$.

When the adsorbed cationic contaminant has its desorption threshold at pH 6.5, it also becomes remobilized by such changes of the environment. Like the

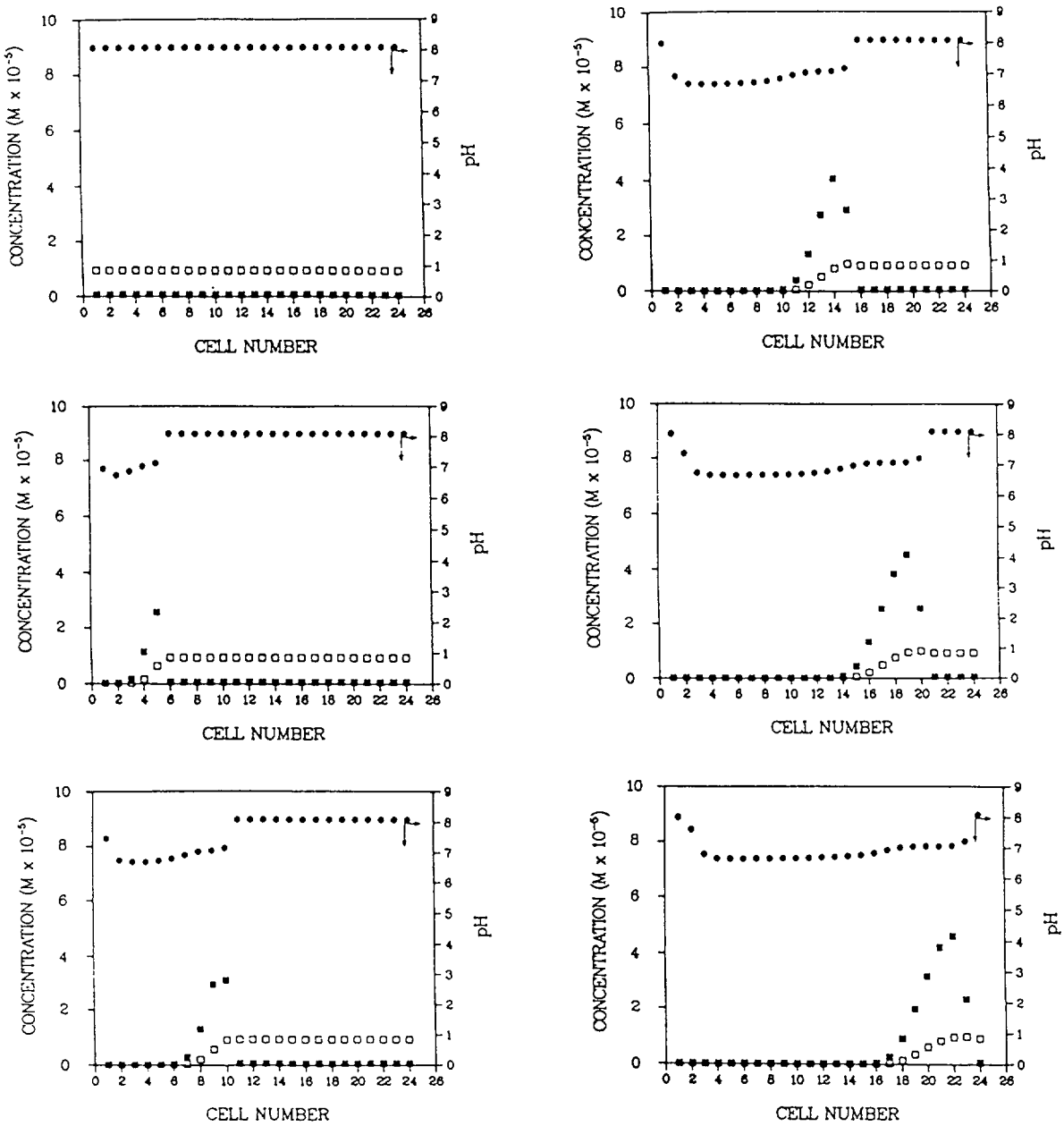

Figure 4. The computed accumulation of protons and contaminant in a water intruding into a chromatographic column of soil where SO_{4T} is 10^{-2}M; in the original water, SO_{4T} is 10^{-6}M. The accumulation is shown as six time steps; the sequence is counterclockwise starting in the upper left corner. The solid circles represent a sequence of pH values, the open squares represent the concentrations of the adsorbed contaminant, and the solid squares represent the concentrations of soluble contaminants.

protons, the contaminant accumulates at the front and migrates with the speed of the front. Such a behavior is in contradiction with the constant K_d model commonly used to quantify waste isolation. The accumulation of a contaminant and its acceleration can potentially breach the isolation that is expected on the basis of the constant K_d model.

4. Possible Mechanisms for Breach of Isolation. In the model calculation (Fig. 4) the retardation of the contaminant in the environment before the appearance of the remobilizing water is

$$R_{rn} = 1 + C^s_{rn}/C^w_{rn} = 2 \times 10^3,$$

where C^s_{rn}, C^w_{rn} are the concentrations of the radionuclide on goethite and in solution, respectively ($C^w_{rn} = 6 \times 10^{-9}$ M, $C^w_{rn} = 10^{-5}$ M).

The retardation of the pH front, on the other hand, can be approximated by

$$R_w = 1 + \Delta C^s_h / C^w_h,$$

where C^w_h is the sum of the concentrations of the free and complexed protons, ΔC^s_h is the increase of the surface proton pool during the passing of the front. With C^w_h (pH 6.6) = 2×10^{-6} M and with $\Delta C^s_h = C^s_h$ (pH 6.6) - C^s_h (pH 8.0) $\approx 10^{-7}$ M, the retardation of the pH front is R = 1.

The contaminant retardation, which is equal to that of the pH front, is therefore

$$R_{rn} = R_h = 1.$$

This means that the contaminant will move with no retardation at all (R = 1). These results are contrary to the results of the constant K_d model, which would give a retardation factor R = 2000.

In addition to this breach of the retardation barrier, the pH front will also induce a breach of the chemical isolation by reconcentrating the contaminant when the minimum pH in the front is below the contaminant

desorption threshold. Note that in Fig. 4 the minimum pH is at or near the desorption threshold. Under these conditions none of the contaminant is left on the goethite after the pH front has passed through the repository environment; the front has accumulated the entire inventory of the contaminant plume.

F. Conclusions

Because front formation has been observed [19,20] and could well be the common case rather than an anomaly, repository environments that provide various degrees of chemical isolation should be investigated with respect to their stability against accumulation scenarios such as the one discussed in this report.

The interpretations presented in this report are based on simple systems. It is not yet possible to model or quantitatively describe real soil or rock systems by today's geochemical speciation codes.[15] However, the interpretation of the behavior of simple systems, with the help of geochemical models, is important because it will aid in constructing more complex scenarios, in interpreting observed system behavior, and in designing new experiments in order to better predict the effect of changing environments on contaminant transport.

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TABLE I
OBJECTIVES OF SORPTION MODELING SUBTASK FOR BATCH DATA

Objective	Description
1	Selection of well-documented data sets
2	Quantitative and qualitative inventory of data base
3	Modeling of individual and combined data sets by various simple expressions
4	Comparison of the models' effectiveness
5	Quality assurance and sensitivity studies

TABLE II
DATA SETS WITH AT LEAST THREE POINTS FOR
ISOTHERM ANALYSIS IN SPECIFIC PARTICLE SIZE RANGES

Sample	Size (μm)	Elements
YM-22	<75	Sr, Cs, Ba, Eu
	75-500	Sr, Cs, Ba, Eu
YM-38	<75	Sr, Cs, Ba, Eu
	75-500	Sr, Cs, Ba, Eu
G1-2840	75-500	Sr, Cs

TABLE III-1

DEPTH INTERVALS AND SAMPLES OF MAJOR TUFF STRATIGRAPHIC UNITS[a]

Stratigraphic Unit (formation)	Symbol	Drill Hole USW-G1 (ft)	Samples
Yucca Mountain	Tpy	60-235	JA-8, YM-5
Tiva Canyon	Tpc		
Topopah Spring	Tpt	235-1426	YM-22, G1-1292, YM-30, JA-18
Calico Hills	Tht	1426-1802	G1-1436, YM-38, YM-42
Prow Pass	Tcp	1802-2173	G1-1854, YM-45, G1-1883, YM-46, G1-1982, YM-48, YM-49, JA-26
Bullfrog	Tcb	2173-2640	JA-28, G1-2233, G1-2289, YM-54, G1-2333, G1-2363, G1-2410, JA-32, G1-2476
Tram	Tct	2640-3558	G1-2698, G1-2840, G1-2854, G1-2901, G1-3116, JA-37
Dacite Flow-Breccia	T1	3558-3946	G1-3658

[a]This information was obtained from Ref. 1.

TABLE III-2
PETROLOGIC CHARACTERIZATION OF TUFF SAMPLES[a,b]

Sample	Particle Size (μm)	Abundance (%) Smectite	Illite Muscovite	Clinoptil-olite	Quartz	Cristob-alite	Alkali Feldspar	Glass	Other[c]	Dry Bulk Density (g/cm^3)	Crystals (%)	Lithics (%)	Unit
JA-8	all	25-50	--	--	--	10-20	tr	25-50	--		8.9	6.7	Tpc
"	75-500	30-60	--	--	<5	10-20	--	20-50	--				"
"	<75	30-60	--	--	--	10-20	--	30-60	--				"
YM-5	all[g]	10	--	--	<5	<5	10-20	~70	--		10.9	4.3	Tpc
YM-22	all	5-10	--	--	40-60	--	40-60	--	--	2.3	1.0	0.4	Tpt
"	106-500	<5	<2	--	30-50	--	30-50	--	--,				"
"	38-106	<2	tr	--	30-50	--	30-50	--	--				"
"	<38	<5	<2	--	30-50	--	30-50	--	--				"
G1-1292	all	tr	--	--	--	5-10	10-20	80-90	--				
"	75-500	--	--	--	--	15-30	10-20	40-60	--				
YM-30	all	5-10	5	5-10	40-60	5-15	30-50	--	--	2.1	2.1	21.6	"
"	75-500	--	--	15	30	20	35	--	--				
"	<75	--	--	15	30	20	35	--	--				
JA-18	all	5	5	5-10	--	15-25	15-25	~50	--		1.8	11.9	"
"	355-500	~5	--	10-20	--	30-50	30-50	~40	--				"
"	106-500	~5	~5	10-20	--	30-50	30-50	~40	--				"
G1-1436	75-500	<5	<5	75-90	5-10	--	~5	--	--	1.6	5.2	3.2	Tht
YM-38	106-500	5-10	<2	30-50	15-30	10-20	5-15	--	A, tr	1.8	4.0	7.7	"
"	38-106	5-10	<5	40-60	2-10	10-20	5-15	--	--				"
"	<38	5-15	<5	40-60	2-10	10-20	10-20	--	A, tr				"
YM-42	75-500	tr	<5	20	35-40	--	40	--	--	2.3	15.6	46.6	"
"	<75	tr	tr	20	40	--	40	--	--				"
G1-1854	75-500	5-10	--	30-50	5-15	15-30	20-40	--	--				Tcp
"	<75	5-10	--	40-60	20-40	15-30	10-30	--	--				"
YM-45	all	1-5	--	--	40-60	tr	30-50	--			13.5	0.6	"
G1-1883	75-500	<2	<5	--	30-50	--	50-70	--	--	1.7	16.6	1.0	"
"	106-500	<2	<2	--	20-40	0-10	40-60	--	--				"
"	38-106	<2	<5	--	30-50	0-10	30-50	--	--				"
"	<38	2-5	<2	--	20-40	0-10	40-60	--	--				"
YM-46	all	<5	<5	--	40-60	--	35-55	--	--	2.1	12.7	0.3	"
"	75-500	<5	--	--	50	--	45	--	--				"

TABLE III-2 (cont)

Sample	Particle Size (µm)	Abundance (%) Smectite	Illite Muscovite	Clinoptil-olite	Quartz	Cristob-alite	Alkali Feldspar	Glass	Other[c]	Dry Bulk Density (g/cm^3)	Crystals (%)	Lithics (%)	Unit
G1-1982	all	tr	<5	--	5-15	40-60	30-50	--	--	1.8	13.2	0.4	"
"	75-500	5-10	<2	--	--	--	70-90	--	--				"
"	38-106	<2	--	--	--	40-60	40-60	--	--				"
"	<38	10-20	--	--	--	30-50	20-40	--	C,<2				"
YM-48	all	tr	--	10-20	--	--	20-30	40-60	--				"
"	106-500	<2	--	20-40	5-10	5-15	20-40	10-30	--				"
YM-49	all	tr	tr	10-20	--	--	20-30	40-60	--	2.0	8.0	1.4	Tcp
JA-26	all	--	--	tr	30-50	tr	10-20	--	A,30-50		18.3	1.0	"
JA-28	all	tr	2.5	--	30-50	--	10-20	--	A,30-50		20	5	Tcb
G1-2233	<500	<5	<5	20-40	15-20	10-20	10-20	--	M,20-40	1.5	15.4	0.4	"
"	75-500	<5	5-15	15-30	5-10	--	40-60	--	M,<5				"
"	38-106	<5	~5	20-40	15-30	10-20	10-20	--	M,20-40				"
G1-2289	75-500	--	5-10	30-50	<5	--	30-50	--	M,10-20	1.6	15.8	1.0	"
YM-54	all	tr	tr	--	50-70	--	20-40	--	--	2.1	17.8	0	"
"	106-500	5-10	2-5	--	30-50	--	25-45	--	--				
"	38-106	5-10	5-10	--	30-50	--	30-50	--	--				
"	<38	5-10	2-10	--	15-30	--	40-60	--	--				
G1-2333	75-500	2-5	2-5	--	15-30	10-30	50-70	--	--				
"	<75	5-10	<5	--	15-30	20-40	20-40	--	--				
G1-2363	all	10-20	5-10	--	30-50	--	30-50	--	--	1.9	20.4	0.2	"
"	106-500	5	<2	--	30-50	0-10	30-50	--	--				"
"	38-106	5	<2	--	30-50	0-10	30-50	--	--				"
"	<38	5-10	<2	--	20-40	0-10	40-60	--	--				"
G1-2410	75-500	5-10	<2	--	20-40	0-10	30-50	--	--				"
"	<75	5-10	<5	--	20-40	5-15	30-50	--	--				"
JA-32	106-500	<5	5-15	--	30-50	--	30-50	--	--				"
"	355-500	--	5-10	--	40-50	--	30-40	--	--				"
"	150-180	--	10-15	--	35-50	--	40-65	--	--				"
"	106-150	<5	5-15	--	30-50	--	30-50	--	--				"
"	38-106	<2	tr	--	30-50	--	30-50	--	--				"
"	<38	5-10	--	--	20-40	--	40-60	--	A,tr				"
G1-2476	75-500	<2	~2	--	30-50	5-15	40-60	--	--				"
"	<75	2-5	~2	--	30-50	5-15	40-60	--	--				"

TABLE III-2 (cont)

Sample	Particle Size (μm)	Abundance (%) Smectite	Illite Muscovite	Clinoptil-olite	Quartz	Cristob-alite	Alkali Feldspar	Glass	Other[c]	Dry Bulk Density (g/cm^3)	Crystals (%)	Lithics (%)	Unit
G1-2698	all	<5	10-15	30-50	<5	--	30-50	--	M,<5	1.8	13.2	1	Tct
G1-2840	75-500	2-5	2-5	--	40-60	0-10	30-50	--	--				"
"	<75	2-5	2-5	--	40-60	0-10	30-50	--	--				"
G1-2854	75-500	<2	5-10	--	30-50	0-10	30-50	--	--				"
"	<75	<2	5-10	--	30-50	0-10	30-50	--	--				"
G1-2901	all	5-10	5-10	--	20-40	--	40-60	--	--		16.5	2	"
G1-3116	all	5-10	5-10	5-15	20-40	--	20-40	--	A,10-30	1.9	4.0	21.4	"
JA-37	all	20-40	5	~5	30-60	--	15-30	--	--				Tct
"	355-500	10-15	--	tr	40-50	--	30-40	--	C,tr				"
"	106-150	5-10	--	--	40-50	--	30-40	--	C,tr				"
G1-3658	75-500	40-60	--	--	--	--	40-60			2.3	23.4	0	Tl
"	106-500	40-60	--	--	--	--	40-60						"
"	38-106	30-50	--	--	--	--	50-70						"
"	<38	50-70	--	--	--	--	30-50						"

[a]This information is reproduced from Ref. 1.
[b]A blank indicates that no analysis was performed, and a dash indicates that the mineral was not detected.
[c]A = analcime; C = calcite; and M = mordenite; tr = trace ($\lesssim$ 1%).

TABLE IV
STRATEGY FOR MODELING OF ADSORPTION BATCH DATA

Case	Description	No. of CEC's Tested	Isotherms	Achieved Objective
1	Data sets with at least three points in individual particle size ranges. Adsorbed values are less than or equal to CEC	2	Linear Langmuir Freundlich Modified Freundlich	3, 4, 5[a]
2	Data sets with at least three points whose adsorbed values are less, equal, or greater than CEC	1	Linear Langmuir Freundlich	4, 5
3	Data sets with at least three points when all size ranges are combined	1	Linear Langmuir Freundlich Modified Freundlich	4, 5
4	Data sets with at least three points when all size ranges are combined in a particular geological formation	1	Linear Langmuir Freundlich	4, 5

[a]Refer to Table I.

TABLE V
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS,

CASE 1 (ADSORBED CONCENTRATIONS < CEC)[a]

Samples	Element	Linear R^2	Linear SSE	Langmuir R^2	Langmuir SSE
YM-22, <75 μm	Sr	0.999	0.0053	0.781	1.46E-03
CEC = 20	Cs	0.999	0.182	0.995	2.81E-03
μmol(p+)/g	Ba	0.998	0.107	0.935	2.09E-04
	Eu	0.381	0.315	0.603	4.22E-04
75-500 μm	Sr	0.999	0.00669	0.601	2.43E-03
	Cs	0.999	0.177	0.995	3.41E-03
	Ba	0.997	0.123	0.967	3.02E-04
	Eu	0.999	0.008	0.786	1.08E-04
YM-38, <75 μm	Sr	0.999	0.408	0.866	1.06E-04
CEC = 1,220	Cs	0.999	0.018	0.0017	8.91E-05
μmol(p+)/g	Ba	0.999	0.018	0.297	1.57E-06
	Eu	0.792	0.106	0.028	1.10E-04
75-500 μm	Sr	0.999	0.363	0.547	2.51E-04
	Cs	1.000	0.150	0.261	5.03E-05
	Ba	0.999	0.058	0.247	8.58E-06
	Eu	0.788	0.114	0.066	1.95E-04
G1-2840, 75-500 μm	Sr	0.866	3.043	0.988	3.00E-03
CEC = 430	Cs	0.988	0.470	0.703	9.37E-03
μmol(p+)/g					

[a]R = correlation coefficient.
R^2 = coefficient of determination.
SSE = standard error.

TABLE V (cont.)
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS,

CASE 1 (ADSORBED CONCENTRATIONS < CEC)[a]

Sample	Element	Freundlich R^2	Freundlich SSE	Modified Freundlich R^2	Modified Freundlich SSE
YM-22, <75 μm	Sr	0.998	4.13E-02	0.998	4.25E-02
CEC = 20	Cs	0.988	0.330	0.996	0.200
μmol(p+)/g	Ba	0.998	5.79E-02	0.999	4.71E-02
	Eu	0.931	0.461	0.930	0.465
75-500 μm	Sr	0.994	8.09E-02	0.994	0.081
	Cs	0.993	0.245	0.999	0.115
	Ba	0.976	7.79E-02	0.998	6.42E-02
	Eu	0.999	2.22E-02	0.999	2.14E-02
YM-38, <75 μm	Sr	0.996	0.358	0.976	0.353
CEC = 1,220	Cs	0.998	0.156	0.998	0.154
μmol(p+)/g	Ba	0.999	4.23E-02	0.999	4.21E-02
	Eu	0.982	0.199	0.982	0.200
75-500 μm	Sr	0.974	0.369	0.974	0.366
	Cs	0.999	0.112	0.999	0.105
	Ba	0.975	0.179	0.975	0.179
	Eu	0.979	0.222	0.979	0.223
G1-2840, 75-500 μm	Sr	0.983	0.138	0.983	0.136
CEC = 430	Cs	0.996	0.119	0.996	0.120
μmol(p+)/g					

[a]R = correlation coefficient.
R^2 = coefficient of determination.
SSE = standard error.

TABLE VI
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS, CASE 1 (ADSORBED CONCENTRATIONS < CEC)

Sample	Element	Linear Kd	Langmuir b	Langmuir k
YM-22, <75 μm	Sr	5.41E+01	3.536	2.03E+01
CEC = 20	Cs	1.20E+01	1.57E+01	1.90E+01
μmol(p+)/g	Ba	4.01E+02	6.103	1.72E+02
	Eu	1.29E+03	0.281	9.92E+03
75-500 μm	Sr	5.50E+01	3.230	2.33E+01
	Cs	1.00E+01	1.39E-01	1.81E+01
	Ba	2.10E+02	5.451	1.15E+02
	Eu	1.11E+03	1.170	1.56E+03
YM-38, <75 μm	Sr	1.50E+03	1.01E+02	6.85E+01
CEC = 1,220	Cs	3.51E+03	2.39E+03	1.509
μmol(p+)/g	Ba	9.99E+04	-1.96E+01	-4.28E+03
	Eu	4.18E+03	2.071	1.92E+03
75-500 μm	Sr	1.20E+03	1.23E+02	2.72E+01
	Cs	3.41E+03	3.00E+02	1.42E+01
	Ba	7.89E+04	-5.123	-8.85E+03
	Eu	2.38E+03	1.410	1.89E+03
G1-2840, 75-500	Sr	1.18E+01	20.95	2.74
CEC = 430	Cs	2.04E+01	1.33E+01	8.670
μmol(p+)/g				

TABLE VI (cont.)
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS, CASE 1 (ADSORBED CONCENTRATION < CEC)

Sample	Element	Freundlich K	Freundlich N	Modified Frendlich A	Modified Frendlich β	Modified Frendlich KD
YM-22, <75 μm	Sr	4.01E+01	0.930	4.38E+01	0.940	2.303
CEC = 20	Cs	2.31E+01	0.799	5.97E+01	0.864	3.549
μmol(p^+)/g	Ba	2.14E+02	0.850	2.87E+02	0.877	2.09E+01
	Eu	1.46E+03	0.975	1.52E+03	0.978	8.39E+01
75-500 μm	Sr	3.91E+01	0.920	4.27E+01	0.931	2.260
	Cs	1.79E+01	0.787	3.72E+01	0.836	2.098
	Ba	1.23E+02	0.840	1.60E+02	0.865	1.11E+01
	Eu	6.14E+02	0.923	6.39E+02	0.925	4.22E+01
YM-38, <75 μm	Sr	1.60E+03	0.885	1.72E+03	0.891	1.468
CEC = 1,220	Cs	4.22E+03	1.010	4.40E+03	1.012	3.552
μmol(p^+)/g	Ba	1.73E+05	1.050	1.74E+05	1.051	1.12E-02
	Eu	3.85E+03	0.997	3.85E+03	0.997	3.172
75-500 μm	Sr	1.22E+03	0.907	1.31E+03	0.913	1.084
	Cs	4.48E+03	1.006	4.68E+03	1.009	3.796
	Ba	2.29E+05	1.111	2.31E+05	1.112	1.12E+02
	Eu	1.96E+03	0.975	1.96E+03	0.975	1.625
G1-2840	Sr	1.90E-01	0.800	1.16E-01	0.717	0.010
CEC = 430	Cs	1.60E-01	0.716	1.62E-01	0.717	0.010
μmol(p^+)/g						

TABLE VII
QUALITATIVE EVALUATION OF THE EFFECTIVENESS
OF MODELING YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS (CASE 1)[a]

Sample	Element	Linear	Langmuir	Freundlich	Modified Freundlich
YM-22, <75 μm	Sr	E	A	E	E
	Cs	E	E	E	E
	Ba	E	E	E	E
	Eu	P	P	E	E
75-500 μm	Sr	E	P	E	E
	Cs	E	E	E	E
	Ba	E	E	E	E
	Eu	E	A	E	E
YM-38, <75 μm	Sr	E	G	E	E
	Cs	E	P	E	E
	Ba	E	P	E	E
	Eu	A	P	E	E
75-500 μm	Sr	E	P	E	E
	Cs	E	P	E	E
	Ba	E	P	E	E
	EU	A	P	E	E
G1-2840,75-500	SR	G	P	E	E
μm	CS	E	A	E	E

[a]E = Excellent, $R^2 \geq 0.90$.

G = Good, $0.80 \leq R^2 < 0.90$.

A = Acceptable, $0.65 \leq R^2 < 0.80$.

P = Poor, $R^2 < 0.65$.

TABLE VIII
EFFECT OF CEC ON THE STATISTICS OF THE MODIFIED
FREUNDLICH ISOTHERM (ADSORBED CONCENTRATIONS < CEC)[a]

Sample	CEC μmol(p+)/g	Element	R^2	SSE
YM-22				
	20[b]	Sr	0.998	4.25E-02
<75 μm		Cs	0.996	0.200
		Ba	0.999	4.71E-02
		Eu	0.930	0.465
	14[c]	Sr	0.998	4.29E-02
		Cs	0.993	0.221
		Ba	0.999	4.44E-02
		Eu	0.929	0.467
75-500 μm	20[b]	Sr	0.994	0.081
		Cs	0.999	0.115
		Ba	0.998	6.42E-02
		Eu	1.000	2.14E-02
	8[c]	Sr	0.994	0.082
		Cs	0.998	0.105
		Ba	0.998	4.97E-02
		Eu	0.999	2.11E-02
YM-38				
	1,220[b]	Sr	0.976	0.353
<75 μm		Cs	0.998	0.154
		Ba	0.999	4.19E-02
		Eu	0.982	0.200
	1,520[c]	Sr	0.976	0.354
		Cs	0.998	0.134
		Ba	0.999	4.19E-02
		Eu	0.982	0.200
G1-2840				
75-500 μm	430[b]	Sr	0.983	0.136
		Cs	0.996	0.120
	3[c]	Sr	0.969	0.187
		Cs	0.991	0.162

[a]R = correlation coefficient.

R = coefficient of determination.

SSE = standard error.

[b]CEC determined by the NH_4AC test.

[c]CEC estimated from the sum of cations.

TABLE IX
EFFECT OF CEC ON THE CONSTANTS OF THE MODIFIED FREUNDLICH ISOTHERM (ADSORBED CONCENTRATIONS < CEC)

Sample	CEC μmol(p+)/g	Element	A	β	K_D
YM-22					
<75 μm	20[a]	Sr	4.38E+01	0.940	2.303
		Cs	5.97E+01	0.864	3.546
		Ba	2.88E+02	0.877	2.09E+01
		Eu	1.52E+03	0.978	8.39E+01
	14[b]	Sr	4.55E+01	0.945	3.485
		Cs	9.19E+01	0.892	8.167
		Ba	3.33E+02	0.890	3.52E+01
		Eu	1.55E+03	0.979	1.22E+02
75-500 μm	20[a]	Sr	4.27E+01	0.930	2.260
		Cs	3.71E+01	0.836	2.098
		Ba	1.61E+02	0.865	1.11E+01
		Eu	6.40E+02	0.926	4.23E+01
	8[b]	Sr	4.91E+01	0.947	6.79
		Cs	5.45E+01	0.862	9.27
		Ba	2.74E+02	0.916	4.73E+01
		Eu	6.79E+02	0.930	1.19E+02
YM-38					
<75 μm	1,220[a]	Sr	1.72E+03	0.891	1.468
		Cs	4.40E+03	1.012	3.551
		Ba	1.74E+05	1.051	1.12E-02
		Eu	3.86E+03	0.997	3.179
	1.520[b]	Sr	1.69E+03	0.889	1.128
		Cs	4.36E+03	1.012	2.837
		Ba	1.74E+05	1.051	9.09E+01
		Eu	3.85E+03	0.997	2.543
G1-2840					
75-500 μm	430[a]	Sr	1.90E+01	0.805	2.15E-02
		Cs	1.62E+01	0.717	0.0103
	3[b]	Sr	2.30E+02	1.167	4.13E+01
		Cs	2.57E+01	0.751	1.17E+01

[a]CEC determined by the NH_4AC test.

[b]CEC estimated from the sum of cations.

TABLE X
COMPARISON OF STATISTICAL PARAMETERS FROM TWO DATA SETS OF STRONTIUM FOR THE YM-22 TUFF SAMPLE (CASE 2): (1) CONCENTRATIONS ADSORBED < CEC AND (2) CONCENTRATIONS ADSORBED < CEC AND ≥ CEC[a]

Data Set	Particle Size (μm)	Linear R^2	Linear SSE	Langmuir R^2	Langmuir SSE	Freundlich R^2	Freundlich SSE
Conc. Ads. <CEC	<75	0.999	0.0053	0.781	1.46E-03	0.998	4.25
	75-500	0.999	0.0067	0.601	2.43E-03	0.994	8.09E-02
Conc. Ads. <CEC + ≥CEC	<75	0.999	0.319	0.982	2.47E-03	0.999	6.99E-02
	75-500	0.999	0.421	0.996	3.01E-03	0.993	0.141

[a]R = correlation coefficient.

R^2 = coefficient of determination.

SSE = standard error.

TABLE XI
COMPARISON OF ISOTHERM CONSTANTS FROM TWO DATA SETS OF STRONTIUM FOR THE YM-22 TUFF SAMPLE (CASE 2): (1) CONCENTRATIONS ADSORBED < CEC AND (2) CONCENTRATIONS ADSORBED < CEC AND ≥ CEC

Data Set	Particle Size (μm)	Linear	Langmuir		Freundlich	
		Kd	b	k	K	N
Conc. Ads. <CEC	<75	5.41E+01	3.54	2.03E+01	4.03E+01	0.930
	75-500	5.50E+01	3.23	2.33E+01	3.90E+01	0.920
Conc. Ads. <CEC + ≥CEC	<75	2.00E+01	8.58E+01	0.773	2.54E+01	0.870
	75-500	9.412	4.46E+01	1.553	1.51E+01	0.796

TABLE XII

QUALITATIVE COMPARISON OF THE EFFECTIVENESS OF ISOTHERMS FROM TWO DATA SETS OF STRONTIUM FOR YM-22 TUFF SAMPLE (CASE 2): (1) CONCENTRATIONS ADSORBED < CEC AND (2) CONCENTRATIONS ADSORBED < CEC AND ≥ CEC[a]

Data Set	Particle Size (μm)	Linear	Langmuir	Freundlich
Conc. Ads. <CEC	<75	E	A	E
	75-500	E	P	E
Conc. Ads. <CEC + ≥CEC	<75	E	E	E
	75-500	E	E	E

[a]E = Excellent, $R^2 \geq 0.90$.

G = Good, $0.80 \leq R^2 < 0.90$.

A = Acceptable, $0.65 \leq R^2 < 0.80$.

P = Poor, $R^2 < 0.65$.

TABLE XIII
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS, CASE 3 (COMBINATION OF ALL SIZES WITH AVAILABLE DATA)[a]

Sample[b]	Element	Linear		Langmuir	
		R^2	SSE	R^2	SSE
YM-22	Sr	0.999	0.006	0.133	3.40E-03
CEC = 20	Cs	0.991	0.593	0.990	3.57E-03
μmol(p+)/g	Ba	0.9066	0.513	0.880	4.00E-04
	Eu	0.6831	0.149	0.290	2.94E-04
YM-38	Sr	0.986	3.191	0.638	1.58E-04
CEC = 1,520	Cs	0.999	0.340	0.134	1.05E-04
μmol(p+)/g	Ba	0.986	0.168	0.024	7.46E-06
	Eu	0.736	0.078	7.98E-03	2.17E-04
G1-2363[c]	Ba	0.998	0.009	0.288	1.56E-03
CEC = 48					
μmol(p+)/g					

[a]R = correlation coefficient.

R^2 = coefficient of determination.

SSE = standard error.

[b]Data for sample G1-2840 (75-500 μm) remain the same as the data in cases 1 and 2.

[c]In combining all particle size ranges, modeling becomes possible for G1-2363.

TABLE XIII (cont.)
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS, CASE 3 (COMBINATION OF ALL SIZES WITH AVAILABLE DATA)

Sample[b]	Element	Freundlich		Modified Freundlich	
		R^2	SSE	R^2	SSE
YM-22	Sr	0.986	8.88E-02	0.986	8.95E-02
CEC = 20	Cs	0.990	0.258	0.996	0.174
μmol(p+)/g	Ba	0.989	0.114	0.990	0.113
	Eu	0.969	0.238	0.969	0.240
YM-38	Sr	0.951	0.333	0.952	0.333
CEC = 1,520	Sr	0.987	0.278	0.987	0.278
μmol(p+)/g	Ba	0.945	0.200	0.945	0.200
	Eu	0.946	0.229	0.946	0.229
G1-2363[b]	Ba	0.888	0.322	0.888	0.322
CEC = 48					
μmol(p+)/g					

[a]R = correlation coefficient.

R^2 = coefficient of determination.

SSE = standard error.

[b]Data for sample G1-2840 (75-500 μM) remains the same as the data in cases 1 and 2.

[c]In combining all particle size ranges, modeling becomes possible for G1-2363.

TABLE XIV
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS, CASE 3 (COMBINATION OF ALL SIZES WITH AVAILABLE DATA)

Sample[a]	Element	Linear	Langmuir	
		Kd	b	k
YM-22	Sr	5.45E+01	5.299	1.23E+01
	Cs	1.09E+01	1.46E+01	1.92E+01
	Ba	2.54E+02	5.280	1.55E+02
	Eu	1.15E+03	0.868	1.97E+03
YM-38	Sr	1.32E+03	9.71E+01	7.14E+01
	Cs	3.46E+03	1.43E+02	4.12E+01
	Ba	8.70E+04	-1.274E+01	-5.17E+03
	Eu	2.78E+03	-2.119	-1.05E+03
G1-2363[b]	Ba	8.51E+02	-1.79E-01	-1.70E+03

Sample[a]	Element	Freundlich		Modified Frendlich		
		K	N	A	β	KD
YM-22	Sr	4.00E+01	0.937	4.36E+01	0.947	2.280
	Cs	2.11E+01	0.807	4.86E+01	0.861	2.802
	Ba	1.53E+02	0.840	2.02E+02	0.865	1.45E+01
	Eu	9.18E+02	0.952	9.57E+02	0.955	5.74E+01
YM-38	Sr	1.03E+03	0.835	1.11E+03	0.840	0.673
	Cs	2.71E+03	0.942	2.83E+03	0.944	1.911
	Ba	5.13E+04	0.973	5.14E+04	0.973	3.728E+01
	Eu	2.07E+03	0.983	2.06E+03	0.983	1.36
G1-2363[b]	Ba	1.39E+03	1.107	1.41E+03	1.108	2.12E+01

[a]Data for sample G1-2840 (75-500 μm) remain the same as the data in cases 1 and 2.

[b]In combining all particle size ranges, modeling becomes possible for G1-2363.

TABLE XV
QUALITATIVE EVALUATION OF THE EFFECTIVENESS
OF MODELING YUCCA MOUNTAIN SAMPLES BY VARIOUS ISOTHERMS (CASE 3)[a]

Sample	Element	Linear	Langmuir	Freundlich	Modified Freundlich
YM-22	Sr	E	P	E	E
	Cs	E	E	E	E
	Ba	G	G	E	E
	Eu	P	P	E	E
YM-38	Sr	E	P	E	E
	Cs	E	P	E	E
	Ba	E	P	E	E
	Eu	A	P	E	E
G1-2363	Ba	E	P	G	G

[a]E = Excellent, $R^2 \geq 0.90$.

G = Good, $0.80 \leq R^2 < 0.90$.

A = Acceptable, $0.65 \leq R^2 < 0.80$.

P = Poor, $R^2 < 0.65$.

TABLE XVI
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF STRONTIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)[a, b]

	Linear		Langmuir		Freundlich	
Unit	R^2	SSE	R^2	SSE	R^2	SSE
Tpt	0.871 (G)	6.402	0.864 (G)	9.37E-03	0.984 (G)	0.621
Tht	0.988 (E)	2.913	0.606 (P)	1.56E-04	0.943 (E)	0.402
Tct	0.866 (G)	2.503	0.936 (E)	6.61E-03	0.900 (E)	0.382
Tcp	0.425 (P)	0.006	0.744 (A)	8.55E-03	0.576 (P)	0.861
Tcb	0.809 (G)	0.010	0.560 (P)	5.60E-03	0.696 (A)	0.629

[a]E = Excellent, $R^2 \geq 0.90$.
G = Good, $0.80 \leq R^2 < 0.90$.
A = Acceptable, $0.65 \leq R^2 < 0.80$.
P = Poor, $R^2 < 0.65$.
[b]R = correlation coefficient.
R^2 = coefficient of determination
SSE = standard error.

TABLE XVII
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF STRONTIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)

Unit	Linear	Langmuir		Freundlich	
	K_D	b	k	K	N
Tpt	1.31E+01	5.06E+01	1.81	1.26E+01	0.717
Tht	1.32E+03	9.70E+01	7.23E+01	1.66E+03	0.874
Tct	1.18E+01	1.95E+01	3.914	9.694	0.601
Tcp	3.77E+01	7.50E-03	3.64E+04	2.563	0.616
Tcb	5.56E+01	4.15E-02	4.66E-03	2.555	0.556

TABLE XVIII
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF BARIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)[a, b]

	Linear		Langmuir		Freundlich	
Unit	R^2	SSE	R^2	SSE	R^2	SSE
Tpt	0.903 (E)	0.402	0.760 (A)	5.51E-04	0.948 (E)	0.318
Tht	0.985 (E)	0.160	1.41E-02 (P)	7.28E-06	0.965 (E)	0.205
Tct	0.050 (P)	0.213	0.640 (P)	3.32E-04	2.00E-02 (P)	0.803
Tcp	0.656 (A)	0.105	0.731 (A)	1.16E-03	0.752 (A)	0.643
Tcb	0.599 (P)	0.065	1.50E-02 (P)	2.00E-03	0.318 (P)	0.718

[a]E = Excellent, $R^2 \geq 0.90$.
G = Good, $0.80 \leq R^2 < 0.90$.
A = Acceptable, $0.65 \leq r^2 < 0.80$.
P = Poor, $R^2 < 0.65$.
[b]R = correlation coefficient.
R^2 = coefficient of determination.
SSE = standard error.

TABLE XIX
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF BARIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)

Unit	Linear	Langmuir		Freundlich	
	K_D	b	k	K	N
Tpt	2.55E-02	4.631	2.55E+02	7.42E+1	0.734
Tht	8.71E+04	-1.59E+01	-4.41E+03	8.43E+04	1.004
Tct	9.49E+02	0.097	3.30E+04	0.375	0.178
Tcp	2.10E+02	0.300	4.84E+03	4.05E+01	0.659
Tcb	7.82E+02	0.374	1.53E+03	0.912	0.381

TABLE XX
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF CESIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)[a, b]

	Linear		Langmuir		Freundlich	
Unit	R^2	SSE	R^2	SSE	R^2	SSE
Tpt	0.991 (E)	0.469	0.989 (E)	3.10E-03	0.947 (E)	0.495
Tht	0.9998 (E)	0.311	0.147 (P)	9.93E-05	0.987 (E)	0.263
Tct	0.989 (E)	0.386	0.699 (A)	8.54E-03	0.991 (E)	0.174
Tcp	0.595 (P)	0.000	0.924 (E)	5.18E-04	0.507 (P)	0.181
Tcb	0.268 (P)	0.0001	0.688 (P)	1.53E-03	0.061 (P)	0.220

[a]E = Excellent, $R^2 \geq 0.90$.
G = Good, $0.80 \leq R^2 < 0.90$.
A = Acceptable, $0.65 \leq R^2 < 0.80$.
P = Poor, $R^2 < 0.65$.
[b]R = correlation coefficient.
R^2 = coefficient of determination.
SSE = standard error.

TABLE XXI
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF CESIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)

Unit	Linear	Langmuir		Freundlich	
	K_D	b	k	K	N
Tpt	1.09E+01	1.45E+01	2.65E+01	1.44E+01	0.741
Tht	3.46E+03	1.33E+02	4.73E+01	2.64E+03	0.939
Tct	2.08E+01	1.25E+01	1.36E+01	1.40E+01	0.697
Tcp	2.73E+02	7.86E-05	5.37E+07	1.53E-03	0.199
Tcb	3.00E+02	5.02E-05	-2.91E+08	2.06E-5	-0.073

TABLE XXII
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF EUROPIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)[a, b]

	Linear		Langmuir		Freundlich	
Unit	R^2	SSE	R^2	SSE	R^2	SSE
Tpt	0.151 (P)	0.183	0.780 (A)	7.03E-03	0.861 (G)	0.605
Tht	0.736 (A)	0.071	3.30E-03 (P)	2.52E-04	0.889 (G)	0.382
Tct	0.558 (P)	0.009	0.980 (E)	3.62E-04	0.527 (P)	0.380
Tcp	0.411 (P)	0.003	0.061 (P)	4.64E-03	0.496 (P)	0.635
Tcb	0.862 (E)	0.16	0.924 (E)	8.04E-04	0.814 (G)	0.317

[a]E = Excellent, $R^2 \geq 0.90$.
G = Good, $0.80 \leq R^2 < 0.90$.
A = Acceptable, $0.65 \leq R^2 < 0.80$.
P = Poor, $R^2 < 0.65$.
[b]R = correlation coefficient.
R^2 = coefficient of determination.
SSE = standard error.

TABLE XXIII
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF EUROPIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)

Unit	Linear	Langmuir		Freundlich	
	K_D	b	k	K	N
Tpt	2.34E+02	0.022	-5.92E+04	2.48E+01	0.713
Tht	2.78E+03	2.652	1.01E+03	2.19E+02	0.789
Tct	1.59E+02	0.022	1.31E+05	0.226	0.284
Tcp	2.71E+02	6.91E-03	6.42E+04	1.039	0.480
Tcb	7.93E+01	0.031	2.72E+04	1.65E+01	0.696

TABLE XXIV
SUMMARY TABLE FOR THE STATISTICS FROM THE MODELING OF CERIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)[a, b]

	Linear		Langmuir		Freundlich	
Unit	R^2	SSE	R^2	SSE	R^2	SSE
Tpt	0.452 (P)	0.024	0.768 (A)	7.25E-03 (E)	0.938	0.703
Tht	0.980 (E)	0.006	1.000 (E)	7.85E-06 (E)	0.935	0.863
Tct	0.849 (G)	0.002	0.996 (E)	3.77E-04 (E)	0.984	7.05E-02
Tcp	0.925 (E)	0.009	4.05E-02 (P)	7.27E-04 (E)	0.992	0.182
Tcb	0.828 (G)	0.014	0.915 (E)	1.92E-03 (G)	0.890	0.236

[a]E= Excellent, $R^2 \geq 0.90$.
G = Good, $0.80 \leq R^2 < 0.90$.
A = Acceptable, $0.65 \leq R^2 < 0.80$.
P = Poor, $R^2 < 0.65$.
[b]R = correlation coefficient.
R^2 = coefficient of determination.
SSE = standard error.

TABLE XXV
SUMMARY TABLE FOR THE CONSTANTS FROM THE MODELING OF CERIUM ADSORPTION ON COMBINED SAMPLES OF THE SAME STRATIGRAPHIC UNIT BY VARIOUS ISOTHERMS (CASE 4)

Unit	Linear	Langmuir		Freundlich	
	K_D	b	k	K	N
Tpt	3.37E+01	0.042	5.19E+03	8.909	0.707
Tht	9.01E+02	0.060	8.58E+05	1.05E+03	0.835
Tct	1.05E+02	4.85E-03	-1.05E+06	0.088	0.281
Tcp	6.53E+02	0.205	3.60E+03	3.48E+01	0.723
Tcb	8.31E+01	0.044	1.40E+04	4.045	0.596

TABLE XXVI

CHEMICAL COMPOSITION OF WELL J-13 WATER[a]

Constituent	Original	Precontacted with Tuff Samples G1-2840	YM-22	YM-38
Mg	7.24×10^{-5}	6.83×10^{-5}	9.87×10^{-5}	4.11×10^{-6}
Mn	2.18×10^{-7}	1.64×10^{-7}	1.82×10^{-8}	1.82×10^{-8}
H_4SiO_4	1.13×10^{-3}	(1.13×10^{-3})	(1.13×10^{-3})	(1.13×10^{-3})
Fe	1.97×10^{-7}	$<1.25 \times 10^{-7}$	1.79×10^{-7}	1.79×10^{-7}
Sr	4.45×10^{-7}			
Ba	7.28×10^{-9}			
Ca	2.87×10^{-4}	2.97×10^{-4}	3.24×10^{-4}	3.49×10^{-4}
Li	8.65×10^{-6}	8.21×10^{-6}	(8.65×10^{-6})	(8.65×10^{-6})
K	1.35×10^{-4}	1.30×10^{-4}	1.36×10^{-4}	1.48×10^{-4}
Al	9.27×10^{-7}	3.71×10^{-7}	(9.27×10^{-7})	(9.27×10^{-7})
Na	1.96×10^{-3}	2.10×10^{-3}	2.35×10^{-3}	2.48×10^{-3}
F	1.11×10^{-4}	(1.11×10^{-4})	1.37×10^{-4}	1.32×10^{-4}
Cl	1.81×10^{-4}	(1.81×10^{-4})	2.06×10^{-4}	2.12×10^{-4}
PO_4^{3-}	(ND)[b]	(ND)	(ND)	(ND)
NO_3^{2-}	1.63×10^{-4}	(1.63×10^{-4})	(1.63×10^{-4})	(1.63×10^{-4})
SO_4	1.88×10^{-4}	(1.88×10^{-4})	2.50×10^{-4}	2.71×10^{-4}
Total CO_3	2.40×10^{-3}	(2.40×10^{-3})	(2.40×10^{-3})	(2.40×10^{-3})
pH	7.0	(7.0)	(7.0)	(7.0)
O_2	1.78×10^{-4}	(1.78×10^{-4})	1.78×10^{-4}	(1.78×10^{-4})
HPO_4^{2-}	1.04×10^{-6}	(1.04×10^{-6})	(1.04×10^{-6})	(1.04×10^{-6})

[a]Data expressed as moles/L with exception of pH.

[b]ND = nondetectable.

TABLE XXVII
CONCENTRATIONS OF BA AND SR ORIGINALLY ADDED
AND AFTER EQUILIBRATION WITH J-13 WELL
WATER/YM-22 TUFF SAMPLES

Sr (moles/L)		Ba (moles/L)	
Original	Equilibrated	Original	Equilibrated
(<75-μm Tuff Size Fraction)			
5.0×10^{-7}	2.00×10^{-7}	3.0×10^{-7} [b]	4.55×10^{-9}
6.0×10^{-7}	1.41×10^{-7}	3.0×10^{-7} [b]	5.90×10^{-9}
6.0×10^{-7}	1.34×10^{-7}	4.0×10^{-7} [b]	6.55×10^{-9}
3.0×10^{-5}	8.10×10^{-6}	1.0×10^{-5} [b]	2.57×10^{-7} [b]
3.0×10^{-3} [a]	1.50×10^{-3} [a]	1.0×10^{-4} [b]	4.77×10^{-6} [b]
(75- to 500-μm Tuff Size Fraction)			
5.0×10^{-7}	1.10×10^{-7}	3.0×10^{-7} [b]	8.70×10^{-9}
6.0×10^{-7}	1.41×10^{-7}	3.0×10^{-7} [b]	9.70×10^{-9}
6.0×10^{-7}	1.05×10^{-7}	4.0×10^{-7} [b]	9.85×10^{-9}
3.0×10^{-5}	8.00×10^{-6}	1.0×10^{5} [b]	4.07×10^{-7} [b]
3.0×10^{-3} [a]	2.04×10^{-3} [a]	1.0×10^{-4} [b]	8.70×10^{-6} [b]

[a] Concentration greater than the solubility of Sr (3.55×10^{-4} moles/L) in equilibrium with $SrSO_4$.

[b] Concentration greater than the solubility of Ba (4.60×10^{-8} moles/L) in equilibrium with $BaSO_4$.

TABLE XXVIII
CONCENTRATIONS OF BA AND SR ORIGINALLY ADDED
AND AFTER EQUILIBRATION WITH J-13 WELL
WATER/YM-38 TUFF SAMPLES

Sr (moles/L)		Ba (moles/L)	
Original	Equilibrated	Original	Equilibrated
(<75-μm Tuff Size Fraction)			
7.0×10^{-8}	1.40×10^{-10}	4.0×10^{-7} [b]	1.10×10^{-10}
2.0×10^{-7}	4.00×10^{-10}	6.0×10^{-7} [b]	1.49×10^{-10}
5.0×10^{-7}	3.02×10^{-10}	2.0×10^{-6} [b]	4.11×10^{-10}
2.0×10^{-5}	3.06×10^{-8}	1.0×10^{-5} [b]	2.16×10^{-9}
2.0×10^{-3} [a]	2.63×10^{-5}	1.0×10^{-4} [b]	2.00×10^{-8}
(75- to 500-μm Tuff Size Fraction)			
6.0×10^{-8}	7.85×10^{-10}	4.0×10^{-7} [b]	2.42×10^{-10}
7.0×10^{-8}	3.40×10^{-10}	6.0×10^{-7} [b]	1.76×10^{-10}
2.0×10^{-7}	4.43×10^{-10}	2.0×10^{-6} [b]	1.19×10^{-9}
2.0×10^{-5}	7.00×10^{-8}	1.0×10^{-5} [b]	2.67×10^{-9}
$2.0 \times 1-^{-3}$ [a]	3.29×10^{-5}	1.0×10^{-4} [b]	2.54×10^{-8}

[a] Concentration greater than the solubility of Sr (3.30×10^{-4} moles/L) in equilibrium with $SrSO_4$.

[b] Concentration greater than the solubility of Ba (4.3×10^{-8} moles/L) in equilibrium with $BaSO_4$.

TABLE XXIX
CONCENTRATIONS OF SR ORIGINALLY ADDED AND AFTER
EQUILIBRATION WITH J-13 WELL WATER/G1-2840 TUFF SAMPLES

Sr (moles/L)			
Original	Equilibrated	Original	Equilibrated
	(75- to 500-μm Tuff Size Fraction)		
8.10×10^{-7}	2.05×10^{-7}	8.3×10^{-5}	2.50×10^{-5}
8.10×10^{-7}	2.11×10^{-7}	8.3×10^{-5}	2.47×10^{-5}
1.00×10^{-6}	1.12×10^{-7}	2.1×10^{-4}	7.10×10^{-5}
1.40×10^{-6}	3.52×10^{-7}	2.1×10^{-4}	7.25×10^{-5}
1.40×10^{-6}	3.35×10^{-7}	3.3×10^{-4}	1.31×10^{-4}
2.8×10^{-6}	6.85×10^{-7}	3.3×10^{-4}	1.30×10^{-4}
2.8×10^{-6}	6.90×10^{-7}	6.0×10^{-4}	2.87×10^{-4}
1.2×10^{-5}	3.13×10^{-6}	6.0×10^{-4}[a]	3.01×10^{-4}
1.2×10^{-5}	3.11×10^{-6}	8.5×10^{-4}[a]	4.89×10^{-4}[a]
2.4×10^{-5}	6.40×10^{-6}	8.5×10^{-4}[a]	4.74×10^{-4}[a]
2.4×10^{-5}	6.30×10^{-6}	1.4×10^{-3}[a]	9.60×10^{-4}[a]
7.7×10^{-5}	2.30×10^{-5}	1.4×10^{-3}[a]	9.40×10^{-4}[a]
7.7×10^{-5}	2.17×10^{-5}		

[a] Concentration greater than the solubility of Sr (4.75×10^{-4} moles/L) in equilibrium with $SrSO_4$.

TABLE XXX
TRACER SOLUBILITIES AS CALCULATED FROM THE CHEMICAL COMPOSITION OF J-13 WELL WATERS EQUILIBRATED WITH SPECIFIED MINERAL SOLIDS

Mineral Solids	J-13 Well Waters Original	YM-22	YM-38	G1-2840
Strontium (moles/L)				
$SrCO_3$(EQ 3/6)	7.93×10^{-4}	8.12×10^{-4}	8.12×10^{-4}	7.96×10^{-4}
$SrCO_3$ (Robie)	2.64×10^{-3}	2.69×10^{-3}	2.69×10^{-3}	2.65×10^{-3}
$SrSO_4$	4.68×10^{-4}	3.55×10^{-4}	3.30×10^{-4}	4.75×10^{-4}
Barium (moles/L)				
$BaCO_3$	1.41×10^{-4}	1.47×10^{-4}	1.48×10^{-4}	1.41×10^{-4}
$BaSO_4$	5.92×10^{-8}	4.60×10^{-8}	4.31×10^{-8}	5.95×10^{-8}

Appendix A

Experimental Raw Data Sets

This Appendix is a data base of experimental laboratory sorption data. The data were retrieved from INC-11 computer files and records. The entries in the data base are defined for each solid matrix and element studied by the following experimental factors: temperature, atmosphere, sampling time, initial element concentration, and particle size range. The following information is included in Tables A-I through A-V: solid matrix (SAMPLE), element (EL), retardation factor (Rd expressed as mL/g), time (TI expressed in days), atmosphere (ATM expressed as air or ca), size (SIZE expressed as μm diameter), initial concentration (Co expressed as moles/L), equilibrated concentration [C expressed as μmoles(p+)/g], equilibrated amount sorbed [S expressed as μmoles(p+)/g], and temperature (T expressed in ^{o}C). A temperature is not given in the tables for experiments conducted at ambient laboratory conditions. Data for experiments conducted in a nitrogen atmosphere are noted by the symbol ca.

Table A-I

Data Base Entries of Experimental Sorption Data for the Element Strontium

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-1292	sr	200.0	21	air	-500	2.00E-07	3.64E-05	7.27E-03	
gl-1292	sr	200.0	21	air	-500	2.00E-07	3.64E-05	7.27E-03	
gl-1292	sr	190.0	42	air	-500	2.00E-07	3.81E-05	7.24E-03	
gl-1292	sr	220.0	42	air	-500	2.00E-07	3.33E-05	7.33E-03	
gl-1436	sr	31000.0	21	air	-500	1.00E-07	1.29E-07	4.00E-03	
gl-1436	sr	36000.0	21	air	-500	1.00E-07	1.11E-07	4.00E-03	
gl-1436	sr	33000.0	42	air	-500	1.00E-07	1.21E-07	4.00E-03	
gl-1436	sr	45000.0	42	air	-500	1.00E-07	8.88E-08	4.00E-03	
gl-1854	sr	71000.0	21	air	- 75	3.00E-08	1.69E-08	1.20E-03	
gl-1854	sr	32000.0	21	air	75-500	3.00E-08	3.75E-08	1.20E-03	
gl-1854	sr	92000.0	42	air	- 75	3.00E-08	1.30E-08	1.20E-03	
gl-1854	sr	43000.0	42	air	75-500	3.00E-08	2.79E-08	1.20E-03	
gl-1883	sr	26.0	21	air	- 38	3.00E-07	2.61E-04	6.78E-03	
gl-1883	sr	80.0	21	air	- 38	3.00E-07	1.20E-04	9.60E-03	
gl-1883	sr	58.0	21	air	-500	2.00E-07	1.03E-04	5.95E-03	
gl-1883	sr	59.0	21	air	-500	2.00E-07	1.01E-04	5.97E-03	
gl-1883	sr	22.0	21	air	38-106	3.00E-07	2.86E-04	6.29E-03	
gl-1883	sr	22.0	21	air	38-106	3.00E-07	2.86E-04	6.29E-03	
gl-1883	sr	22.0	21	air	106-500	3.00E-07	2.86E-04	6.29E-03	
gl-1883	sr	22.0	21	air	106-500	3.00E-07	2.86E-04	6.29E-03	
gl-1883	sr	57.0	42	air	-500	2.00E-07	1.04E-04	5.92E-03	
gl-1883	sr	58.0	42	air	-500	2.00E-07	1.03E-04	5.95E-03	
gl-1982	sr	1200.0	14	air	- 38	2.00E-07	6.56E-06	7.87E-03	
gl-1982	sr	59.0	14	air	38- 75	2.00E-07	1.01E-04	5.97E-03	
gl-1982	sr	49.0	14	air	75-250	2.00E-07	1.16E-04	5.68E-03	
gl-1982	sr	51.0	14	air	250-500	2.00E-07	1.13E-04	5.75E-03	
gl-1982	sr	1200.0	21	air	- 38	2.00E-07	6.56E-06	7.87E-03	
gl-1982	sr	430.0	21	air	-500	2.00E-07	1.78E-05	7.64E-03	
gl-1982	sr	430.0	21	air	-500	2.00E-07	1.78E-05	7.64E-03	
gl-1982	sr	66.0	21	air	38- 75	2.00E-07	9.30E-05	6.14E-03	
gl-1982	sr	53.0	21	air	75-250	2.00E-07	1.10E-04	5.81E-03	
gl-1982	sr	66.0	21	air	250-500	2.00E-07	9.30E-05	6.14E-03	
gl-1982	sr	450.0	42	air	-500	2.00E-07	1.70E-05	7.66E-03	
gl-1982	sr	450.0	42	air	-500	2.00E-07	1.70E-05	7.66E-03	
gl-2233	sr	40000.0	21	air	-500	1.00E-07	1.00E-07	4.00E-03	
gl-2233	sr	55000.0	21	air	-500	1.00E-07	7.27E-08	4.00E-03	
gl-2233	sr	50000.0	42	air	-500	1.00E-07	8.00E-08	4.00E-03	
gl-2233	sr	49000.0	42	air	-500	1.00E-07	8.16E-08	4.00E-03	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-2289	sr	17000.0	21	air	- 38	3.00E-08	7.05E-08	1.20E-03	
gl-2289	sr	12000.0	21	air	- 38	3.00E-08	9.98E-08	1.20E-03	
gl-2289	sr	6300.0	21	air	38-106	3.00E-08	1.90E-07	1.20E-03	
gl-2289	sr	6400.0	21	air	38-106	3.00E-08	1.87E-07	1.20E-03	
gl-2289	sr	7800.0	21	air	106-500	3.00E-08	1.53E-07	1.20E-03	
gl-2289	sr	8400.0	21	air	106-500	3.00E-08	1.43E-07	1.20E-03	
gl-2333	sr	220.0	21	air	- 75	1.00E-06	1.67E-04	3.67E-02	
gl-2333	sr	150.0	21	air	75-500	1.00E-06	2.35E-04	3.53E-02	
gl-2333	sr	220.0	42	air	- 75	1.00E-06	1.67E-04	3.67E-02	
gl-2333	sr	140.0	42	air	75-500	1.00E-06	2.50E-04	3.50E-02	
gl-2363	sr	170.0	21	air	- 38	5.00E-07	1.05E-04	1.79E-02	
gl-2363	sr	180.0	21	air	- 38	5.00E-07	1.00E-04	1.80E-02	
gl-2363	sr	170.0	21	air	-500	4.00E-07	8.42E-05	1.43E-02	
gl-2363	sr	180.0	21	air	-500	4.00E-07	8.00E-05	1.44E-02	
gl-2363	sr	74.0	21	air	38-106	5.00E-07	2.13E-04	1.57E-02	
gl-2363	sr	62.0	21	air	38-106	5.00E-07	2.44E-04	1.51E-02	
gl-2363	sr	58.0	21	air	106-500	5.00E-07	2.56E-04	1.49E-02	
gl-2363	sr	61.0	21	air	106-500	5.00E-07	2.47E-04	1.51E-02	
gl-2363	sr	170.0	42	air	-500	4.00E-07	8.42E-05	1.43E-02	
gl-2363	sr	170.0	42	air	-500	4.00E-07	8.42E-05	1.43E-02	
gl-2410	sr	280.0	21	air	- 75	4.00E-07	5.33E-05	1.49E-02	
gl-2410	sr	170.0	21	air	75-500	4.00E-07	8.42E-05	1.43E-02	
gl-2410	sr	280.0	42	air	- 75	4.00E-07	5.33E-05	1.49E-02	
gl-2410	sr	170.0	42	air	75-500	4.00E-07	8.42E-05	1.43E-02	
gl-2476	sr	49.0	21	air	- 75	9.00E-07	5.22E-04	2.56E-02	
gl-2476	sr	41.0	21	air	75-500	9.00E-07	5.90E-04	2.42E-02	
gl-2476	sr	51.0	42	air	- 75	9.00E-07	5.07E-04	2.59E-02	
gl-2476	sr	40.0	42	air	75-500	9.00E-07	6.00E-04	2.40E-02	
gl-2698	sr	39000.0	21	air	-500	2.00E-07	2.05E-07	8.00E-03	
gl-2698	sr	49000.0	21	air	-500	2.00E-07	1.63E-07	8.00E-03	
gl-2698	sr	43000.0	42	air	-500	2.00E-07	1.86E-07	8.00E-03	
gl-2698	sr	37000.0	42	air	-500	2.00E-07	2.16E-07	8.00E-03	
gl-2840	sr	170.0	21	air	- 75	1.00E-06	2.11E-04	3.58E-02	
gl-2840	sr	9.2	21	air	75-500	1.40E-03	1.92E+00	1.76E+01	
gl-2840	sr	9.7	21	air	75-500	1.40E-03	1.89E+00	1.83E+01	
gl-2840	sr	14.8	21	air	75-500	8.50E-04	9.77E-01	1.45E+01	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-2840	sr	15.9	21	air	75-500	8.50E-04	9.47E-01	1.51E+01	
gl-2840	sr	19.9	21	air	75-500	6.00E-04	6.02E-01	1.20E+01	
gl-2840	sr	21.9	21	air	75-500	6.00E-04	5.73E-01	1.25E+01	
gl-2840	sr	30.5	21	air	75-500	3.30E-04	2.61E-01	7.97E+00	
gl-2840	sr	30.7	21	air	75-500	3.30E-04	2.60E-01	7.99E+00	
gl-2840	sr	38.1	21	air	75-500	2.10E-04	1.45E-01	5.51E+00	
gl-2840	sr	39.5	21	air	75-500	2.10E-04	1.41E-01	5.58E+00	
gl-2840	sr	46.6	21	air	75-500	8.30E-05	4.98E-02	2.32E+00	
gl-2840	sr	47.0	21	air	75-500	7.70E-05	4.60E-02	2.16E+00	
gl-2840	sr	47.3	21	air	75-500	8.30E-05	4.93E-02	2.33E+00	
gl-2840	sr	51.0	21	air	75-500	7.70E-05	4.34E-02	2.21E+00	
gl-2840	sr	55.3	21	air	75-500	2.40E-05	1.27E-02	7.05E-01	
gl-2840	sr	56.4	21	air	75-500	2.40E-05	1.26E-02	7.09E-01	
gl-2840	sr	56.7	21	air	75-500	1.20E-05	6.26E-03	3.55E-01	
gl-2840	sr	57.0	21	air	75-500	8.10E-07	4.21E-04	2.40E-02	
gl-2840	sr	57.1	21	air	75-500	1.20E-05	6.23E-03	3.55E-01	
gl-2840	sr	59.0	21	air	75-500	8.10E-07	4.10E-04	2.42E-02	
gl-2840	sr	59.6	21	air	75-500	1.40E-06	7.04E-04	4.19E-02	
gl-2840	sr	61.2	21	air	75-500	2.80E-06	1.38E-03	8.44E-02	
gl-2840	sr	61.7	21	air	75-500	2.80E-06	1.37E-03	8.46E-02	
gl-2840	sr	63.6	21	air	75-500	1.40E-06	6.70E-04	4.26E-02	
gl-2840	sr	160.0	21	air	75-500	1.00E-06	2.22E-04	3.56E-02	
gl-2840	sr	170.0	42	air	- 75	1.00E-06	2.11E-04	3.58E-02	
gl-2840	sr	159.0	42	air	75-500	1.00E-06	2.23E-04	3.55E-02	
gl-2854	sr	120.0	21	air	- 75	5.00E-07	1.43E-04	1.71E-02	
gl-2854	sr	94.0	21	air	75-500	5.00E-07	1.75E-04	1.65E-02	
gl-2854	sr	60.0	42	air	- 75	5.00E-07	2.50E-04	1.50E-02	
gl-2854	sr	93.0	42	air	75-500	5.00E-07	1.77E-04	1.65E-02	
gl-2901	sr	68.0	21	air	-500	1.00E-06	4.55E-04	3.09E-02	
gl-2901	sr	69.0	21	air	-500	1.00E-06	4.49E-04	3.10E-02	
gl-2901	sr	66.0	42	air	-500	1.00E-06	4.65E-04	3.07E-02	
gl-2901	sr	71.0	42	air	-500	1.00E-06	4.40E-04	3.12E-02	
gl-3116	sr	2500.0	21	air	-500	2.00E-07	3.17E-06	7.94E-03	
gl-3116	sr	2500.0	21	air	-500	2.00E-07	3.17E-06	7.94E-03	
gl-3116	sr	2200.0	42	air	-500	2.00E-07	3.60E-06	7.93E-03	
gl-3116	sr	2400.0	42	air	-500	2.00E-07	3.31E-06	7.93E-03	
gl-3658	sr	160000.0	21	air	- 38	3.00E-07	7.50E-08	1.20E-02	
gl-3658	sr	98000.0	21	air	- 38	3.00E-07	1.22E-07	1.20E-02	
gl-3658	sr	10000.9	21	air	-500	3.00E-07	1.20E-06	1.20E-02	
gl-3658	sr	14000.0	21	air	-500	3.00E-07	8.56E-07	1.20E-02	
gl-3658	sr	120000.0	21	air	38-106	3.00E-07	1.00E-07	1.20E-02	
gl-3658	sr	140000.0	21	air	38-106	3.00E-07	8.57E-08	1.20E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-3658	sr	130000.0	21	air	106-500	3.00E-07	9.23E-08	1.20E-02	
gl-3658	sr	130000.0	21	air	106-500	3.00E-07	9.23E-08	1.20E-02	
gl-3658	sr	12000.0	42	air	-500	3.00E-07	9.98E-07	1.20E-02	
gl-3658	sr	11000.0	42	air	-500	3.00E-07	1.09E-06	1.20E-02	
g2-1952	sr	1940.0	42	air	-500	2.00E-06	4.08E-05	7.92E-02	
g2-1952	sr	2560.0	42	air	-500	2.00E-06	3.10E-05	7.94E-02	
g2-3933	sr	192.0	42	air	-500	2.00E-06	3.77E-04	7.25E-02	
g2-3933	sr	299.0	42	air	-500	2.00E-06	2.51E-04	7.50E-02	
g2-547	sr	256.0	42	air	-500	2.60E-06	3.77E-04	9.65E-02	
g2-547	sr	275.0	42	air	-500	2.60E-06	3.53E-04	9.69E-02	
g2-723	sr	248.0	42	air	-500	2.00E-06	2.99E-04	7.40E-02	
g2-723	sr	326.0	42	air	-500	2.00E-06	2.31E-04	7.54E-02	
gu3-1203	sr	42.0	42	air	75-500	1.00E-06	6.45E-04	2.71E-02	
gu3-1203	sr	43.0	42	air	75-500	1.00E-06	6.35E-04	2.73E-02	
GU3-1301	sr	23.0	42	air	75-500	2.00E-06	1.86E-03	4.28E-02	
GU3-1301	sr	25.0	42	air	75-500	2.00E-06	1.78E-03	4.44E-02	
GU3-1301	sr	25.0	42	air	75-500	2.00E-06	1.78E-03	4.44E-02	
GU3-1301	sr	40.0	42	air	75-500	2.00E-06	1.33E-03	5.33E-02	
gu3-433	sr	28.2	42	air	75-500	2.00E-06	1.66E-03	4.68E-02	
gu3-433	sr	31.6	42	air	75-500	2.00E-06	1.55E-03	4.90E-02	
gu3-433	sr	56.0	42	air	75-500	2.00E-06	1.05E-03	5.89E-02	
gu3-433	sr	66.0	42	air	75-500	2.00E-06	9.30E-04	6.14E-02	
ja-18	sr	11000.0	14	air	106-150	1.00E-06	3.63E-06	3.99E-02	
ja-18	sr	8900.0	14	air	355-500	1.00E-06	4.48E-06	3.99E-02	
ja-18	sr	16000.0	21	air	75-500	8.00E-11	2.00E-10	3.20E-06	
ja-18	sr	13000.0	21	air	106-150	1.00E-06	3.07E-06	3.99E-02	
ja-18	sr	6500.0	21	air	355-500	1.00E-06	6.13E-06	3.99E-02	
ja-18	sr	5000.0	28	air	250-355	2.00E-06	1.59E-05	7.97E-02	
ja-18	sr	24000.0	28	air	250-355	2.00E-06	3.33E-06	7.99E-02	
ja-18	sr	45000.0	42	air	75-500	8.00E-11	7.11E-11	3.20E-06	
ja-18	sr	18000.0	42	air	106-150	1.00E-06	2.22E-06	4.00E-02	
ja-18	sr	5800.0	42	air	355-500	1.00E-06	6.87E-06	3.99E-02	
ja-18	sr	4900.0	63	air	250-355	2.00E-06	1.63E-05	7.97E-02	
ja-18	sr	27000.0	63	air	250-355	2.00E-06	2.96E-06	7.99E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-18	sr	22000.0	77	air	106-150	1.00E-06	1.82E-06	4.00E-02	
ja-18	sr	16000.0	77	air	355-500	1.00E-06	2.50E-06	4.00E-02	
ja-18	sr	20000.0	84	air	75-500	8.00E-11	1.60E-10	3.20E-06	
ja-26	sr	36.0	21	air	75-500	2.00E-11	1.43E-08	5.14E-07	
ja-26	sr	40.0	21	air	75-500	2.00E-11	1.33E-08	5.33E-07	
ja-26	sr	130.0	42	air	75-500	2.00E-11	5.33E-09	6.93E-07	
ja-26	sr	170.0	42	air	75-500	2.00E-11	4.21E-09	7.16E-07	
ja-28	sr	110.0	21	air	75-500	2.00E-11	6.15E-09	6.77E-07	
ja-28	sr	140.0	21	air	75-500	2.00E-11	5.00E-09	7.00E-07	
ja-28	sr	69.0	42	air	75-500	2.00E-11	8.99E-09	6.20E-07	
ja-28	sr	54.0	42	air	75-500	2.00E-11	1.08E-08	5.84E-07	
ja-32	sr	48.0	7	air	106-150	2.00E-06	1.18E-03	5.65E-02	
ja-32	sr	50.0	7	air	355-500	2.00E-06	1.14E-03	5.71E-02	
ja-32	sr	50.0	21	air	106-150	2.00E-06	1.14E-03	5.71E-02	
ja-32	sr	52.0	21	air	355-500	2.00E-06	1.11E-03	5.78E-02	
ja-32	sr	18.0	28	air	250-355	2.00E-06	2.11E-03	3.79E-02	
ja-32	sr	84.0	28	air	250-355	2.00E-06	7.69E-04	6.46E-02	
ja-32	sr	72.0	35	air	106-150	2.00E-06	8.70E-04	6.26E-02	
ja-32	sr	56.0	35	air	355-500	2.00E-06	1.05E-03	5.89E-02	
ja-32	sr	55.0	56	air	106-150	2.00E-06	1.07E-03	5.87E-02	
ja-32	sr	71.0	56	air	355-500	2.00E-06	8.79E-04	6.24E-02	
ja-32	sr	18.0	63	air	250-355	2.00E-06	2.11E-03	3.79E-02	
ja-32	sr	85.0	63	air	250-355	2.00E-06	7.62E-04	6.48E-02	
ja-37	sr	300.0	14	air	106-150	3.00E-06	3.75E-04	1.13E-01	
ja-37	sr	260.0	14	air	355-500	3.00E-06	4.29E-04	1.11E-01	
ja-37	sr	280.0	21	air	106-150	3.00E-06	4.00E-04	1.12E-01	
ja-37	sr	250.0	21	air	355-500	3.00E-06	4.44E-04	1.11E-01	
ja-37	sr	420.0	28	air	250-355	2.00E-06	1.82E-04	7.64E-02	
ja-37	sr	74.0	28	air	250-355	2.00E-06	8.51E-04	6.30E-02	
ja-37	sr	260.0	35	air	106-150	3.00E-06	4.29E-04	1.11E-01	
ja-37	sr	340.0	35	air	355-500	3.00E-06	3.33E-04	1.13E-01	
ja-37	sr	390.0	63	air	250-355	2.00E-06	1.95E-04	7.61E-02	
ja-37	sr	150.0	63	air	250-355	2.00E-06	4.71E-04	7.06E-02	
ja-37	sr	350.0	70	air	106-150	3.00E-06	3.24E-04	1.14E-01	
ja-37	sr	260.0	70	air	355-500	3.00E-06	4.29E-04	1.11E-01	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-8	sr	260.0	21	air	75-500	2.00E-11	2.86E-09	7.43E-07	
ja-8	sr	270.0	21	air	75-500	2.00E-11	2.76E-09	7.45E-07	
ja-8	sr	270.0	42	air	75-500	2.00E-11	2.76E-09	7.45E-07	
ja-8	sr	290.0	42	air	75-500	2.00E-11	2.58E-09	7.48E-07	
ym-22	sr	73.0	21	ca	- 75	7.00E-07	3.01E-04	2.20E-02	
ym-22	sr	48.0	21	ca	75-500	7.00E-07	4.12E-04	1.98E-02	
ym-22	sr	75.0	42	ca	- 75	7.00E-07	2.95E-04	2.21E-02	
ym-22	sr	53.0	42	ca	75-500	7.00E-07	3.84E-04	2.03E-02	
ym-22	sr	81.0	84	ca	- 75	7.00E-07	2.77E-04	2.25E-02	
ym-22	sr	46.0	84	ca	75-500	7.00E-07	4.24E-04	1.95E-02	
ym-22	sr	20.0	21	air	- 75	3.00E-03	3.00E+00	6.00E+01	
ym-22	sr	81.0	21	air	- 75	5.00E-07	1.98E-04	1.60E-02	
ym-22	sr	65.0	21	air	- 75	6.00E-07	2.82E-04	1.84E-02	
ym-22	sr	54.0	21	air	- 75	3.00E-05	1.62E-02	8.76E-01	
ym-22	sr	70.0	21	air	- 75	6.00E-07	2.67E-04	1.87E-02	
ym-22	sr	9.4	21	air	75-500	3.00E-03	4.08E+00	3.84E+01	
ym-22	sr	55.0	21	air	75-500	3.00E-05	1.60E-02	8.80E-01	
ym-22	sr	71.0	21	air	75-500	5.00E-07	2.20E-04	1.56E-02	
ym-22	sr	65.0	21	air	75-500	6.00E-07	2.82E-04	1.84E-02	
ym-22	sr	95.0	21	air	75-500	6.00E-07	2.09E-04	1.98E-02	
ym-22	sr	48.0	21	air	106-500	7.00E-07	4.12E-04	1.98E-02	
ym-22	sr	48.0	21	air	106-500	7.00E-07	4.12E-04	1.98E-02	
ym-22	sr	66.0	42	air	-106	7.00E-07	3.26E-04	2.15E-02	
ym-22	sr	55.0	42	air	106-500	7.00E-07	3.73E-04	2.05E-02	
ym-22	sr	62.0	42	air	106-500	7.00E-07	3.41E-04	2.12E-02	
ym-30	sr	100.0	21	air	75-500	8.00E-11	2.67E-08	2.67E-06	
ym-30	sr	320.0	42	air	75-500	8.00E-11	9.41E-09	3.01E-06	
ym-30	sr	360.0	84	air	75-500	8.00E-11	8.42E-09	3.03E-06	
ym-38	sr	9100.0	21	ca	- 75	1.00E-07	4.39E-07	3.99E-03	
ym-38	sr	7200.0	21	ca	75-500	1.00E-07	5.54E-07	3.99E-03	
ym-38	sr	23000.0	42	ca	- 75	1.00E-07	1.74E-07	4.00E-03	
ym-38	sr	8500.0	42	ca	75-500	1.00E-07	4.69E-07	3.99E-03	
ym-38	sr	8000.0	84	ca	- 75	1.00E-07	4.99E-07	3.99E-03	
ym-38	sr	7500.0	84	ca	75-500	1.00E-07	5.32E-07	3.99E-03	
ym-38	sr	20000.0	21	air	- 38	4.00E-07	7.99E-07	1.60E-02	
ym-38	sr	14000.0	21	air	- 38	4.00E-07	1.14E-06	1.60E-02	
ym-38	sr	3300.0	21	air	- 75	5.00E-08	6.02E-07	1.99E-03	
ym-38	sr	10000.0	21	air	- 75	7.00E-08	2.79E-07	2.79E-03	
ym-38	sr	1500.0	21	air	- 75	2.00E-03	5.26E-02	7.89E+01	
ym-38	sr	10000.0	21	air	- 75	2.00E-07	7.98E-07	7.98E-03	
ym-38	sr	13000.0	21	air	- 75	2.00E-05	6.14E-05	7.99E-01	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-38	sr	20000.0	21	air	38-106	4.00E-07	7.99E-07	1.60E-02	
ym-38	sr	20000.0	21	air	38-106	4.00E-07	7.99E-07	1.60E-02	
ym-38	sr	1200.0	21	air	75-500	2.00E-03	6.56E-02	7.87E+01	
ym-38	sr	1500.0	21	air	75-500	6.00E-08	1.58E-06	2.37E-03	
ym-38	sr	4100.0	21	air	75-500	7.00E-08	6.80E-07	2.79E-03	
ym-38	sr	9000.0	21	air	75-500	2.00E-07	8.87E-07	7.98E-03	
ym-38	sr	5700.0	21	air	75-500	2.00E-05	1.40E-04	7.97E-01	
ym-38	sr	17000.0	21	air	106-500	4.00E-07	9.40E-07	1.60E-02	
ym-38	sr	18000.0	21	air	106-500	4.00E-07	8.88E-07	1.60E-02	
ym-38	sr	18000.0	21	air	106-500	6.00E-08	1.33E-07	2.40E-03	
ym-38	sr	10000.0	42	air	106-500	6.00E-08	2.40E-07	2.40E-03	
ym-38	sr	7400.0	42	air	-106	6.00E-08	3.23E-07	2.39E-03	
ym-42	sr	2900.0	21	air	75-500	8.00E-11	1.10E-09	3.18E-06	
ym-42	sr	3900.0	42	air	75-500	8.00E-11	8.16E-10	3.18E-06	
ym-42	sr	5000.0	84	air	75-500	8.00E-11	6.37E-10	3.19E-06	
ym-45	sr	220.0	21	air	-106	6.00E-07	1.00E-04	2.20E-02	
ym-45	sr	170.0	21	air	106-500	6.00E-07	1.26E-04	2.15E-02	
ym-45	sr	220.0	42	air	-106	6.00E-07	1.00E-04	2.20E-02	
ym-45	sr	170.0	42	air	106-500	6.00E-07	1.26E-04	2.15E-02	
ym-46	sr	90.0	21	air	75-500	8.00E-11	2.91E-08	2.62E-06	
ym-46	sr	170.0	42	air	75-500	8.00E-11	1.68E-08	2.86E-06	
ym-46	sr	300.0	84	air	75-500	8.00E-11	1.00E-08	3.00E-06	
ym-48	sr	15000.0	21	air	106-500	7.00E-08	1.86E-07	2.80E-03	
ym-48	sr	1200.0	42	air	-106	7.00E-08	2.30E-06	2.75E-03	
ym-48	sr	2500.0	42	air	106-500	7.00E-08	1.11E-06	2.78E-03	
ym-49	sr	1500.0	21	air	-106	6.00E-08	1.58E-06	2.37E-03	
ym-49	sr	2600.0	21	air	106-500	6.00E-08	9.16E-07	2.38E-03	
ym-49	sr	2700.0	21	air	106-500	6.00E-08	8.82E-07	2.38E-03	
ym-49	sr	2400.0	42	air	-106	6.00E-08	9.92E-07	2.38E-03	
ym-49	sr	3800.0	42	air	106-500	6.00E-08	6.28E-07	2.39E-03	
ym-49	sr	3800.0	42	air	106-500	6.00E-08	6.28E-07	2.39E-03	
ym-54	sr	56.0	21	air	38-106	6.00E-07	3.16E-04	1.77E-02	
ym-54	sr	57.0	21	air	38-106	6.00E-07	3.12E-04	1.78E-02	
ym-54	sr	42.0	21	air	106-500	6.00E-07	3.87E-04	1.63E-02	
ym-54	sr	37.0	21	air	106-500	6.00E-07	4.21E-04	1.56E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-54	sr	100.0	21	ca	- 75	8.00E-08	2.67E-05	2.67E-03	
ym-54	sr	76.0	21	ca	75-500	8.00E-08	3.33E-05	2.53E-03	
ym-54	sr	150.0	42	ca	- 75	8.00E-08	1.88E-05	2.82E-03	
ym-54	sr	130.0	42	ca	75-500	8.00E-08	2.13E-05	2.77E-03	
ym-54	sr	130.0	84	ca	- 75	8.00E-08	2.13E-05	2.77E-03	
ym-54	sr	70.0	84	ca	75-500	8.00E-08	3.56E-05	2.49E-03	
ym-54	sr	270.0	21	air	- 38	6.00E-07	8.28E-05	2.23E-02	
ym-54	sr	280.0	21	air	- 38	6.00E-07	8.00E-05	2.24E-02	
ym-54	sr	95.0	21	air	-106	6.00E-07	2.09E-04	1.98E-02	
ym-54	sr	88.0	21	air	106-500	6.00E-07	2.22E-04	1.96E-02	
ym-54	sr	97.0	42	air	-106	6.00E-07	2.05E-04	1.99E-02	
ym-54	sr	80.0	42	air	106-500	6.00E-07	2.40E-04	1.92E-02	
ja-18	sr	13000.0	14	air	106-150	1.00E-06	3.07E-06	3.99E-02	70
ja-18	sr	19000.0	14	air	355-500	1.00E-06	2.10E-06	4.00E-02	70
ja-18	sr	22000.0	21	air	106-150	1.00E-06	1.82E-06	4.00E-02	70
ja-18	sr	15000.0	21	air	355-500	1.00E-06	2.66E-06	3.99E-02	70
ja-18	sr	15000.0	35	air	106-150	1.00E-06	2.66E-06	3.99E-02	70
ja-18	sr	22000.0	35	air	355-500	1.00E-06	1.82E-06	4.00E-02	70
ja-18	sr	4700.0	63	air	106-150	1.00E-06	8.47E-06	3.98E-02	70
ja-18	sr	4300.0	63	air	355-500	1.00E-06	9.26E-06	3.98E-02	70
ja-32	sr	82.0	7	air	106-150	2.00E-06	7.84E-04	6.43E-02	70
ja-32	sr	93.0	7	air	355-500	2.00E-06	7.08E-04	6.58E-02	70
ja-32	sr	92.0	14	air	106-150	2.00E-06	7.14E-04	6.57E-02	70
ja-32	sr	110.0	14	air	355-500	2.00E-06	6.15E-04	6.77E-02	70
ja-32	sr	120.0	28	air	106-150	2.00E-06	5.71E-04	6.86E-02	70
ja-32	sr	110.0	28	air	355-500	2.00E-06	6.15E-04	6.77E-02	70
ja-32	sr	160.0	56	air	106-150	2.00E-06	4.44E-04	7.11E-02	70
ja-32	sr	140.0	56	air	355-500	2.00E-06	5.00E-04	7.00E-02	70
ja-37	sr	770.0	7	air	106-150	2.00E-06	1.01E-04	7.80E-02	70
ja-37	sr	660.0	7	air	355-500	2.00E-06	1.18E-04	7.76E-02	70
ja-37	sr	820.0	14	air	106-150	2.00E-06	9.52E-05	7.81E-02	70
ja-37	sr	790.0	14	air	355-500	2.00E-06	9.88E-05	7.80E-02	70
ja-37	sr	1200.0	21	air	106-150	2.00E-06	6.56E-05	7.87E-02	70
ja-37	sr	1000.0	21	air	355-500	2.00E-06	7.84E-05	7.84E-02	70
ja-37	sr	1600.0	49	air	106-150	2.00E-06	4.94E-05	7.90E-02	70
ja-37	sr	1500.0	49	air	355-500	2.00E-06	5.26E-05	7.89E-02	70

Table A-II

Data Base Entries of Experimental Sorption Data for the Element Cesium

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
GU3-1301	cs	109.0	42	air	75-500	3.00E-09	4.65E-07	5.07E-05	
GU3-1301	cs	125.0	42	air	75-500	3.00E-09	4.14E-07	5.17E-05	
GU3-1301	cs	135.0	42	air	75-500	3.00E-09	3.87E-07	5.23E-05	
GU3-1301	cs	195.0	42	air	75-500	3.00E-09	2.79E-07	5.44E-05	
gl-1292	cs	390.0	21	air	-500	3.00E-09	1.46E-07	5.71E-05	
gl-1292	cs	450.0	21	air	-500	3.00E-09	1.28E-07	5.74E-05	
gl-1292	cs	380.0	42	air	-500	3.00E-09	1.50E-07	5.70E-05	
gl-1292	cs	500.0	42	air	-500	3.00E-09	1.15E-07	5.77E-05	
gl-1436	cs	7000.0	21	air	-500	3.00E-09	8.55E-09	5.98E-05	
gl-1436	cs	7900.0	21	air	-500	3.00E-09	7.58E-09	5.98E-05	
gl-1436	cs	7400.0	42	air	-500	3.00E-09	8.09E-09	5.98E-05	
gl-1436	cs	9000.0	42	air	-500	3.00E-09	6.65E-09	5.99E-05	
gl-1854	cs	15000.0	21	air	- 75	4.00E-09	5.33E-09	7.99E-05	
gl-1854	cs	11000.0	21	air	75-500	4.00E-09	7.26E-09	7.99E-05	
gl-1854	cs	15000.0	42	air	- 75	4.00E-09	5.33E-09	7.99E-05	
gl-1854	cs	10000.0	42	air	75-500	4.00E-09	7.98E-09	7.98E-05	
gl-1883	cs	720.0	21	air	- 38	4.00E-09	1.08E-07	7.78E-05	
gl-1883	cs	310.0	21	air	- 38	4.00E-09	2.42E-07	7.52E-05	
gl-1883	cs	350.0	21	air	-500	3.00E-09	1.62E-07	5.68E-05	
gl-1883	cs	380.0	21	air	-500	3.00E-09	1.50E-07	5.70E-05	
gl-1883	cs	180.0	21	air	38-106	4.00E-09	4.00E-07	7.20E-05	
gl-1883	cs	200.0	21	air	38-106	4.00E-09	3.64E-07	7.27E-05	
gl-1883	cs	180.0	21	air	106-500	4.00E-09	4.00E-07	7.20E-05	
gl-1883	cs	190.0	21	air	106-500	4.00E-09	3.81E-07	7.24E-05	
gl-1883	cs	440.0	42	air	-500	3.00E-09	1.30E-07	5.74E-05	
gl-1883	cs	440.0	42	air	-500	3.00E-09	1.30E-07	5.74E-05	
gl-1982	cs	3800.0	14	air	- 38	3.00E-09	1.57E-08	5.97E-05	
gl-1982	cs	1200.0	14	air	38- 75	3.00E-09	4.92E-08	5.90E-05	
gl-1982	cs	960.0	14	air	75-250	3.00E-09	6.12E-08	5.88E-05	
gl-1982	cs	1200.0	14	air	250-500	3.00E-09	4.92E-08	5.90E-05	
gl-1982	cs	3500.0	21	air	- 38	3.00E-09	1.70E-08	5.97E-05	
gl-1982	cs	1400.0	21	air	-500	3.00E-09	4.23E-08	5.92E-05	
gl-1982	cs	1400.0	21	air	-500	3.00E-09	4.23E-08	5.92E-05	
gl-1982	cs	1300.0	21	air	38- 75	3.00E-09	4.55E-08	5.91E-05	
gl-1982	cs	1100.0	21	air	75-250	3.00E-09	5.36E-08	5.89E-05	
gl-1982	cs	1200.0	21	air	250-500	3.00E-09	4.92E-08	5.90E-05	
gl-1982	cs	1800.0	42	air	-500	3.00E-09	3.30E-08	5.93E-05	
gl-1982	cs	1800.0	42	air	-500	3.00E-09	3.30E-08	5.93E-05	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-2233	cs	11000.0	21	air	-500	3.00E-09	5.44E-09	5.99E-05	
gl-2233	cs	13000.0	21	air	-500	3.00E-09	4.61E-09	5.99E-05	
gl-2233	cs	14000.0	42	air	-500	3.00E-09	4.28E-09	5.99E-05	
gl-2233	cs	15000.0	42	air	-500	3.00E-09	3.99E-09	5.99E-05	
gl-2289	cs	27000.0	21	air	- 38	4.00E-09	2.96E-09	7.99E-05	
gl-2289	cs	43000.0	21	air	- 38	4.00E-09	1.86E-09	8.00E-05	
gl-2289	cs	29000.0	21	air	38-106	4.00E-09	2.76E-09	7.99E-05	
gl-2289	cs	34000.0	21	air	38-106	4.00E-09	2.35E-09	8.00E-05	
gl-2289	cs	12000.0	21	air	106-500	4.00E-09	6.66E-09	7.99E-05	
gl-2289	cs	72000.0	21	air	106-500	4.00E-09	1.11E-09	8.00E-05	
gl-2333	cs	1700.0	21	air	- 75	5.00E-09	5.81E-08	9.88E-05	
gl-2333	cs	1200.0	21	air	75-500	5.00E-09	8.20E-08	9.84E-05	
gl-2363	cs	380.0	21	air	106-500	4.00E-09	2..00E-07	7.60E-05	
gl-2333	cs	1500.0	42	air	- 75	5.00E-09	6.58E-08	9.87E-05	
gl-2333	cs	1100.0	42	air	75-500	5.00E-09	8.93E-08	9.82E-05	
gl-2363	cs	1400.0	21	air	- 38	4.00E-09	5.63E-08	7.89E-05	
gl-2363	cs	1300.0	21	air	- 38	4.00E-09	6.06E-08	7.88E-05	
gl-2363	cs	1200.0	21	air	-500	7.00E-09	1.15E-07	1.38E-04	
gl-2363	cs	1300.0	21	air	-500	7.00E-09	1.06E-07	1.38E-04	
gl-2363	cs	550.0	21	air	38-106	4.00E-09	1.40E-07	7.72E-05	
gl-2363	cs	520.0	21	air	38-106	4.00E-09	1.48E-07	7.70E-05	
gl-2363	cs	410.0	21	air	106-500	4.00E-09	1.86E-07	7.63E-05	
gl-2363	cs	1400.0	42	air	-500	7.00E-09	9.86E-08	1.38E-04	
gl-2363	cs	1400.0	42	air	-500	7.00E-09	9.86E-08	1.38E-04	
gl-2410	cs	2000.0	21	air	- 75	4.00E-09	3.96E-08	7.92E-05	
gl-2410	cs	1200.0	21	air	75-500	4.00E-09	6.56E-08	7.87E-05	
gl-2410	cs	2000.0	42	air	- 75	4.00E-09	3.96E-08	7.92E-05	
gl-2410	cs	1300.0	42	air	75-500	4.00E-09	6.06E-08	7.88E-05	
gl-2476	cs	810.0	21	air	- 75	5.00E-09	1.20E-07	9.76E-05	
gl-2476	cs	660.0	21	air	75-500	5.00E-09	1.47E-07	9.71E-05	
gl-2476	cs	920.0	42	air	- 75	5.00E-09	1.06E-07	9.79E-05	
gl-2476	cs	740.0	42	air	75-500	5.00E-09	1.32E-07	9.74E-05	
gl-2698	cs	7400.0	21	air	-500	5.00E-09	1.35E-08	9.97E-05	
gl-2698	cs	8200.0	21	air	-500	5.00E-09	1.22E-08	9.98E-05	
gl-2698	cs	6600.0	42	air	-500	5.00E-09	1.51E-08	9.97E-05	
gl-2698	cs	8500.0	42	air	-500	5.00E-09	1.17E-08	9.98E-05	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-2840	cs	2800.0	21	air	- 75	5.00E-09	3.55E-08	9.93E-05	
gl-2840	cs	19.0	21	air	75-500	1.30E-03	6.67E-01	1.27E+01	
gl-2840	cs	21.0	21	air	75-500	1.30E-03	6.34E-01	1.33E+01	
gl-2840	cs	24.0	21	air	75-500	6.30E-04	2.86E-01	6.87E+00	
gl-2840	cs	25.0	21	air	75-500	6.30E-04	2.80E-01	7.00E+00	
gl-2840	cs	31.0	21	air	75-500	1.60E-04	6.27E-02	1.95E+00	
gl-2840	cs	32.0	21	air	75-500	1.60E-04	6.15E-02	1.97E+00	
gl-2840	cs	45.0	21	air	75-500	6.30E-05	1.94E-02	8.72E-01	
gl-2840	cs	49.0	21	air	75-500	6.30E-05	1.83E-02	8.95E-01	
gl-2840	cs	65.0	21	air	75-500	1.60E-05	3.76E-03	2.45E-01	
gl-2840	cs	68.0	21	air	75-500	1.60E-05	3.64E-03	2.47E-01	
gl-2840	cs	78.0	21	air	75-500	6.30E-06	1.29E-03	1.00E-01	
gl-2840	cs	81.0	21	air	75-500	6.30E-06	1.25E-03	1.01E-01	
gl-2840	cs	179.0	21	air	75-500	1.60E-06	1.61E-04	2.88E-02	
gl-2840	cs	182.0	21	air	75-500	1.60E-06	1.58E-04	2.88E-02	
gl-2840	cs	366.0	21	air	75-500	6.30E-07	3.26E-05	1.19E-02	
gl-2840	cs	371.0	21	air	75-500	6.30E-07	3.22E-05	1.20E-02	
gl-2840	cs	942.0	21	air	75-500	1.30E-07	2.70E-06	2.55E-03	
gl-2840	cs	961.0	21	air	75-500	1.30E-07	2.65E-06	2.55E-03	
gl-2840	cs	1060.0	21	air	75-500	6.30E-08	1.17E-06	1.24E-03	
gl-2840	cs	1130.0	21	air	75-500	1.80E-09	3.13E-08	3.54E-05	
gl-2840	cs	1170.0	21	air	75-500	6.30E-08	1.06E-06	1.24E-03	
gl-2840	cs	1330.0	21	air	75-500	6.98E-09	1.03E-07	1.38E-04	
gl-2840	cs	1430.0	21	air	75-500	1.80E-09	2.48E-08	3.55E-05	
gl-2840	cs	1580.0	21	air	75-500	6.98E-09	8.73E-08	1.38E-04	
gl-2840	cs	2000.0	42	air	75-500	5.00E-09	4.95E-08	9.90E-05	
gl-2840	cs	2400.0	21	air	75-500	5.00E-09	4.13E-08	9.92E-05	
gl-2840	cs	2500.0	42	air	- 75	5.00E-09	3.97E-08	9.92E-05	
gl-2854	cs	1700.0	21	air	- 75	5.00E-09	5.81E-08	9.88E-05	
gl-2854	cs	1200.0	21	air	75-500	5.00E-09	8.20E-08	9.84E-05	
gl-2854	cs	510.0	42	air	- 75	5.00E-09	1.89E-07	9.62E-05	
gl-2854	cs	950.0	42	air	75-500	5.00E-09	1.03E-07	9.79E-05	
gl-2901	cs	950.0	21	air	-500	6.00E-09	1.24E-07	1.18E-04	
gl-2901	cs	1400.0	21	air	-500	6.00E-09	8.45E-08	1.18E-04	
gl-2901	cs	1400.0	42	air	-500	6.00E-09	8.45E-08	1.18E-04	
gl-2901	cs	1400.0	42	air	-500	6.00E-09	8.45E-08	1.18E-04	
gl-3116	cs	7000.0	21	air	-500	5.00E-09	1.42E-08	9.97E-05	
gl-3116	cs	7600.0	21	air	-500	5.00E-09	1.31E-08	9.97E-05	
gl-3116	cs	6200.0	42	air	-500	5.00E-09	1.61E-08	9.97E-05	
gl-3116	cs	5500.0	42	air	-500	5.00E-09	1.81E-08	9.96E-05	
gl-3658	cs	140000.0	21	air	- 38	8.00E-09	1.14E-09	1.60E-04	
gl-3658	cs	180000.0	21	air	- 38	7.00E-09	7.78E-10	1.40E-04	
gl-3658	cs	7800.0	21	air	-500	7.00E-09	1.79E-08	1.40E-04	
gl-3658	cs	8200.0	21	air	-500	7.00E-09	1.70E-08	1.40E-04	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
g1-3658	cs	61000.0	21	air	38-106	7.00E-09	2.29E-09	1.40E-04	
g1-3658	cs	70000.0	21	air	38-106	7.00E-09	2.00E-09	1.40E-04	
g1-3658	cs	49000.0	21	air	106-500	7.00E-09	2.86E-09	1.40E-04	
g1-3658	cs	50000.0	21	air	106-500	7.00E-09	2.80E-09	1.40E-04	
g1-3658	cs	8500.0	42	air	-500	7.00E-09	1.64E-08	1.40E-04	
g1-3658	cs	7700.0	42	air	-500	7.00E-09	1.81E-08	1.40E-04	
g2-1952	cs	61300.0	42	air	-500	5.00E-09	1.63E-09	1.00E-04	
g2-1952	cs	63400.0	42	air	-500	5.00E-09	1.58E-09	1.00E-04	
g2-3933	cs	1580.0	42	air	-500	5.00E-09	6.25E-08	9.88E-05	
g2-3933	cs	3490.0	42	air	-500	5.00E-09	2.85E-08	9.94E-05	
g2-547	cs	14800.0	42	air	-500	4.80E-09	6.48E-09	9.59E-05	
g2-723	cs	3530.0	42	air	-500	5.00E-09	2.82E-08	9.94E-05	
g2-723	cs	4620.0	42	air	-500	5.00E-09	2.16E-08	9.96E-05	
gu3-1203	cs	330.0	42	air	75-500	4.00E-09	2.29E-07	7.54E-05	
gu3-1203	cs	380.0	42	air	75-500	4.00E-09	2.00E-07	7.60E-05	
gu3-433	cs	370.0	42	air	75-500	3.00E-09	1.54E-07	5.69E-05	
gu3-433	cs	436.0	42	air	75-500	3.00E-09	1.32E-07	5.74E-05	
gu3-433	cs	613.0	42	air	75-500	3.00E-09	9.48E-08	5.81E-05	
gu3-433	cs	651.0	42	air	75-500	3.00E-09	8.94E-08	5.82E-05	
ja-18	cs	12000.0	14	air	106-150	1.00E-08	1.66E-08	2.00E-04	
ja-18	cs	10000.0	14	air	355-500	1.00E-08	2.00E-08	2.00E-04	
ja-18	cs	16000.0	21	air	75-500	3.00E-09	3.75E-09	5.99E-05	
ja-18	cs	13000.0	21	air	106-150	1.00E-08	1.54E-08	2.00E-04	
ja-18	cs	10000.0	21	air	355-500	1.00E-08	2.00E-08	2.00E-04	
ja-18	cs	7400.0	28	air	250-355	1.00E-09	2.70E-09	1.99E-05	
ja-18	cs	11000.0	28	air	250-355	6.00E-10	1.09E-09	1.20E-05	
ja-18	cs	15000.0	42	air	75-500	3.00E-09	3.99E-09	5.99E-05	
ja-18	cs	17000.0	42	air	106-150	1.00E-08	1.18E-08	2.00E-04	
ja-18	cs	19000.0	42	air	355-500	1.00E-08	1.05E-08	2.00E-04	
ja-18	cs	8400.0	63	air	250-355	1.00E-09	2.38E-09	2.00E-05	
ja-18	cs	15000.0	63	air	250-355	6.00E-10	7.99E-10	1.20E-05	
ja-18	cs	18000.0	84	air	75-500	3.00E-09	3.33E-09	5.99E-05	
ja-18	cs	19000.0	77	air	355-500	1.00E-08	1.05E-08	2.00E-04	
ja-18	cs	20000.0	77	air	106-150	1.00E-08	9.99E-09	2.00E-04	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-26	cs	420.0	21	air	75-500	6.00E-09	2.73E-07	1.15E-04	
ja-26	cs	720.0	21	air	75-500	6.00E-09	1.62E-07	1.17E-04	
ja-26	cs	1900.0	42	air	75-500	6.00E-09	6.25E-08	1.19E-04	
ja-26	cs	2900.0	42	air	75-500	6.00E-09	4.11E-08	1.19E-04	
ja-28	cs	1200.0	21	air	75-500	6.00E-09	9.84E-08	1.18E-04	
ja-28	cs	1700.0	21	air	75-500	6.00E-09	6.98E-08	1.19E-04	
ja-28	cs	1500.0	42	air	75-500	6.00E-09	7.89E-08	1.18E-04	
ja-28	cs	2200.0	42	air	75-500	6.00E-09	5.41E-08	1.19E-04	
ja-32	cs	120.0	7	air	106-150	1.00E-09	1.43E-07	1.71E-05	
ja-32	cs	110.0	7	air	355-500	1.00E-09	1.54E-07	1.69E-05	
ja-32	cs	120.0	21	air	106-150	1.00E-09	1.43E-07	1.71E-05	
ja-32	cs	120.0	21	air	355-500	1.00E-09	1.43E-07	1.71E-05	
ja-32	cs	85.0	28	air	250-355	1.00E-09	1.90E-07	1.62E-05	
ja-32	cs	130.0	28	air	250-355	6.00E-10	8.00E-08	1.04E-05	
ja-32	cs	130.0	35	air	106-150	1.00E-09	1.33E-07	1.73E-05	
ja-32	cs	140.0	35	air	355-500	1.00E-09	1.25E-07	1.75E-05	
ja-32	cs	140.0	56	air	106-150	1.00E-09	1.25E-07	1.75E-05	
ja-32	cs	120.0	56	air	355-500	1.00E-09	1.43E-07	1.71E-05	
ja-32	cs	73.0	63	air	250-355	1.00E-09	2.15E-07	1.57E-05	
ja-32	cs	140.0	63	air	250-355	6.00E-10	7.50E-08	1.05E-05	
ja-37	cs	700.0	14	air	355-500	1.00E-07	2.78E-06	1.94E-03	
ja-37	cs	530.0	14	air	106-150	1.00E-07	3.64E-06	1.93E-03	
ja-37	cs	490.0	21	air	106-150	1.00E-07	3.92E-06	1.92E-03	
ja-37	cs	480.0	21	air	355-500	1.00E-07	4.00E-06	1.92E-03	
ja-37	cs	1300.0	28	air	250-355	6.00E-10	9.09E-09	1.18E-05	
ja-37	cs	840.0	28	air	250-355	1.00E-09	2.33E-08	1.95E-05	
ja-37	cs	510.0	35	air	106-150	1.00E-07	3.77E-06	1.92E-03	
ja-37	cs	650.0	35	air	355-500	1.00E-07	2.99E-06	1.94E-03	
ja-37	cs	760.0	63	air	250-355	1.00E-09	2.56E-08	1.95E-05	
ja-37	cs	1400.0	63	air	250-355	6.00E-10	8.45E-09	1.18E-05	
ja-37	cs	780.0	70	air	106-150	1.00E-07	2.50E-06	1.95E-03	
ja-37	cs	750.0	70	air	355-500	1.00E-07	2.60E-06	1.95E-03	
ja-8	cs	2400.0	21	air	75-500	6.00E-09	4.96E-08	1.19E-04	
ja-8	cs	2200.0	21	air	75-500	6.00E-09	5.41E-08	1.19E-04	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-8	cs	2600.0	42	air	75-500	6.00E-09	4.58E-08	1.19E-04	
ja-8	cs	3800.0	42	air	75-500	6.00E-09	3.14E-08	1.19E-04	
ym-22	cs	380.0	21	ca	- 75	2.00E-09	1.00E-07	3.80E-05	
ym-22	cs	200.0	21	ca	75-500	2.00E-09	1.82E-07	3.64E-05	
ym-22	cs	440.0	42	ca	- 75	2.00E-09	8.70E-08	3.83E-05	
ym-22	cs	210.0	42	ca	75-500	2.00E-09	1.74E-07	3.65E-05	
ym-22	cs	480.0	84	ca	- 75	2.00E-09	8.00E-08	3.84E-05	
ym-22	cs	250.0	84	ca	75-500	2.00E-09	1.48E-07	3.70E-05	
ym-22	cs	610.0	21	air	- 75	3.00E-10	9.52E-09	5.81E-06	
ym-22	cs	12.0	21	air	- 75	2.00E-03	1.25E+00	1.50E+01	
ym-22	cs	380.0	21	air	- 75	3.00E-09	1.50E-07	5.70E-05	
ym-22	cs	130.0	21	air	- 75	2.00E-05	2.67E-03	3.47E-01	
ym-22	cs	610.0	21	air	- 75	2.00E-07	6.35E-06	3.87E-03	
ym-22	cs	10.0	21	air	75-500	2.00E-03	1.33E+00	1.33E+01	
ym-22	cs	110.0	21	air	75-500	2.00E-05	3.08E-03	3.38E-01	
ym-22	cs	550.0	21	air	75-500	3.00E-10	1.05E-08	5.79E-06	
ym-22	cs	660.0	21	air	75-500	3.00E-09	8.82E-08	5.82E-05	
ym-22	cs	260.0	21	air	75-500	2.00E-07	1.43E-05	3.71E-03	
ym-22	cs	380.0	21	air	106-500	1.00E-09	5.00E-08	1.90E-05	
ym-22	cs	260.0	21	air	106-500	1.00E-09	7.14E-08	1.86E-05	
ym-22	cs	540.0	42	air	-106	1.00E-09	3.57E-08	1.93E-05	
ym-22	cs	270.0	42	air	106-500	1.00E-09	6.90E-08	1.86E-05	
ym-22	cs	240.0	42	air	106-500	1.00E-09	7.69E-08	1.85E-05	
ym-30	cs	850.0	21	air	75-500	3.00E-09	6.90E-08	5.86E-05	
ym-30	cs	860.0	42	air	75-500	3.00E-09	6.82E-08	5.86E-05	
ym-30	cs	2000.0	84	air	75-500	3.00E-09	2.97E-08	5.94E-05	
ym-38	cs	9500.0	21	ca	- 75	3.00E-09	6.30E-09	5.99E-05	
ym-38	cs	7900.0	21	ca	75-500	3.00E-09	7.58E-09	5.98E-05	
ym-38	cs	14000.0	42	ca	- 75	3.00E-09	4.28E-09	5.99E-05	
ym-38	cs	10000.0	42	ca	75-500	3.00E-09	5.99E-09	5.99E-05	
ym-38	cs	9000.0	84	ca	- 75	3.00E-09	6.65E-09	5.99E-05	
ym-38	cs	5400.0	84	ca	75-500	3.00E-09	1.11E-08	5.98E-05	
ym-38	cs	20000.0	21	air	- 38	4.00E-09	4.00E-09	7.99E-05	
ym-38	cs	11000.0	21	air	- 38	4.00E-09	7.26E-09	7.99E-05	
ym-38	cs	2700.0	21	air	- 75	2.00E-09	1.47E-08	3.97E-05	
ym-38	cs	3200.0	21	air	- 75	2.00E-10	1.24E-09	3.98E-06	
ym-38	cs	3500.0	21	air	- 75	3.00E-03	1.70E-02	5.97E+01	
ym-38	cs	3700.0	21	air	- 75	3.00E-05	1.61E-04	5.97E-01	
ym-38	cs	6300.0	21	air	- 75	3.00E-07	9.49E-07	5.98E-03	
ym-38	cs	17000.0	21	air	38-106	4.00E-09	4.70E-09	7.99E-05	
ym-38	cs	15000.0	21	air	38-106	4.00E-09	5.33E-09	7.99E-05	
ym-38	cs	3400.0	21	air	75-500	3.00E-03	1.75E-02	5.96E+01	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-38	cs	3500.0	21	air	75-500	2.00E-10	1.14E-09	3.98E-06	
ym-38	cs	4000.0	21	air	75-500	2.00E-09	9.95E-09	3.98E-05	
ym-38	cs	4200.0	21	air	75-500	3.00E-07	1.42E-06	5.97E-03	
ym-38	cs	6000.0	21	air	75-500	3.00E-05	9.97E-05	5.98E-01	
ym-38	cs	12000.0	21	air	106-500	1.00E-09	1.66E-09	2.00E-05	
ym-38	cs	14000.0	21	air	106-500	4.00E-09	5.71E-09	7.99E-05	
ym-38	cs	14000.0	21	air	106-500	4.00E-09	5.71E-09	7.99E-05	
ym-38	cs	5900.0	42	air	-106	1.00E-09	3.38E-09	1.99E-05	
ym-38	cs	8200.0	42	air	106-500	1.00E-09	2.43E-09	2.00E-05	
ym-42	cs	16000.0	21	air	75-500	3.00E-09	3.75E-09	5.99E-05	
ym-42	cs	17000.0	42	air	75-500	3.00E-09	3.53E-09	5.99E-05	
ym-42	cs	19000.0	84	air	75-500	3.00E-09	3.15E-09	5.99E-05	
ym-45	cs	740.0	21	air	-106	1.00E-09	2.63E-08	1.95E-05	
ym-45	cs	480.0	21	air	106-500	1.00E-09	4.00E-08	1.92E-05	
ym-45	cs	320.0	42	air	106-500	1.00E-09	5.88E-08	1.88E-05	
ym-45	cs	550.0	42	air	-106	1.00E-09	3.51E-08	1.93E-05	
ym-46	cs	500.0	21	air	75-500	3.00E-09	1.15E-07	5.77E-05	
ym-46	cs	320.0	42	air	75-500	3.00E-09	1.76E-07	5.65E-05	
ym-46	cs	1700.0	84	air	75-500	3.00E-09	3.49E-08	5.93E-05	
ym-48	cs	15000.0	21	air	106-500	1.00E-09	1.33E-09	2.00E-05	
ym-48	cs	6900.0	42	air	-106	1.00E-09	2.89E-09	1.99E-05	
ym-48	cs	22000.0	42	air	106-500	1.00E-09	9.08E-10	2.00E-05	
ym-49	cs	22000.0	21	air	-106	1.00E-09	9.08E-10	2.00E-05	
ym-49	cs	29000.0	21	air	106-500	1.00E-09	6.89E-10	2.00E-05	
ym-49	cs	36000.0	42	air	106-500	1.00E-09	5.55E-10	2.00E-05	
ym-49	cs	37000.0	21	air	106-500	1.00E-09	5.40E-10	2.00E-05	
ym-49	cs	8700.0	42	air	-106	1.00E-09	2.29E-09	2.00E-05	
ym-49	cs	43000.0	42	air	106-500	1.00E-09	4.65E-10	2.00E-05	
ym-54	cs	360.0	21	ca	- 75	3.00E-09	1.58E-07	5.68E-05	
ym-54	cs	210.0	21	ca	75-500	3.00E-09	2.61E-07	5.48E-05	
ym-54	cs	370.0	42	ca	- 75	3.00E-09	1.54E-07	5.69E-05	
ym-54	cs	260.0	42	ca	75-500	3.00E-09	2.14E-07	5.57E-05	
ym-54	cs	390.0	84	ca	- 75	3.00E-09	1.46E-07	5.71E-05	
ym-54	cs	240.0	84	ca	75-500	3.00E-09	2.31E-07	5.54E-05	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-54	cs	940.0	21	air	- 38	3.00E-09	6.25E-08	5.87E-05	
ym-54	cs	890.0	21	air	- 38	3.00E-09	6.59E-08	5.87E-05	
ym-54	cs	270.0	21	air	-106	2.00E-09	1.38E-07	3.72E-05	
ym-54	cs	190.0	21	air	38-106	3.00E-09	2.86E-07	5.43E-05	
ym-54	cs	190.0	21	air	38-106	3.00E-09	2.86E-07	5.43E-05	
ym-54	cs	110.0	21	air	106-500	3.00E-09	4.62E-07	5.08E-05	
ym-54	cs	130.0	21	air	106-500	3.00E-09	4.00E-07	5.20E-05	
ym-54	cs	290.0	21	air	106-500	2.00E-09	1.29E-07	3.74E-05	
ym-54	cs	230.0	42	air	-106	2.00E-09	1.60E-07	3.68E-05	
ym-54	cs	200.0	42	air	106-500	2.00E-09	1.82E-07	3.64E-05	
ja-18	cs	13000.0	14	air	106-150	1.00E-08	1.54E-08	2.00E-04	70
ja-18	cs	21000.0	14	air	355-500	1.00E-08	9.51E-09	2.00E-04	70
ja-18	cs	21000.0	21	air	106-150	1.00E-08	9.51E-09	2.00E-04	70
ja-18	cs	18000.0	21	air	355-500	1.00E-08	1.11E-08	2.00E-04	70
ja-18	cs	16000.0	35	air	106-150	1.00E-08	1.25E-08	2.00E-04	70
ja-18	cs	19000.0	35	air	355-500	1.00E-08	1.05E-08	2.00E-04	70
ja-18	cs	17000.0	63	air	106-150	1.00E-08	1.18E-08	2.00E-04	70
ja-18	cs	19000.0	63	air	355-500	1.00E-08	1.05E-08	2.00E-04	70
ja-32	cs	82.0	7	air	106-150	2.00E-09	3.92E-07	3.22E-05	70
ja-32	cs	82.0	7	air	355-500	2.00E-09	3.92E-07	3.22E-05	70
ja-32	cs	87.0	14	air	106-150	2.00E-09	3.74E-07	3.25E-05	70
ja-32	cs	85.0	14	air	355-500	2.00E-09	3.81E-07	3.24E-05	70
ja-32	cs	120.0	28	air	106-150	2.00E-09	2.86E-07	3.43E-05	70
ja-32	cs	100.0	28	air	355-500	2.00E-09	3.33E-07	3.33E-05	70
ja-32	cs	120.0	56	air	106-150	2.00E-09	2.86E-07	3.43E-05	70
ja-32	cs	100.0	56	air	355-500	2.00E-09	3.33E-07	3.33E-05	70
ja-37	cs	1100.0	7	air	106-150	4.00E-08	7.14E-07	7.86E-04	70
ja-37	cs	1100.0	7	air	355-500	4.00E-08	7.14E-07	7.86E-04	70
ja-37	cs	1300.0	14	air	106-150	4.00E-08	6.06E-07	7.88E-04	70
ja-37	cs	1300.0	14	air	355-500	4.00E-08	6.06E-07	7.88E-04	70
ja-37	cs	1400.0	21	air	106-150	4.00E-08	5.63E-07	7.89E-04	70
ja-37	cs	1400.0	21	air	355-500	4.00E-08	5.63E-07	7.89E-04	70
ja-37	cs	1800.0	49	air	106-150	4.00E-08	4.40E-07	7.91E-04	70
ja-37	cs	1600.0	49	air	355-500	4.00E-08	4.94E-07	7.90E-04	70

Table A-III

Data Base Entries of Experimental Sorption Data for the Element Barium

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-1292	ba	1800.0	21	air	-500	7.00E-06	1.54E-04	2.77E-01	
gl-1292	ba	2200.0	21	air	-500	7.00E-06	1.26E-04	2.77E-01	
gl-1292	ba	1500.0	42	air	-500	7.00E-06	1.84E-04	2.76E-01	
gl-1292	ba	2800.0	42	air	-500	7.00E-06	9.93E-05	2.78E-01	
gl-1436	ba	140000.0	21	air	-500	8.00E-06	2.29E-06	3.20E-01	
gl-1436	ba	150000.0	21	air	-500	8.00E-06	2.13E-06	3.20E-01	
gl-1436	ba	93000.0	42	air	-500	8.00E-06	3.44E-06	3.20E-01	
gl-1436	ba	210000.0	42	air	-500	8.00E-06	1.52E-06	3.20E-01	
gl-1854	ba	63000.0	21	air	- 75	1.00E-07	6.35E-08	4.00E-03	
gl-1854	ba	34000.0	21	air	75-500	1.00E-07	1.18E-07	4.00E-03	
gl-1854	ba	48000.0	42	air	- 75	1.00E-07	8.33E-08	4.00E-03	
gl-1854	ba	34000.0	42	air	75-500	1.00E-07	1.18E-07	4.00E-03	
gl-1883	ba	230.0	21	air	- 38	7.00E-06	1.12E-03	2.58E-01	
gl-1883	ba	750.0	21	air	- 38	7.00E-06	3.64E-04	2.73E-01	
gl-1883	ba	250.0	21	air	-500	8.00E-06	1.19E-03	2.96E-01	
gl-1883	ba	4300.0	21	air	-500	8.00E-06	7.41E-05	3.19E-01	
gl-1883	ba	200.0	21	air	38-106	7.00E-06	1.27E-03	2.55E-01	
gl-1883	ba	210.0	21	air	38-106	7.00E-06	1.22E-03	2.56E-01	
gl-1883	ba	160.0	21	air	106-500	7.00E-06	1.56E-03	2.49E-01	
gl-1883	ba	160.0	21	air	106-500	7.00E-06	1.56E-03	2.49E-01	
gl-1883	ba	480.0	42	air	-500	8.00E-06	6.40E-04	3.07E-01	
gl-1883	ba	490.0	42	air	-500	8.00E-06	6.27E-04	3.07E-01	
gl-1982	ba	10000.0	14	air	- 38	4.00E-06	1.60E-05	1.60E-01	
gl-1982	ba	670.0	14	air	38- 75	4.00E-06	2.32E-04	1.55E-01	
gl-1982	ba	570.0	14	air	75-250	4.00E-06	2.71E-04	1.55E-01	
gl-1982	ba	690.0	14	air	250-500	4.00E-06	2.25E-04	1.55E-01	
gl-1982	ba	10000.0	21	air	- 38	4.00E-06	1.60E-05	1.60E-01	
gl-1982	ba	2500.0	21	air	-500	4.00E-06	6.35E-05	1.59E-01	
gl-1982	ba	2200.0	21	air	-500	4.00E-06	7.21E-05	1.59E-01	
gl-1982	ba	840.0	21	air	38- 75	4.00E-06	1.86E-04	1.56E-01	
gl-1982	ba	780.0	21	air	75-250	4.00E-06	2.00E-04	1.56E-01	
gl-1982	ba	780.0	21	air	250-500	4.00E-06	2.00E-04	1.56E-01	
gl-1982	ba	3100.0	42	air	-500	4.00E-06	5.13E-05	1.59E-01	
gl-1982	ba	3200.0	42	air	-500	4.00E-06	4.97E-05	1.59E-01	
gl-2233	ba	200000.0	21	air	-500	6.00E-06	1.20E-06	2.40E-01	
gl-2233	ba	210000.0	21	air	-500	6.00E-06	1.14E-06	2.40E-01	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-2233	ba	250000.0	42	air	-500	6.00E-06	9.60E-07	2.40E-01	
gl-2233	ba	330000.0	42	air	-500	6.00E-06	7.27E-07	2.40E-01	
gl-2289	ba	170000.0	21	air	- 38	1.00E-07	2.35E-08	4.00E-03	
gl-2289	ba	110000.0	21	air	- 38	1.00E-07	3.64E-08	4.00E-03	
gl-2289	ba	48000.0	21	air	38-106	1.00E-07	8.33E-08	4.00E-03	
gl-2289	ba	54000.0	21	air	38-106	1.00E-07	7.40E-08	4.00E-03	
gl-2289	ba	70000.0	21	air	106-500	1.00E-07	5.71E-08	4.00E-03	
gl-2289	ba	90000.0	21	air	106-500	1.00E-07	4.44E-08	4.00E-03	
gl-2333	ba	1900.0	21	air	- 75	3.00E-07	6.25E-06	1.19E-02	
gl-2333	ba	1200.0	21	air	75-500	3.00E-07	9.84E-06	1.18E-02	
gl-2333	ba	1800.0	42	air	- 75	3.00E-07	6.59E-06	1.19E-02	
gl-2333	ba	1100.0	42	air	75-500	3.00E-07	1.07E-05	1.18E-02	
gl-2363	ba	920.0	21	air	- 38	1.00E-07	4.26E-06	3.91E-03	
gl-2363	ba	860.0	21	air	- 38	1.00E-07	4.55E-06	3.91E-03	
gl-2363	ba	830.0	21	air	-500	8.00E-06	3.76E-04	3.12E-01	
gl-2363	ba	880.0	21	air	-500	8.00E-06	3.56E-04	3.13E-01	
gl-2363	ba	250.0	21	air	38-106	1.00E-07	1.48E-05	3.70E-03	
gl-2363	ba	240.0	21	air	38-106	1.00E-07	1.54E-05	3.69E-03	
gl-2363	ba	210.0	21	air	106-500	1.00E-07	1.74E-05	3.65E-03	
gl-2363	ba	230.0	21	air	106-500	1.00E-07	1.60E-05	3.68E-03	
gl-2363	ba	920.0	42	air	-500	8.00E-06	3.40E-04	3.13E-01	
gl-2363	ba	930.0	42	air	-500	8.00E-06	3.37E-04	3.13E-01	
gl-2410	ba	3000.0	42	air	- 75	2.00E-07	2.65E-06	7.95E-03	
gl-2410	ba	1800.0	42	air	75-500	2.00E-07	4.40E-06	7.91E-03	
gl-2476	ba	480.0	21	air	- 75	1.00E-07	8.00E-06	3.84E-03	
gl-2476	ba	370.0	21	air	75-500	1.00E-07	1.03E-05	3.79E-03	
gl-2476	ba	520.0	42	air	- 75	1.00E-07	7.41E-06	3.85E-03	
gl-2476	ba	400.0	42	air	75-500	1.00E-07	9.52E-06	3.81E-03	
gl-2698	ba	56000.0	21	air	-500	8.00E-06	5.71E-06	3.20E-01	
gl-2698	ba	61000.0	21	air	-500	8.00E-06	5.24E-06	3.20E-01	
gl-2698	ba	58000.0	42	air	-500	8.00E-06	5.52E-06	3.20E-01	
gl-2698	ba	77000.0	42	air	-500	8.00E-06	4.15E-06	3.20E-01	
gl-2840	ba	2300.0	21	air	- 75	2.00E-07	3.45E-06	7.93E-03	
gl-2840	ba	2000.0	21	air	75-500	2.00E-07	3.96E-06	7.92E-03	
gl-2840	ba	2600.0	42	air	- 75	2.00E-07	3.05E-06	7.94E-03	
gl-2840	ba	2100.0	42	air	75-500	2.00E-07	3.77E-06	7.92E-03	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-2854	ba	1600.0	21	air	- 75	1.00E-07	2.47E-06	3.95E-03	
gl-2854	ba	950.0	21	air	75-500	1.00E-07	4.12E-06	3.92E-03	
gl-2854	ba	6500.0	42	air	- 75	1.00E-07	6.13E-07	3.99E-03	
gl-2854	ba	1000.0	42	air	75-500	1.00E-07	3.92E-06	3.92E-03	
gl-2901	ba	1200.0	21	air	-500	1.00E-06	3.28E-05	3.93E-02	
gl-2901	ba	1900.0	21	air	-500	1.00E-06	2.08E-05	3.96E-02	
gl-2901	ba	1900.0	42	air	-500	1.00E-06	2.08E-05	3.96E-02	
gl-2901	ba	1900.0	42	air	-500	1.00E-06	2.08E-05	3.96E-02	
gl-3116	ba	120000.0	21	air	-500	9.00E-06	3.00E-06	3.60E-01	
gl-3116	ba	130000.0	21	air	-500	9.00E-06	2.77E-06	3.60E-01	
gl-3116	ba	120000.0	42	air	-500	9.00E-06	3.00E-06	3.60E-01	
gl-3116	ba	130000.0	42	air	-500	9.00E-06	2.77E-06	3.60E-01	
gl-3658	ba	190000.0	21	air	- 38	9.00E-06	1.89E-06	3.60E-01	
gl-3658	ba	120000.0	21	air	- 38	9.00E-06	3.00E-06	3.60E-01	
gl-3658	ba	8700.0	21	air	-500	9.00E-06	4.13E-05	3.59E-01	
gl-3658	ba	12000.0	21	air	-500	9.00E-06	3.00E-05	3.59E-01	
gl-3658	ba	90000.0	21	air	38-106	9.00E-06	4.00E-06	3.60E-01	
gl-3658	ba	100000.0	21	air	38-106	9.00E-06	3.60E-06	3.60E-01	
gl-3658	ba	130000.0	21	air	106-500	9.00E-06	2.77E-06	3.60E-01	
gl-3658	ba	140000.0	21	air	106-500	9.00E-06	2.57E-06	3.60E-01	
gl-3658	ba	9000.0	42	air	-500	9.00E-06	3.99E-05	3.59E-01	
gl-3658	ba	12000.0	42	air	-500	9.00E-06	3.00E-05	3.59E-01	
g2-1952	ba	21500.0	42	air	-500	7.00E-08	1.30E-07	2.80E-03	
g2-1952	ba	28700.0	42	air	-500	7.00E-08	9.75E-08	2.80E-03	
g2-3933	ba	1240.0	42	air	-500	6.00E-08	1.90E-06	2.36E-03	
g2-3933	ba	2220.0	42	air	-500	6.00E-08	1.07E-06	2.38E-03	
g2-547	ba	3460.0	42	air	-500	7.30E-08	8.39E-07	2.90E-03	
g2-547	ba	3520.0	42	air	-500	7.30E-08	8.25E-07	2.90E-03	
g2-723	ba	3080.0	42	air	-500	7.00E-08	9.03E-07	2.78E-03	
g2-723	ba	3930.0	42	air	-500	7.00E-08	7.09E-07	2.79E-03	
gu3-1203	ba	0.0	42	air	75-500	4.00E-08	8.00E-05	0.00E-01	
gu3-1203	ba	600.0	42	air	75-500	4.00E-08	2.58E-06	1.55E-03	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
GU3-1301	ba	370.0	42	air	75-500	3.00E-08	3.08E-06	1.14E-03	
GU3-1301	ba	460.0	42	air	75-500	3.00E-08	2.50E-06	1.15E-03	
GU3-1301	ba	512.0	42	air	75-500	3.00E-08	2.26E-06	1.15E-03	
GU3-1301	ba	629.0	42	air	75-500	3.00E-08	1.85E-06	1.16E-03	
gu3-433	ba	290.0	42	air	75-500	3.00E-08	3.87E-06	1.12E-03	
gu3-433	ba	392.0	42	air	75-500	3.00E-08	2.91E-06	1.14E-03	
gu3-433	ba	708.0	42	air	75-500	3.00E-08	1.65E-06	1.17E-03	
gu3-433	ba	912.0	42	air	75-500	3.00E-08	1.29E-06	1.17E-03	
ja-18	ba	3100.0	14	air	106-150	2.00E-07	2.56E-06	7.95E-03	
ja-18	ba	3100.0	14	air	106-150	2.00E-07	2.56E-06	7.95E-03	
ja-18	ba	2300.0	14	air	355-500	2.00E-07	3.45E-06	7.93E-03	
ja-18	ba	35000.0	14	air	355-500	2.00E-07	2.28E-07	8.00E-03	
ja-18	ba	35000.0	14	air	355-500	2.00E-07	2.28E-07	8.00E-03	
ja-18	ba	96000.0	21	air	75-500	8.00E-10	3.33E-10	3.20E-05	
ja-18	ba	4500.0	21	air	106-150	2.00E-07	1.77E-06	7.96E-03	
ja-18	ba	4500.0	21	air	106-150	2.00E-07	1.77E-06	7.96E-03	
ja-18	ba	40000.0	21	air	355-500	2.00E-07	2.00E-07	8.00E-03	
ja-18	ba	3300.0	21	air	355-500	2.00E-07	2.41E-06	7.95E-03	
ja-18	ba	40000.0	21	air	355-500	2.00E-07	2.00E-07	8.00E-03	
ja-18	ba	75000.0	35	air	355-500	2.00E-07	1.07E-07	8.00E-03	
ja-18	ba	75000.0	35	air	355-500	2.00E-07	1.07E-07	8.00E-03	
ja-18	ba	46000.0	28	air	250-355	1.00E-06	8.69E-07	4.00E-02	
ja-18	ba	17000.0	28	air	250-355	1.00E-06	2.35E-06	4.00E-02	
ja-18	ba	110000.0	42	air	75-500	8.00E-10	2.91E-10	3.20E-05	
ja-18	ba	4700.0	42	air	106-150	2.00E-07	1.69E-06	7.97E-03	
ja-18	ba	7100.0	42	air	355-500	2.00E-07	1.12E-06	7.98E-03	
ja-18	ba	120000.0	63	air	250-355	1.00E-06	3.33E-07	4.00E-02	
ja-18	ba	82000.0	63	air	250-355	1.00E-06	4.88E-07	4.00E-02	
ja-18	ba	61000.0	63	air	355-500	2.00E-07	1.31E-07	8.00E-03	
ja-18	ba	61000.0	63	air	355-500	2.00E-07	1.31E-07	8.00E-03	
ja-18	ba	6600.0	77	air	106-150	2.00E-07	1.21E-06	7.98E-03	
ja-18	ba	7100.0	77	air	355-500	2.00E-07	1.12E-06	7.98E-03	
ja-18	ba	170000.0	84	air	75-500	8.00E-10	1.88E-10	3.20E-05	
ja-26	ba	210.0	21	air	75-500	1.00E-09	1.74E-07	3.65E-05	
ja-26	ba	270.0	21	air	75-500	1.00E-09	1.38E-07	3.72E-05	
ja-26	ba	1200.0	42	air	75-500	1.00E-09	3.28E-08	3.93E-05	
ja-26	ba	1400.0	42	air	75-500	1.00E-09	2.82E-08	3.94E-05	
ja-28	ba	760.0	21	air	75-500	1.00E-09	5.13E-08	3.90E-05	
ja-28	ba	900.0	21	air	75-500	1.00E-09	4.35E-08	3.91E-05	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-28	ba	720.0	42	air	75-500	1.00E-09	5.41E-08	3.89E-05	
ja-28	ba	900.0	42	air	75-500	1.00E-09	4.35E-08	3.91E-05	
ja-32	ba	370.0	7	air	106-150	1.00E-06	1.03E-04	3.79E-02	
ja-32	ba	270.0	7	air	355-500	1.00E-06	1.38E-04	3.72E-02	
ja-32	ba	900.0	7	air	355-500	1.00E-06	4.35E-05	3.91E-02	
ja-32	ba	900.0	7	air	355-500	1.00E-06	4.35E-05	3.91E-02	
ja-32	ba	1000.0	14	air	355-500	1.00E-06	3.92E-05	3.92E-02	
ja-32	ba	1000.0	14	air	355-500	1.00E-06	3.92E-05	3.92E-02	
ja-32	ba	310.0	21	air	355-500	1.00E-06	1.21E-04	3.76E-02	
ja-32	ba	370.0	21	air	106-150	1.00E-06	1.03E-04	3.79E-02	
ja-32	ba	160.0	28	air	250-355	1.00E-06	2.22E-04	3.56E-02	
ja-32	ba	590.0	28	air	250-355	1.00E-06	6.56E-05	3.87E-02	
ja-32	ba	1100.0	28	air	355-500	1.00E-06	3.57E-05	3.93E-02	
ja-32	ba	1100.0	28	air	355-500	1.00E-06	3.57E-05	3.93E-02	
ja-32	ba	420.0	35	air	106-150	1.00E-06	9.09E-05	3.82E-02	
ja-32	ba	370.0	35	air	355-500	1.00E-06	1.03E-04	3.79E-02	
ja-32	ba	440.0	56	air	106-150	1.00E-06	8.70E-05	3.83E-02	
ja-32	ba	1600.0	56	air	355-500	1.00E-06	2.47E-05	3.95E-02	
ja-32	ba	520.0	56	air	355-500	1.00E-06	7.41E-05	3.85E-02	
ja-32	ba	1600.0	56	air	355-500	1.00E-06	2.47E-05	3.95E-02	
ja-32	ba	660.0	63	air	250-355	1.00E-06	5.88E-05	3.88E-02	
ja-32	ba	180.0	63	air	250-355	1.00E-06	2.00E-04	3.60E-02	
ja-37	ba	1700.0	7	air	355-500	1.00E-06	2.33E-05	3.95E-02	
ja-37	ba	1700.0	7	air	355-500	1.00E-06	2.33E-05	3.95E-02	
ja-37	ba	700.0	14	air	106-150	2.00E-06	1.11E-04	7.78E-02	
ja-37	ba	2400.0	14	air	355-500	1.00E-06	1.65E-05	3.97E-02	
ja-37	ba	2400.0	14	air	355-500	1.00E-06	1.65E-05	3.97E-02	
ja-37	ba	600.0	14	air	355-500	2.00E-06	1.29E-04	7.74E-02	
ja-37	ba	750.0	21	air	106-150	2.00E-06	1.04E-04	7.79E-02	
ja-37	ba	660.0	21	air	355-500	2.00E-06	1.18E-04	7.76E-02	
ja-37	ba	3400.0	21	air	355-500	1.00E-06	1.17E-05	3.98E-02	
ja-37	ba	3400.0	21	air	355-500	1.00E-06	1.17E-05	3.98E-02	
ja-37	ba	840.0	28	air	250-355	1.00E-06	4.65E-05	3.91E-02	
ja-37	ba	380.0	28	air	250-355	1.00E-06	1.00E-04	3.80E-02	
ja-37	ba	710.0	35	air	106-150	2.00E-06	1.10E-04	7.78E-02	
ja-37	ba	830.0	35	air	355-500	2.00E-06	9.41E-05	7.81E-02	
ja-37	ba	6600.0	49	air	355-500	1.00E-06	6.04E-06	3.99E-02	
ja-37	ba	6600.0	49	air	355-500	1.00E-06	6.04E-06	3.99E-02	
ja-37	ba	880.0	63	air	250-355	1.00E-06	4.44E-05	3.91E-02	
ja-37	ba	340.0	63	air	250-355	1.00E-06	1.11E-04	3.78E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-37	ba	1000.0	70	air	106-150	2.00E-06	7.84E-05	7.84E-02	
ja-37	ba	760.0	70	air	355-500	2.00E-06	1.03E-04	7.79E-02	
ja-8	ba	400.0	21	air	75-500	1.00E-09	9.52E-08	3.81E-05	
ja-8	ba	420.0	21	air	75-500	1.00E-09	9.09E-08	3.82E-05	
ja-8	ba	450.0	42	air	75-500	1.00E-09	8.51E-08	3.83E-05	
ja-8	ba	470.0	42	air	75-500	1.00E-09	8.16E-08	3.84E-05	
ym-22	ba	660.0	21	ca	- 75	3.00E-07	1.76E-05	1.16E-02	
ym-22	ba	200.0	21	ca	75-500	3.00E-07	5.45E-05	1.09E-02	
ym-22	ba	900.0	42	ca	- 75	3.00E-07	1.30E-05	1.17E-02	
ym-22	ba	300.0	42	ca	75-500	3.00E-07	3.75E-05	1.13E-02	
ym-22	ba	1000.0	84	ca	- 75	3.00E-07	1.18E-05	1.18E-02	
ym-22	ba	300.0	84	ca	75-500	3.00E-07	3.75E-05	1.13E-02	
ym-22	ba	400.0	21	air	- 75	1.00E-04	9.52E-03	3.81E+00	
ym-22	ba	1000.0	21	air	- 75	3.00E-07	1.18E-05	1.18E-02	
ym-22	ba	1200.0	21	air	- 75	4.00E-07	1.31E-05	1.57E-02	
ym-22	ba	1300.0	21	air	- 75	3.00E-07	9.09E-06	1.18E-02	
ym-22	ba	760.0	21	air	- 75	1.00E-05	5.13E-04	3.90E-01	
ym-22	ba	210.0	21	air	75-500	1.00E-04	1.74E-02	3.65E+00	
ym-22	ba	470.0	21	air	75-500	1.00E-05	8.16E-04	3.84E-01	
ym-22	ba	600.0	21	air	75-500	3.00E-07	1.94E-05	1.16E-02	
ym-22	ba	670.0	21	air	75-500	3.00E-07	1.74E-05	1.17E-02	
ym-22	ba	790.0	21	air	75-500	4.00E-07	1.98E-05	1.56E-02	
ym-22	ba	850.0	21	air	106-500	3.00E-07	1.38E-05	1.17E-02	
ym-22	ba	910.0	21	air	106-500	3.00E-07	1.29E-05	1.17E-02	
ym-22	ba	1300.0	42	air	-106	3.00E-07	9.09E-06	1.18E-02	
ym-22	ba	850.0	42	air	106-500	3.00E-07	1.38E-05	1.17E-02	
ym-22	ba	980.0	42	air	106-500	3.00E-07	1.20E-05	1.18E-02	
ym-30	ba	2000.0	21	air	75-500	8.00E-10	1.58E-08	3.17E-05	
ym-30	ba	1800.0	42	air	75-500	8.00E-10	1.76E-08	3.16E-05	
ym-30	ba	6400.0	84	air	75-500	8.00E-10	4.98E-09	3.19E-05	
ym-38	ba	57000.0	21	ca	- 75	4.00E-07	2.81E-07	1.60E-02	
ym-38	ba	34000.0	21	ca	75-500	4.00E-07	4.70E-07	1.60E-02	
ym-38	ba	210000.0	42	ca	- 75	4.00E-07	7.62E-08	1.60E-02	
ym-38	ba	41000.0	42	ca	75-500	4.00E-07	3.90E-07	1.60E-02	
ym-38	ba	22000.0	84	ca	- 75	4.00E-07	7.27E-07	1.60E-02	
ym-38	ba	11000.0	84	ca	75-500	4.00E-07	1.45E-06	1.60E-02	
ym-38	ba	69000.0	21	air	- 38	4.00E-07	2.32E-07	1.60E-02	
ym-38	ba	190000.0	21	air	- 38	4.00E-07	8.42E-08	1.60E-02	
ym-38	ba	100000.0	21	air	- 75	1.00E-04	4.00E-05	4.00E+00	
ym-38	ba	72000.0	21	air	- 75	4.00E-07	2.22E-07	1.60E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-38	ba	97000.0	21	air	- 75	2.00E-06	8.25E-07	8.00E-02	
ym-38	ba	81000.0	21	air	- 75	6.00E-07	2.96E-07	2.40E-02	
ym-38	ba	93000.0	21	air	- 75	1.00E-05	4.30E-06	4.00E-01	
ym-38	ba	33000.0	21	air	-500	4.00E-07	4.85E-07	1.60E-02	
ym-38	ba	100000.0	21	air	38-106	4.00E-07	1.60E-07	1.60E-02	
ym-38	ba	120000.0	21	air	38-106	4.00E-07	1.33E-07	1.60E-02	
ym-38	ba	33000.0	21	air	75-500	4.00E-07	4.85E-07	1.60E-02	
ym-38	ba	36000.0	21	air	75-500	2.00E-06	2.22E-06	8.00E-02	
ym-38	ba	75000.0	21	air	75-500	1.00E-05	5.33E-06	4.00E-01	
ym-38	ba	79000.0	21	air	75-500	1.00E-04	5.06E-05	4.00E+00	
ym-38	ba	68000.0	21	air	75-500	6.00E-07	3.53E-07	2.40E-02	
ym-38	ba	100000.0	21	air	106-500	4.00E-07	1.60E-07	1.60E-02	
ym-38	ba	57000.0	21	air	106-500	4.00E-07	2.81E-07	1.60E-02	
ym-38	ba	77000.0	21	air	106-500	4.00E-07	2.08E-07	1.60E-02	
ym-38	ba	40000.0	42	air	-106	4.00E-07	4.00E-07	1.60E-02	
ym-38	ba	4000.0	42	air	-106	4.00E-07	3.98E-06	1.59E-02	
ym-38	ba	81000.0	42	air	106-500	4.00E-07	1.97E-07	1.60E-02	
ym-42	ba	72000.0	21	air	75-500	8.00E-10	4.44E-10	3.20E-05	
ym-42	ba	90000.0	42	air	75-500	8.00E-10	3.55E-10	3.20E-05	
ym-42	ba	120000.0	84	air	75-500	8.00E-10	2.67E-10	3.20E-05	
ym-45	ba	970.0	21	air	-106	3.00E-07	1.21E-05	1.18E-02	
ym-45	ba	1200.0	21	air	106-500	3.00E-07	9.84E-06	1.18E-02	
ym-45	ba	1200.0	42	air	-106	3.00E-07	9.84E-06	1.18E-02	
ym-45	ba	1400.0	42	air	106-500	3.00E-07	8.45E-06	1.18E-02	
ym-46	ba	6500.0	21	air	75-500	8.00E-10	4.91E-09	3.19E-05	
ym-46	ba	11000.0	42	air	75-500	8.00E-10	2.90E-09	3.19E-05	
ym-46	ba	25000.0	84	air	75-500	8.00E-10	1.28E-09	3.20E-05	
ym-48	ba	12000.0	21	air	106-500	4.00E-07	1.33E-06	1.60E-02	
ym-48	ba	10000.0	42	air	-106	4.00E-07	1.60E-06	1.60E-02	
ym-48	ba	23000.0	42	air	106-500	4.00E-07	6.95E-07	1.60E-02	
ym-49	ba	17000.0	21	air	-106	4.00E-07	9.40E-07	1.60E-02	
ym-49	ba	26000.0	21	air	106-500	4.00E-07	6.15E-07	1.60E-02	
ym-49	ba	30000.0	21	air	106-500	4.00E-07	5.33E-07	1.60E-02	
ym-49	ba	9200.0	42	air	-106	4.00E-07	1.74E-06	1.60E-02	
ym-49	ba	54000.0	42	air	106-500	4.00E-07	2.96E-07	1.60E-02	
ym-49	ba	59000.0	42	air	106-500	4.00E-07	2.71E-07	1.60E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-54	ba	610.0	21	ca	- 75	1.00E-07	6.35E-06	3.87E-03	
ym-54	ba	870.0	21	ca	75-500	1.00E-07	4.49E-06	3.91E-03	
ym-54	ba	740.0	42	ca	- 75	1.00E-07	5.26E-06	3.89E-03	
ym-54	ba	620.0	42	ca	75-500	1.00E-07	6.25E-06	3.87E-03	
ym-54	ba	660.0	84	ca	- 75	1.00E-07	5.88E-06	3.88E-03	
ym-54	ba	350.0	84	ca	75-500	1.00E-07	1.08E-05	3.78E-03	
ym-54	ba	1700.0	21	air	- 38	3.00E-07	6.98E-06	1.19E-02	
ym-54	ba	1600.0	21	air	- 38	3.00E-07	7.41E-06	1.19E-02	
ym-54	ba	520.0	21	air	-106	3.00E-07	2.22E-05	1.16E-02	
ym-54	ba	470.0	21	air	38-106	3.00E-07	2.45E-05	1.15E-02	
ym-54	ba	480.0	21	air	38-106	3.00E-07	2.40E-05	1.15E-02	
ym-54	ba	130.0	21	air	106-500	3.00E-07	8.00E-05	1.04E-02	
ym-54	ba	150.0	21	air	106-500	3.00E-07	7.06E-05	1.06E-02	
ym-54	ba	720.0	21	air	106-500	3.00E-07	1.62E-05	1.17E-02	
ym-54	ba	650.0	42	air	-106	3.00E-07	1.79E-05	1.16E-02	
ym-54	ba	590.0	42	air	106-500	3.00E-07	1.97E-05	1.16E-02	
ja-18	ba	23000.0	14	air	106-150	2.00E-07	3.48E-07	7.99E-03	70
ja-18	ba	35000.0	14	air	355-500	2.00E-07	2.28E-07	8.00E-03	70
ja-18	ba	29000.0	21	air	106-150	2.00E-07	2.76E-07	7.99E-03	70
ja-18	ba	40000.0	21	air	355-500	2.00E-07	2.00E-07	8.00E-03	70
ja-18	ba	64000.0	35	air	106-150	2.00E-07	1.25E-07	8.00E-03	70
ja-18	ba	75000.0	35	air	355-500	2.00E-07	1.07E-07	8.00E-03	70
ja-18	ba	64000.0	63	air	106-150	2.00E-07	1.25E-07	8.00E-03	70
ja-18	ba	61000.0	63	air	355-500	2.00E-07	1.31E-07	8.00E-03	70
ja-32	ba	560.0	7	air	106-150	1.00E-06	6.90E-05	3.86E-02	70
ja-32	ba	900.0	7	air	355-500	1.00E-06	4.35E-05	3.91E-02	70
ja-32	ba	660.0	14	air	106-150	1.00E-06	5.88E-05	3.88E-02	70
ja-32	ba	1000.0	14	air	355-500	1.00E-06	3.92E-05	3.92E-02	70
ja-32	ba	940.0	28	air	106-150	1.00E-06	4.17E-05	3.92E-02	70
ja-32	ba	1100.0	28	air	355-500	1.00E-06	3.57E-05	3.93E-02	70
ja-32	ba	1300.0	56	air	106-150	1.00E-06	3.03E-05	3.94E-02	70
ja-32	ba	1600.0	56	air	355-500	1.00E-06	2.47E-05	3.95E-02	70
ja-37	ba	2000.0	7	air	106-150	2.00E-06	3.96E-05	7.92E-02	70
ja-37	ba	1700.0	7	air	355-500	1.00E-06	2.33E-05	3.95E-02	70
ja-37	ba	2500.0	14	air	106-150	2.00E-06	3.17E-05	7.94E-02	70
ja-37	ba	2400.0	14	air	355-500	1.00E-06	1.65E-05	3.97E-02	70
ja-37	ba	4200.0	21	air	106-150	2.00E-06	1.90E-05	7.96E-02	70
ja-37	ba	3400.0	21	air	355-500	1.00E-06	1.17E-05	3.98E-02	70
ja-37	ba	6600.0	49	air	106-150	2.00E-06	1.21E-05	7.98E-02	70
ja-37	ba	6600.0	49	air	355-500	1.00E-06	6.04E-06	3.99E-02	70

Table A-IV

Data Base Entries of Experimental Sorption Data for the Element Europium

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
GU3-1301	eu	31.0	42	air	75-500	1.00E-07	1.18E-04	3.65E-03	
GU3-1301	eu	44.0	42	air	75-500	1.00E-07	9.38E-05	4.12E-03	
GU3-1301	eu	64.0	42	air	75-500	1.00E-07	7.14E-05	4.57E-03	
GU3-1301	eu	87.0	42	air	75-500	1.00E-07	5.61E-05	4.88E-03	
g1-1292	eu	140.0	21	air	-500	1.00E-07	3.75E-05	5.25E-03	
g1-1292	eu	160.0	21	air	-500	1.00E-07	3.33E-05	5.33E-03	
g1-1292	eu	100.0	42	air	-500	1.00E-07	5.00E-05	5.00E-03	
g1-1292	eu	160.0	42	air	-500	1.00E-07	3.33E-05	5.33E-03	
g1-1436	eu	30000.0	21	air	-500	1.00E-07	2.00E-07	6.00E-03	
g1-1436	eu	32000.0	21	air	-500	1.00E-07	1.87E-07	6.00E-03	
g1-1436	eu	25000.0	42	air	-500	1.00E-07	2.40E-07	6.00E-03	
g1-1436	eu	34000.0	42	air	-500	1.00E-07	1.76E-07	6.00E-03	
g1-1854	eu	130000.0	21	air	- 75	3.00E-08	1.38E-08	1.80E-03	
g1-1854	eu	120000.0	21	air	75-500	3.00E-08	1.50E-08	1.80E-03	
g1-1854	eu	110000.0	42	air	- 75	3.00E-08	1.64E-08	1.80E-03	
g1-1854	eu	14000.0	42	air	75-500	3.00E-08	1.28E-07	1.80E-03	
g1-1883	eu	650.0	21	air	- 38	3.00E-08	2.69E-06	1.75E-03	
g1-1883	eu	370.0	21	air	- 38	3.00E-08	4.62E-06	1.71E-03	
g1-1883	eu	180.0	21	air	-500	1.00E-07	3.00E-05	5.40E-03	
g1-1883	eu	180.0	21	air	-500	1.00E-07	3.00E-05	5.40E-03	
g1-1883	eu	110.0	21	air	38-106	3.00E-08	1.38E-05	1.52E-03	
g1-1883	eu	120.0	21	air	38-106	3.00E-08	1.29E-05	1.54E-03	
g1-1883	eu	150.0	21	air	106-500	3.00E-08	1.06E-05	1.59E-03	
g1-1883	eu	170.0	21	air	106-500	3.00E-08	9.47E-06	1.61E-03	
g1-1883	eu	300.0	42	air	-500	1.00E-07	1.88E-05	5.63E-03	
g1-1883	eu	330.0	42	air	-500	1.00E-07	1.71E-05	5.66E-03	
g1-1982	eu	1200.0	14	air	- 38	1.00E-07	4.92E-06	5.90E-03	
g1-1982	eu	530.0	14	air	38- 75	1.00E-07	1.09E-05	5.78E-03	
g1-1982	eu	610.0	14	air	75-250	1.00E-07	9.52E-06	5.81E-03	
g1-1982	eu	860.0	14	air	250-500	1.00E-07	6.82E-06	5.86E-03	
g1-1982	eu	2500.0	21	air	- 38	1.00E-07	2.38E-06	5.95E-03	
g1-1982	eu	1500.0	21	air	-500	1.00E-07	3.95E-06	5.92E-03	
g1-1982	eu	1300.0	21	air	-500	1.00E-07	4.55E-06	5.91E-03	
g1-1982	eu	880.0	21	air	38- 75	1.00E-07	6.67E-06	5.87E-03	
g1-1982	eu	1300.0	21	air	75-250	1.00E-07	4.55E-06	5.91E-03	
g1-1982	eu	1100.0	21	air	250-500	1.00E-07	5.36E-06	5.89E-03	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-1982	eu	2000.0	42	air	-500	1.00E-07	2.97E-06	5.94E-03	
gl-1982	eu	1900.0	42	air	-500	1.00E-07	3.13E-06	5.94E-03	
gl-2233	eu	520.0	21	air	-500	9.00E-08	1.00E-05	5.20E-03	
gl-2233	eu	920.0	21	air	-500	9.00E-08	5.74E-06	5.29E-03	
gl-2233	eu	890.0	42	air	-500	9.00E-08	5.93E-06	5.28E-03	
gl-2233	eu	1300.0	42	air	-500	9.00E-08	4.09E-06	5.32E-03	
gl-2289	eu	1400.0	21	air	- 38	2.00E-08	8.45E-07	1.18E-03	
gl-2289	eu	1600.0	21	air	- 38	2.00E-08	7.41E-07	1.19E-03	
gl-2289	eu	780.0	21	air	38-106	2.00E-08	1.50E-06	1.17E-03	
gl-2289	eu	780.0	21	air	38-106	2.00E-08	1.50E-06	1.17E-03	
gl-2289	eu	810.0	21	air	106-500	2.00E-08	1.45E-06	1.17E-03	
gl-2289	eu	820.0	21	air	106-500	2.00E-08	1.43E-06	1.17E-03	
gl-2333	eu	2000.0	21	air	- 75	3.00E-08	8.91E-07	1.78E-03	
gl-2333	eu	1400.0	21	air	75-500	3.00E-08	1.27E-06	1.77E-03	
gl-2333	eu	3100.0	42	air	- 75	3.00E-08	5.77E-07	1.79E-03	
gl-2333	eu	2900.0	42	air	75-500	3.00E-08	6.16E-07	1.79E-03	
gl-2363	eu	5400.0	21	air	- 38	5.00E-08	5.54E-07	2.99E-03	
gl-2363	eu	5600.0	21	air	- 38	5.00E-08	5.34E-07	2.99E-03	
gl-2363	eu	1300.0	21	air	-500	8.00E-08	3.64E-06	4.73E-03	
gl-2363	eu	1300.0	21	air	-500	8.00E-08	3.64E-06	4.73E-03	
gl-2363	eu	790.0	21	air	38-106	5.00E-08	3.70E-06	2.93E-03	
gl-2363	eu	780.0	21	air	38-106	5.00E-08	3.75E-06	2.92E-03	
gl-2363	eu	580.0	21	air	106-500	5.00E-08	5.00E-06	2.90E-03	
gl-2363	eu	780.0	21	air	106-500	5.00E-08	3.75E-06	2.92E-03	
gl-2363	eu	1600.0	42	air	-500	8.00E-08	2.96E-06	4.74E-03	
gl-2363	eu	1900.0	42	air	-500	8.00E-08	2.50E-06	4.75E-03	
gl-2410	eu	390.0	21	air	- 75	2.00E-08	2.93E-06	1.14E-03	
gl-2410	eu	360.0	21	air	75-500	2.00E-08	3.16E-06	1.14E-03	
gl-2410	eu	440.0	42	air	- 75	2.00E-08	2.61E-06	1.15E-03	
gl-2410	eu	510.0	42	air	75-500	2.00E-08	2.26E-06	1.15E-03	
gl-2476	eu	4600.0	21	air	- 75	6.00E-08	7.79E-07	3.58E-03	
gl-2476	eu	3300.0	21	air	75-500	6.00E-08	1.08E-06	3.58E-03	
gl-2476	eu	5100.0	42	air	- 75	6.00E-08	7.03E-07	3.59E-03	
gl-2476	eu	3100.0	42	air	75-500	6.00E-08	1.15E-06	3.58E-03	
gl-2698	eu	130.0	21	air	-500	4.00E-07	1.60E-04	2.08E-02	
gl-2698	eu	180.0	21	air	-500	4.00E-07	1.20E-04	2.16E-02	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
g1-2698	eu	230.0	42	air	-500	4.00E-07	9.60E-05	2.21E-02	
g1-2698	eu	260.0	42	air	-500	4.00E-07	8.57E-05	2.23E-02	
g1-2840	eu	5000.0	21	air	- 75	3.00E-08	3.59E-07	1.79E-03	
g1-2840	eu	4500.0	21	air	75-500	3.00E-08	3.98E-07	1.79E-03	
g1-2840	eu	6200.0	42	air	- 75	3.00E-08	2.89E-07	1.79E-03	
g1-2840	eu	5300.0	42	air	75-500	3.00E-08	3.38E-07	1.79E-03	
g1-2854	eu	1100.0	21	air	- 75	2.00E-08	1.07E-06	1.18E-03	
g1-2854	eu	1100.0	21	air	75-500	2.00E-08	1.07E-06	1.18E-03	
g1-2854	eu	2600.0	42	air	- 75	2.00E-08	4.58E-07	1.19E-03	
g1-2854	eu	1500.0	42	air	75-500	2.00E-08	7.89E-07	1.18E-03	
g1-2901	eu	195000.0	21	air	-500	4.00E-08	1.23E-08	2.40E-03	
g1-2901	eu	230000.0	21	air	-500	4.00E-08	1.04E-08	2.40E-03	
g1-2901	eu	210000.0	42	air	-500	4.00E-08	1.14E-08	2.40E-03	
g1-2901	eu	210000.0	42	air	-500	4.00E-08	1.14E-08	2.40E-03	
g1-3116	eu	660.0	21	air	-500	2.00E-07	1.76E-05	1.16E-02	
g1-3116	eu	680.0	21	air	-500	2.00E-07	1.71E-05	1.17E-02	
g1-3116	eu	790.0	42	air	-500	2.00E-07	1.48E-05	1.17E-02	
g1-3116	eu	900.0	42	air	-500	2.00E-07	1.30E-05	1.17E-02	
g1-3658	eu	490.0	21	air	-500	4.00E-07	4.71E-05	2.31E-02	
g1-3658	eu	510.0	21	air	-500	4.00E-07	4.53E-05	2.31E-02	
g1-3658	eu	1000.0	42	air	-500	4.00E-07	2.35E-05	2.35E-02	
g1-3658	eu	1200.0	42	air	-500	4.00E-07	1.97E-05	2.36E-02	
g1-3658	eu	150000.0	21	air	- 38	4.00E-07	1.60E-07	2.40E-02	
g1-3658	eu	160000.0	21	air	- 38	4.00E-07	1.50E-07	2.40E-02	
g1-3658	eu	4100.0	21	air	38-106	4.00E-07	5.83E-06	2.39E-02	
g1-3658	eu	4800.0	21	air	38-106	4.00E-07	4.98E-06	2.39E-02	
g1-3658	eu	4900.0	21	air	106-500	4.00E-07	4.88E-06	2.39E-02	
g1-3658	eu	5700.0	21	air	106-500	4.00E-07	4.20E-06	2.39E-02	
g2-1952	eu	75.0	42	air	-500	7.00E-08	4.42E-05	3.32E-03	
g2-1952	eu	103.0	42	air	-500	7.00E-08	3.41E-05	3.52E-03	
g2-3933	eu	887.0	42	air	-500	6.00E-08	3.97E-06	3.52E-03	
g2-3933	eu	2230.0	42	air	-500	6.00E-08	1.60E-06	3.57E-03	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
g2-547	eu	360.0	42	air	-500	5.90E-08	9.32E-06	3.35E-03	
g2-547	eu	414.0	42	air	-500	5.90E-08	8.16E-06	3.38E-03	
g2-723	eu	10000.0	42	air	-500	3.00E-08	1.80E-07	1.80E-03	
g2-723	eu	10000.0	42	air	-500	3.00E-08	1.80E-07	1.80E-03	
gu3-1203	eu	190.0	42	air	75-500	9.00E-08	2.57E-05	4.89E-03	
gu3-1203	eu	192.0	42	air	75-500	9.00E-08	2.55E-05	4.89E-03	
gu3-433	eu	55.0	42	air	75-500	9.00E-08	7.20E-05	3.96E-03	
gu3-433	eu	82.0	42	air	75-500	9.00E-08	5.29E-05	4.34E-03	
gu3-433	eu	86.0	42	air	75-500	9.00E-08	5.09E-05	4.38E-03	
gu3-433	eu	113.0	42	air	75-500	9.00E-08	4.06E-05	4.59E-03	
ja-18	eu	14.0	14	air	106-150	6.00E-07	1.06E-03	1.48E-02	
ja-18	eu	14.0	14	air	355-500	6.00E-07	1.06E-03	1.48E-02	
ja-18	eu	1700.0	21	air	75-500	1.00E-10	3.49E-09	5.93E-06	
ja-18	eu	1700.0	21	air	75-500	1.00E-10	3.49E-09	5.93E-06	
ja-18	eu	30.0	21	air	106-150	6.00E-07	7.20E-04	2.16E-02	
ja-18	eu	18.0	21	air	355-500	6.00E-07	9.47E-04	1.71E-02	
ja-18	eu	130.0	28	air	250-355	8.00E-09	3.20E-06	4.16E-04	
ja-18	eu	4600.0	28	air	250-355	3.00E-08	3.90E-07	1.79E-03	
ja-18	eu	1100.0	42	air	75-500	1.00E-10	5.36E-09	5.89E-06	
ja-18	eu	32.0	42	air	106-150	6.00E-07	6.92E-04	2.22E-02	
ja-18	eu	26.0	42	air	355-500	6.00E-07	7.83E-04	2.03E-02	
ja-18	eu	66.0	77	air	106-150	6.00E-07	4.19E-04	2.76E-02	
ja-18	eu	37.0	77	air	355-500	6.00E-07	6.32E-04	2.34E-02	
ja-18	eu	1700.0	63	air	250-355	8.00E-09	2.79E-07	4.74E-04	
ja-18	eu	15000.0	63	air	250-355	3.00E-08	1.20E-07	1.80E-03	
ja-18	eu	1400.0	84	air	75-500	1.00E-10	4.23E-09	5.92E-06	
ja-26	eu	47.0	21	air	75-500	3.00E-10	2.69E-07	1.26E-05	
ja-26	eu	220.0	21	air	75-500	3.00E-10	7.50E-08	1.65E-05	
ja-26	eu	1200.0	42	air	75-500	3.00E-10	1.48E-08	1.77E-05	
ja-26	eu	15000.0	42	air	75-500	3.00E-10	1.20E-09	1.80E-05	
ja-28	eu	1200.0	21	air	75-500	1.00E-10	4.92E-09	5.90E-06	
ja-28	eu	1500.0	21	air	75-500	1.00E-10	3.95E-09	5.92E-06	
ja-28	eu	600.0	42	air	75-500	1.00E-10	9.68E-09	5.81E-06	
ja-28	eu	5200.0	42	air	75-500	1.00E-10	1.15E-09	5.98E-06	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-32	eu	51.0	7	air	106-150	6.00E-07	5.07E-04	2.59E-02	
ja-32	eu	48.0	7	air	355-500	6.00E-07	5.29E-04	2.54E-02	
ja-32	eu	69.0	21	air	106-150	6.00E-07	4.04E-04	2.79E-02	
ja-32	eu	92.0	21	air	355-500	6.00E-07	3.21E-04	2.96E-02	
ja-32	eu	1700.0	28	air	250-355	8.00E-09	2.79E-07	4.74E-04	
ja-32	eu	24000.0	28	air	250-355	8.00E-09	2.00E-08	4.80E-04	
ja-32	eu	73.0	35	air	106-150	6.00E-07	3.87E-04	2.83E-02	
ja-32	eu	88.0	35	air	355-500	6.00E-07	3.33E-04	2.93E-02	
ja-32	eu	190.0	56	air	106-150	6.00E-07	1.71E-04	3.26E-02	
ja-32	eu	120.0	56	air	355-500	6.00E-07	2.57E-04	3.09E-02	
ja-32	eu	4200.0	63	air	250-355	8.00E-09	1.14E-07	4.78E-04	
ja-32	eu	61000.0	63	air	250-355	8.00E-09	7.87E-09	4.80E-04	
ja-37	eu	2100.0	14	air	106-150	3.00E-07	8.49E-06	1.78E-02	
ja-37	eu	4100.0	14	air	355-500	3.00E-07	4.37E-06	1.79E-02	
ja-37	eu	7600.0	21	air	106-150	3.00E-07	2.36E-06	1.80E-02	
ja-37	eu	4000.0	21	air	355-500	3.00E-07	4.48E-06	1.79E-02	
ja-37	eu	12000.0	28	air	250-355	8.00E-09	3.99E-08	4.79E-04	
ja-37	eu	13000.0	28	air	250-355	3.00E-08	1.38E-07	1.80E-03	
ja-37	eu	7300.0	35	air	106-150	3.00E-07	2.46E-06	1.80E-02	
ja-37	eu	6400.0	35	air	355-500	3.00E-07	2.80E-06	1.79E-02	
ja-37	eu	26000.0	63	air	250-355	8.00E-09	1.84E-08	4.80E-04	
ja-37	eu	51000.0	63	air	250-355	3.00E-08	3.53E-08	1.80E-03	
ja-37	eu	9500.0	70	air	106-150	3.00E-07	1.89E-06	1.80E-02	
ja-37	eu	6900.0	70	air	355-500	3.00E-07	2.60E-06	1.79E-02	
ja-8	eu	1800.0	21	air	75-500	3.00E-10	9.89E-09	1.78E-05	
ja-8	eu	2100.0	21	air	75-500	3.00E-10	8.49E-09	1.78E-05	
ja-8	eu	1700.0	42	air	75-500	3.00E-10	1.05E-08	1.78E-05	
ja-8	eu	2900.0	42	air	75-500	3.00E-10	6.16E-09	1.79E-05	
ym-22	eu	800.0	21	ca	- 75	2.00E-08	1.46E-06	1.17E-03	
ym-22	eu	710.0	21	ca	75-500	2.00E-08	1.64E-06	1.17E-03	
ym-22	eu	990.0	42	ca	- 75	2.00E-08	1.19E-06	1.18E-03	
ym-22	eu	1000.0	84	ca	- 75	2.00E-08	1.18E-06	1.18E-03	
ym-22	eu	1300.0	84	ca	75-500	2.00E-08	9.09E-07	1.18E-03	
ym-22	eu	690.0	21	air	- 75	3.00E-06	2.54E-04	1.75E-01	
ym-22	eu	1900.0	21	air	- 75	4.00E-08	1.25E-06	2.37E-03	
ym-22	eu	1900.0	21	air	- 75	1.00E-08	3.12E-07	5.94E-04	
ym-22	eu	5800.0	21	air	- 75	9.00E-06	9.28E-05	5.38E-01	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-22	eu	1100.0	21	air	75-500	9.00E-06	4.82E-04	5.30E-01	
ym-22	eu	1200.0	21	air	75-500	3.00E-06	1.48E-04	1.77E-01	
ym-22	eu	1900.0	21	air	75-500	1.00E-08	3.12E-07	5.94E-04	
ym-22	eu	1900.0	21	air	75-500	4.00E-08	1.25E-06	2.37E-03	
ym-22	eu	2100.0	21	air	75-500	3.00E-09	8.49E-08	1.78E-04	
ym-22	eu	1200.0	21	air	106-500	5.00E-08	2.46E-06	2.95E-03	
ym-22	eu	1300.0	21	air	106-500	5.00E-08	2.27E-06	2.95E-03	
ym-22	eu	1500.0	42	air	-106	5.00E-08	1.97E-06	2.96E-03	
ym-22	eu	1400.0	42	air	106-500	5.00E-08	2.11E-06	2.96E-03	
ym-22	eu	1700.0	42	air	106-500	5.00E-08	1.74E-06	2.97E-03	
ym-30	eu	94000.0	21	air	75-500	1.00E-10	6.38E-11	6.00E-06	
ym-30	eu	120000.0	42	air	75-500	1.00E-10	5.00E-11	6.00E-06	
ym-30	eu	260000.0	84	air	75-500	1.00E-10	2.31E-11	6.00E-06	
ym-38	eu	1100.0	21	ca	- 75	9.00E-08	4.82E-06	5.30E-03	
ym-38	eu	840.0	21	ca	75-500	9.00E-08	6.28E-06	5.27E-03	
ym-38	eu	560.0	42	ca	- 75	9.00E-08	9.31E-06	5.21E-03	
ym-38	eu	1000.0	42	ca	75-500	9.00E-08	5.29E-06	5.29E-03	
ym-38	eu	1000.0	84	ca	- 75	9.00E-08	5.29E-06	5.29E-03	
ym-38	eu	470.0	84	ca	75-500	9.00E-08	1.10E-05	5.18E-03	
ym-38	eu	3000.0	21	air	- 38	7.00E-08	1.39E-06	4.17E-03	
ym-38	eu	2200.0	21	air	- 38	7.00E-08	1.89E-06	4.16E-03	
ym-38	eu	7100.0	21	air	- 75	6.00E-06	5.06E-05	3.59E-01	
ym-38	eu	2600.0	21	air	- 75	3.00E-06	6.87E-05	1.79E-01	
ym-38	eu	5000.0	21	air	- 75	6.00E-09	7.17E-08	3.59E-04	
ym-38	eu	3700.0	21	air	- 75	6.00E-08	9.68E-07	3.58E-03	
ym-38	eu	3100.0	21	air	- 75	4.00E-08	7.69E-07	2.38E-03	
ym-38	eu	1300.0	21	air	38-106	7.00E-08	3.18E-06	4.14E-03	
ym-38	eu	1300.0	21	air	38-106	7.00E-08	3.18E-06	4.14E-03	
ym-38	eu	1700.0	21	air	75-500	4.00E-06	1.40E-04	2.37E-01	
ym-38	eu	1700.0	21	air	75-500	6.00E-08	2.09E-06	3.56E-03	
ym-38	eu	2700.0	21	air	75-500	4.00E-08	8.82E-07	2.38E-03	
ym-38	eu	4600.0	21	air	75-500	6.00E-06	7.79E-05	3.58E-01	
ym-38	eu	3700.0	21	air	75-500	6.00E-09	9.68E-08	3.58E-04	
ym-38	eu	1300.0	21	air	106-500	7.00E-08	3.18E-06	4.14E-03	
ym-38	eu	1500.0	21	air	106-500	7.00E-08	2.76E-06	4.14E-03	
ym-38	eu	2600.0	21	air	106-500	7.00E-08	1.60E-06	4.17E-03	
ym-38	eu	4900.0	42	air	-106	7.00E-08	8.54E-07	4.18E-03	
ym-38	eu	1500.0	42	air	106-500	7.00E-08	2.76E-06	4.14E-03	
ym-42	eu	45000.0	21	air	75-500	1.00E-10	1.33E-10	6.00E-06	
ym-42	eu	53000.0	84	air	75-500	1.00E-10	1.13E-10	6.00E-06	
ym-42	eu	58000.0	42	air	75-500	1.00E-10	1.03E-10	6.00E-06	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-45	eu	990.0	21	air	-106	1.00E-07	5.94E-06	5.88E-03	
ym-45	eu	2100.0	21	air	106-500	1.00E-07	2.83E-06	5.94E-03	
ym-45	eu	1700.0	42	air	-106	1.00E-07	3.49E-06	5.93E-03	
ym-45	eu	1600.0	42	air	106-500	1.00E-07	3.70E-06	5.93E-03	
ym-46	eu	110000.0	21	air	75-500	1.00E-10	5.45E-11	6.00E-06	
ym-46	eu	320000.0	42	air	75-500	1.00E-10	1.87E-11	6.00E-06	
ym-46	eu	490000.0	84	air	75-500	1.00E-10	1.22E-11	6.00E-06	
ym-48	eu	1700.0	21	air	106-500	5.00E-08	1.74E-06	2.97E-03	
ym-48	eu	3100.0	42	air	-106	5.00E-08	9.62E-07	2.98E-03	
ym-48	eu	2700.0	42	air	106-500	5.00E-08	1.10E-06	2.98E-03	
ym-49	eu	1400.0	21	air	-106	1.00E-07	4.23E-06	5.92E-03	
ym-49	eu	1000.0	21	air	106-500	1.00E-07	5.88E-06	5.88E-03	
ym-49	eu	1200.0	21	air	106-500	1.00E-07	4.92E-06	5.90E-03	
ym-49	eu	1300.0	42	air	-106	1.00E-07	4.55E-06	5.91E-03	
ym-49	eu	1000.0	42	air	106-500	1.00E-07	5.88E-06	5.88E-03	
ym-49	eu	1500.0	42	air	106-500	1.00E-07	3.95E-06	5.92E-03	
ym-54	eu	530.0	21	ca	- 75	2.00E-07	2.18E-05	1.16E-02	
ym-54	eu	330.0	21	ca	75-500	2.00E-07	3.43E-05	1.13E-02	
ym-54	eu	1400.0	42	ca	- 75	2.00E-07	8.45E-06	1.18E-02	
ym-54	eu	850.0	42	ca	75-500	2.00E-07	1.38E-05	1.17E-02	
ym-54	eu	1500.0	84	ca	- 75	2.00E-07	7.89E-06	1.18E-02	
ym-54	eu	770.0	84	ca	75-500	2.00E-07	1.52E-05	1.17E-02	
ym-54	eu	1600.0	21	air	- 38	4.00E-08	1.48E-06	2.37E-03	
ym-54	eu	1600.0	21	air	- 38	4.00E-08	1.48E-06	2.37E-03	
ym-54	eu	390.0	21	air	-106	1.00E-07	1.46E-05	5.71E-03	
ym-54	eu	260.0	21	air	38-106	4.00E-08	8.57E-06	2.23E-03	
ym-54	eu	420.0	21	air	38-106	4.00E-08	5.45E-06	2.29E-03	
ym-54	eu	440.0	21	air	106-500	4.00E-08	5.22E-06	2.30E-03	
ym-54	eu	490.0	21	air	106-500	4.00E-08	4.71E-06	2.31E-03	
ym-54	eu	580.0	21	air	106-500	1.00E-07	1.00E-05	5.80E-03	
ym-54	eu	700.0	42	air	-106	1.00E-07	8.33E-06	5.83E-03	
ym-54	eu	370.0	42	air	106-500	1.00E-07	1.54E-05	5.69E-03	
ja-18	eu	63.0	14	air	106-150	3.00E-07	2.17E-04	1.37E-02	70
ja-18	eu	61.0	14	air	355-500	3.00E-07	2.22E-04	1.36E-02	70

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ja-18	eu	76.0	21	air	106-150	3.00E-07	1.88E-04	1.43E-02	70
ja-18	eu	62.0	21	air	355-500	3.00E-07	2.20E-04	1.36E-02	70
ja-18	eu	110.0	35	air	106-150	3.00E-07	1.38E-04	1.52E-02	70
ja-18	eu	76.0	35	air	355-500	3.00E-07	1.88E-04	1.43E-02	70
ja-18	eu	130.0	63	air	106-150	3.00E-07	1.20E-04	1.56E-02	70
ja-18	eu	89.0	63	air	355-500	3.00E-07	1.65E-04	1.47E-02	70
ja-32	eu	120.0	7	air	106-150	6.00E-07	2.57E-04	3.09E-02	70
ja-32	eu	93.0	7	air	355-500	6.00E-07	3.19E-04	2.96E-02	70
ja-32	eu	180.0	14	air	106-150	6.00E-07	1.80E-04	3.24E-02	70
ja-32	eu	130.0	14	air	355-500	6.00E-07	2.40E-04	3.12E-02	70
ja-32	eu	220.0	28	air	106-150	6.00E-07	1.50E-04	3.30E-02	70
ja-32	eu	380.0	28	air	355-500	6.00E-07	9.00E-05	3.42E-02	70
ja-32	eu	240.0	56	air	106-150	6.00E-07	1.38E-04	3.32E-02	70
ja-32	eu	130.0	56	air	355-500	6.00E-07	2.40E-04	3.12E-02	70
ja-37	eu	4000.0	7	air	106-150	1.00E-07	1.49E-06	5.97E-03	70
ja-37	eu	2100.0	7	air	355-500	1.00E-07	2.83E-06	5.94E-03	70
ja-37	eu	4100.0	14	air	106-150	1.00E-07	1.46E-06	5.97E-03	70
ja-37	eu	4400.0	14	air	355-500	1.00E-07	1.36E-06	5.97E-03	70
ja-37	eu	4000.0	21	air	106-150	1.00E-07	1.49E-06	5.97E-03	70
ja-37	eu	4500.0	21	air	355-500	1.00E-07	1.33E-06	5.97E-03	70
ja-37	eu	5200.0	49	air	106-150	1.00E-07	1.15E-06	5.98E-03	70
ja-37	eu	5500.0	49	air	355-500	1.00E-07	1.09E-06	5.98E-03	70

Table A-V

Data Base Entries of Experimental Sorption Data for the Element Cerium

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-1292	ce	54.0	21	air	-500	7.00E-08	5.68E-05	3.06E-03	
gl-1292	ce	79.0	21	air	-500	7.00E-08	4.24E-05	3.35E-03	
gl-1292	ce	50.0	42	air	-500	7.00E-08	6.00E-05	3.00E-03	
gl-1292	ce	82.0	42	air	-500	7.00E-08	4.12E-05	3.38E-03	
gl-1436	ce	58000.0	21	air	-500	1.00E-07	1.03E-07	6.00E-03	
gl-1436	ce	62000.0	21	air	-500	1.00E-07	9.67E-08	6.00E-03	
gl-1436	ce	41000.0	42	air	-500	1.00E-07	1.46E-07	6.00E-03	
gl-1436	ce	74000.0	42	air	-500	1.00E-07	8.11E-08	6.00E-03	
gl-1982	ce	450.0	21	air	-500	1.00E-07	1.28E-05	5.74E-03	
gl-1982	ce	520.0	21	air	-500	1.00E-07	1.11E-05	5.78E-03	
gl-1982	ce	600.0	42	air	-500	1.00E-07	9.68E-06	5.81E-03	
gl-1982	ce	640.0	42	air	-500	1.00E-07	9.09E-06	5.82E-03	
gl-2233	ce	840.0	21	air	-500	7.00E-08	4.88E-06	4.10E-03	
gl-2233	ce	1300.0	21	air	-500	7.00E-08	3.18E-06	4.14E-03	
gl-2233	ce	1200.0	42	air	-500	7.00E-08	3.44E-06	4.13E-03	
gl-2233	ce	2100.0	42	air	-500	7.00E-08	1.98E-06	4.16E-03	
gl-2363	ce	270.0	21	air	-500	3.00E-08	6.21E-06	1.68E-03	
gl-2363	ce	290.0	21	air	-500	3.00E-08	5.81E-06	1.68E-03	
gl-2363	ce	310.0	42	air	-500	3.00E-08	5.45E-06	1.69E-03	
gl-2363	ce	370.0	42	air	-500	3.00E-08	4.62E-06	1.71E-03	
gl-2698	ce	170.0	21	air	-500	1.00E-07	3.16E-05	5.37E-03	
gl-2698	ce	220.0	21	air	-500	1.00E-07	2.50E-05	5.50E-03	
gl-2698	ce	270.0	42	air	-500	1.00E-07	2.07E-05	5.59E-03	
gl-2698	ce	310.0	42	air	-500	1.00E-07	1.82E-05	5.64E-03	
gl-2901	ce	35000.0	21	air	-500	9.00E-09	1.54E-08	5.40E-04	
gl-2901	ce	40000.0	21	air	-500	9.00E-09	1.35E-08	5.40E-04	
gl-2901	ce	45000.0	42	air	-500	9.00E-09	1.20E-08	5.40E-04	
gl-2901	ce	49000.0	42	air	-500	9.00E-09	1.10E-08	5.40E-04	
gl-3116	ce	80.0	21	air	-500	1.00E-07	6.00E-05	4.80E-03	
gl-3116	ce	89.0	21	air	-500	1.00E-07	5.50E-05	4.90E-03	
gl-3116	ce	100.0	42	air	-500	1.00E-07	5.00E-05	5.00E-03	
gl-3116	ce	120.0	42	air	-500	1.00E-07	4.29E-05	5.14E-03	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
gl-3658	ce	630.0	21	air	-500	3.00E-07	2.77E-05	1.74E-02	
gl-3658	ce	640.0	21	air	-500	2.00E-07	1.82E-05	1.16E-02	
gl-3658	ce	1300.0	42	air	-500	2.00E-07	9.09E-06	1.18E-02	
gl-3658	ce	1500.0	42	air	-500	2.00E-07	7.89E-06	1.18E-02	
ja-18	ce	20.0	14	air	355-500	1.00E-06	1.50E-03	3.00E-02	
ja-18	ce	26.0	14	air	106-150	1.00E-06	1.30E-03	3.39E-02	
ja-18	ce	1400.0	21	air	75-500	8.00E-13	3.38E-11	4.73E-08	
ja-18	ce	26.0	21	air	355-500	1.00E-06	1.30E-03	3.39E-02	
ja-18	ce	46.0	21	air	106-150	1.00E-06	9.09E-04	4.18E-02	
ja-18	ce	950.0	28	air	250-355	1.00E-08	6.19E-07	5.88E-04	
ja-18	ce	5200.0	28	air	250-355	2.00E-08	2.30E-07	1.20E-03	
ja-18	ce	5700.0	42	air	75-500	8.00E-13	8.39E-12	4.78E-08	
ja-18	ce	43.0	42	air	106-150	1.00E-06	9.52E-04	4.10E-02	
ja-18	ce	41.0	42	air	355-500	1.00E-06	9.84E-04	4.03E-02	
ja-18	ce	1500.0	63	air	250-355	1.00E-08	3.95E-07	5.92E-04	
ja-18	ce	34000.0	63	air	250-355	2.00E-08	3.53E-08	1.20E-03	
ja-18	ce	70.0	77	air	355-500	1.00E-06	6.67E-04	4.67E-02	
ja-18	ce	78.0	77	air	106-150	1.00E-06	6.12E-04	4.78E-02	
ja-18	ce	1300.0	84	air	75-500	8.00E-13	3.64E-11	4.73E-08	
ja-32	ce	43.0	7	air	106-150	8.00E-07	7.62E-04	3.28E-02	
ja-32	ce	66.0	7	air	355-500	8.00E-07	5.58E-04	3.68E-02	
ja-32	ce	53.0	21	air	106-150	8.00E-07	6.58E-04	3.48E-02	
ja-32	ce	90.0	21	air	355-500	8.00E-07	4.36E-04	3.93E-02	
ja-32	ce	30000.0	28	air	250-355	1.00E-08	2.00E-08	6.00E-04	
ja-32	ce	2900.0	28	air	250-355	1.00E-08	2.05E-07	5.96E-04	
ja-32	ce	48.0	35	air	106-150	8.00E-07	7.06E-04	3.39E-02	
ja-32	ce	90.0	35	air	355-500	8.00E-07	4.36E-04	3.93E-02	
ja-32	ce	160.0	56	air	106-150	8.00E-07	2.67E-04	4.27E-02	
ja-32	ce	110.0	56	air	355-500	8.00E-07	3.69E-04	4.06E-02	
ja-32	ce	45000.0	63	air	250-355	1.00E-08	1.33E-08	6.00E-04	
ja-32	ce	55000.0	63	air	250-355	1.00E-08	1.09E-08	6.00E-04	
ja-37	ce	27000.0	28	air	250-355	1.00E-08	2.22E-08	6.00E-04	
ja-37	ce	36000.0	28	air	250-355	2.00E-08	3.33E-08	1.20E-03	
ja-37	ce	33000.0	63	air	250-355	2.00E-08	3.63E-08	1.20E-03	
ja-37	ce	48000.0	63	air	250-355	1.00E-08	1.25E-08	6.00E-04	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-22	ce	630.0	21	ca	- 75	2.00E-08	1.85E-06	1.16E-03	
ym-22	ce	760.0	21	ca	75-500	2.00E-08	1.54E-06	1.17E-03	
ym-22	ce	860.0	42	ca	- 75	2.00E-08	1.36E-06	1.17E-03	
ym-22	ce	760.0	84	ca	- 75	2.00E-08	1.54E-06	1.17E-03	
ym-22	ce	1600.0	84	ca	75-500	2.00E-08	7.41E-07	1.19E-03	
ym-22	ce	1400.0	21	air	106-500	7.00E-07	2.96E-05	4.14E-02	
ym-22	ce	1200.0	21	air	106-500	7.00E-07	3.44E-05	4.13E-02	
ym-22	ce	1600.0	42	air	-106	7.00E-07	2.59E-05	4.15E-02	
ym-22	ce	1200.0	42	air	106-500	7.00E-07	3.44E-05	4.13E-02	
ym-22	ce	1300.0	42	air	106-500	7.00E-07	3.18E-05	4.14E-02	
ym-30	ce	130000.0	21	air	75-500	8.00E-13	3.69E-13	4.80E-08	
ym-30	ce	999999.0	42	air	75-500	8.00E-13	4.80E-14	4.80E-08	
ym-30	ce	330000.0	84	air	75-500	8.00E-13	1.45E-13	4.80E-08	
ym-38	ce	650.0	21	ca	- 75	7.00E-08	6.27E-06	4.07E-03	
ym-38	ce	560.0	21	ca	75-500	7.00E-08	7.24E-06	4.06E-03	
ym-38	ce	320.0	42	ca	- 75	7.00E-08	1.24E-05	3.95E-03	
ym-38	ce	740.0	84	ca	- 75	7.00E-08	5.53E-06	4.09E-03	
ym-38	ce	320.0	84	ca	75-500	7.00E-08	1.24E-05	3.95E-03	
ym-38	ce	900.0	21	air	106-500	1.00E-06	6.52E-05	5.87E-02	
ym-38	ce	850.0	42	ca	75-500	7.00E-08	4.83E-06	4.10E-03	
ym-38	ce	620.0	42	air	106-500	1.00E-06	9.38E-05	5.81E-02	
ym-38	ce	950.0	42	air	-106	1.00E-06	6.19E-05	5.88E-02	
ym-42	ce	35000.0	21	air	75-500	8.00E-13	1.37E-12	4.80E-08	
ym-42	ce	47000.0	42	air	75-500	8.00E-13	1.02E-12	4.80E-08	
ym-42	ce	29000.0	84	air	75-500	8.00E-13	1.65E-12	4.80E-08	
ym-45	ce	540.0	21	air	-106	9.00E-07	9.64E-05	5.21E-02	
ym-45	ce	1000.0	21	air	106-500	9.00E-07	5.29E-05	5.29E-02	
ym-45	ce	670.0	42	air	-106	9.00E-07	7.83E-05	5.24E-02	
ym-45	ce	710.0	42	air	106-500	9.00E-07	7.40E-05	5.25E-02	
ym-46	ce	97000.0	21	air	75-500	8.00E-13	4.95E-13	4.80E-08	
ym-46	ce	360000.0	42	air	75-500	8.00E-13	1.33E-13	4.80E-08	
ym-46	ce	470000.0	84	air	75-500	8.00E-13	1.02E-13	4.80E-08	

SAMPLE	EL	Rd	TI	ATM	SIZE	Co	C	S	T
ym-48	ce	870.0	21	air	106-500	7.00E-07	4.72E-05	4.11E-02	
ym-48	ce	2900.0	42	air	-106	7.00E-07	1.44E-05	4.17E-02	
ym-48	ce	1900.0	42	air	106-500	7.00E-07	2.19E-05	4.16E-02	
ym-49	ce	570.0	21	air	-106	3.00E-07	3.05E-05	1.74E-02	
ym-49	ce	490.0	21	air	106-500	3.00E-07	3.53E-05	1.73E-02	
ym-49	ce	560.0	21	air	106-500	3.00E-07	3.10E-05	1.74E-02	
ym-49	ce	530.0	42	air	-106	3.00E-07	3.27E-05	1.73E-02	
ym-49	ce	350.0	42	air	106-500	3.00E-07	4.86E-05	1.70E-02	
ym-49	ce	810.0	42	air	106-500	3.00E-07	2.17E-05	1.76E-02	
ym-54	ce	150.0	21	ca	- 75	1.00E-07	3.53E-05	5.29E-03	
ym-54	ce	110.0	21	ca	75-500	1.00E-07	4.62E-05	5.08E-03	
ym-54	ce	860.0	42	ca	- 75	1.00E-07	6.82E-06	5.86E-03	
ym-54	ce	540.0	42	ca	75-500	1.00E-07	1.07E-05	5.79E-03	
ym-54	ce	970.0	84	ca	- 75	1.00E-07	6.06E-06	5.88E-03	
ym-54	ce	490.0	84	ca	75-500	1.00E-07	1.18E-05	5.76E-03	
ym-54	ce	110.0	21	air	-106	9.00E-07	4.15E-04	4.57E-02	
ym-54	ce	180.0	21	air	106-500	9.00E-07	2.70E-04	4.86E-02	
ym-54	ce	170.0	42	air	-106	9.00E-07	2.84E-04	4.83E-02	
ym-54	ce	110.0	42	air	106-500	9.00E-07	4.15E-04	4.57E-02	
ja-18	ce	40.0	14	air	106-150	9.00E-07	9.00E-04	3.60E-02	70
ja-18	ce	40.0	14	air	355-500	9.00E-07	9.00E-04	3.60E-02	70
ja-18	ce	36.0	21	air	106-150	9.00E-07	9.64E-04	3.47E-02	70
ja-18	ce	45.0	21	air	355-500	9.00E-07	8.31E-04	3.74E-02	70
ja-18	ce	46.0	34	air	106-150	9.00E-07	8.18E-04	3.76E-02	70
ja-18	ce	40.0	35	air	355-500	9.00E-07	9.00E-04	3.60E-02	70
ja-18	ce	51.0	63	air	106-150	9.00E-07	7.61E-04	3.88E-02	70
ja-18	ce	42.0	63	air	355-500	9.00E-07	8.71E-04	3.66E-02	70
ja-32	ce	53.0	7	air	106-150	1.00E-06	8.22E-04	4.36E-02	70
ja-32	ce	51.0	7	air	355-500	1.00E-06	8.45E-04	4.31E-02	70
ja-32	ce	64.0	14	air	106-150	1.00E-06	7.14E-04	4.57E-02	70
ja-32	ce	61.0	14	air	355-500	1.00E-06	7.41E-04	4.52E-02	70
ja-32	ce	64.0	28	air	106-150	1.00E-06	7.14E-04	4.57E-02	70
ja-32	ce	130.0	28	air	355-500	1.00E-06	4.00E-04	5.20E-02	70
ja-32	ce	67.0	56	air	106-150	1.00E-06	6.90E-04	4.62E-02	70
ja-32	ce	170.0	56	air	355-500	1.00E-06	3.16E-04	5.37E-02	70

Appendix B

A Fortran 77 Computer Program Named SOSCOCO

The SOSCOCO program operates in three sequential subroutines:

1. GET - Data are sorted from a workable data base in accordance with desired combinations, e.g., size.
2. AN - Isotherms are fitted to the same data sets by linear regressional analysis; empirical constants, correlation coefficients, and standard errors are estimated.
3. MAP - Raw data sets and those predicted from isotherms are graphed by this subroutine. Predicted versus observed amounts adsorbed are also plotted.

Table B-I

Subroutine GET

```
      Program getdata

*****************************************************************************
*                                                                           *
*     Algorithm by Hector R. Fuentes                                        *
*     Program by Jan Gorlitz with additions and revisions by Bernie Lauctes.  *
*                                                                           *
*     This program sorts data according to user inputs from the terminal.   *
*     The output is in file data6.dat which is the input for ANALYSIS.FOR.  *
*                                                                           *
*****************************************************************************

      character*2 t,time
      character*2 el,element
      character*3 atm,ambient,size,temp,temper
      character*7 ssize(13)
      character*8 samp,sample(20)
      character*14 rc(2000),rcc
      character*48 ra(2000),raa
      dimension rb(2000)
c
c  gather parameters to search on from users
c
      call getinfo(sample,element,time,ambient,ssize,temper)
c
c  search input file - pull out data meeting criteria
c
      call search1(7,8,'el',element,'inc.dat','data1.dat')
      call search2(8,9,'samp',sample,'data1.dat','data2.dat')
      call search1(9,10,'temp',temper,'data2.dat','data3.dat')
      call search2(10,11,'t',time,'data3.dat','data4.dat')
      call search1(11,12,'atm',ambient,'data4.dat','data5.dat')
      call search2(12,13,'size',ssize,'data5.dat','data6.dat')
c
c  write out data for mapper file
c
      n=0
      i=1

      open(13,file='data6.dat',status='old')
   23 read(13,100,end=11)raa,rbb,rcc
      ra(i)=raa
      rb(i)=rbb
      rc(i)=rcc
  100 format(a48,1pe10.2,a14)
      n=n+1
      i=i+1
      go to 23
   11 call sort(n,ra,rb,rc)
      rewind 13
      do 20 j=1,n
      write(13,100)ra(j),rb(j),rc(j)
   20 continue
      end

      subroutine getinfo(sample,element,time,ambient,ssize,temper)
```

```
c
c  subroutine written to accept information from user
c
      character*8 sample(20)
      character*3 time(3),ambient,temper
      character*7 ssize(13)
      character*2 element
c
c  prompt user for data
c
      write(6,*)'ELEMENT:'
      read(5,10)element
10    format(a2)
      write(6,*)'SAMPLE: (up to 5)'
      do 12 i = 1,20
        read(5,20)sample(i)
20      format(a8)
        if(sample(i).eq.' ')goto 100
12     continue
100   write(6,*)'ENTER TEMPERATURE: (70,ambient(cr),or both)'
      read(5,21)temper
      write(6,*)'TIME: (up to 3 or all)'
      do 14 i = 1,3
        read(5,21)time(i)
21      format(a3)
        if(time(i).eq.' ')goto 200
14    continue
200   write(6,*)'ATMOSPHERE: (air,ca or both)'
      read(5,21)ambient
      write(6,*) 'SIZE: (up to 10)'
      do 16 i= 1,13
        read(5,22)ssize(i)
22       format(a7)
        if (ssize(i).eq.' ') goto 300
16    continue
      write(6,*)'i just finished size'
300   continue
      return
      end
      subroutine search1(unitin,unitout,field1,field2,infile,outfile)
      integer*2 unitin,unitout
      character*8 samp,sample(20)
      character*10 el,element
      character*2 t,time
      character*3 atm,ambient,temp,temper
      character*7 size,ssize
      character*(*) field1,field2
      character*9 files(10)
      character*10 ch(3)
      open(unit=unitin,file=infile,status='old')
      open(unit=unitout,file=outfile,status='new')
      if(field1.eq.'el')then
        ipt=1
      else if(field1.eq.'atm')then
        ipt=2
      else if(field1.eq.'temp')then
116     ipt = 3
```

```
      endif
      do i = 1,2000
        read(unitin,20,end=200)samp,ch(1),rf,t,ch(2),size,co,c,s,ch(3)
        if(field2.eq.'bot')write(unitout,20)samp,ch(1),rf,t,ch(2),
     1 size,co,c,s,ch(3)
        if(field2.eq.ch(ipt))write(unitout,20)samp,ch(1),rf,t,ch(2),
     1  size,co,c,s,ch(3)
20      format(a9,1x,a2,1x,f8.1,1x,a3,1x,a3,1x,a7,1x,1pe10.2,
     1  e10.2,e10.2,1x,a2)
      enddo
200       continue
      close(unit=unitout)
      close(unit=unitin)
      return
      end
      subroutine search2(unitin,unitout,field1,field2,infile,outfile)
      integer*2 unitin,unitout
      character*8 samp,sample(20)
      character*10 el,element
      character*2 t,time
      character*3 atm,ambient,ite
      character*7 size,ssize
      character*(*) field1,field2(*)
      character*9 files(10)
      character*13 ch(3)
      open(unit=unitin,file=infile,status='old')
      open(unit=unitout,file=outfile,status='new')
20      format(1x,a8,1x,a2,1x,f8.1,2x,a2,1x,a3,1x,a7,1x,1pe10.2,
     1  e10.2,e10.2,1x,a2)
      if(field1.eq.'samp')then
        ipt=1
      else if(field1.eq.'t')then
        ipt=2
      else if(field1.eq.'size')then
        ipt=3
      endif
      do i = 1,2000
        read(unitin,20,end=200)ch(1),el,rf,ch(2),atm,ch(3),co,c,s,ite
        if(field2(1).eq.'all')then
          write(unitout,20)ch(1),el,rf,ch(2),atm,ch(3),co,c,s,ite
          goto 100
        endif
        do j=1,10
          if(field2(j) .eq. ' ')goto 100
          if(field2(j)(3:3).eq.' '.and.field1.eq.'samp')then
            k = 1
            k1 =2
            k2=3
            if(field2(j)(k:k).eq.ch(ipt)(k:k).and.
     1        field2(j)(k1:k1).eq.ch(ipt)(k1:k1))then
              write(unitout,20)ch(1),el,rf,ch(2),atm,ch(3),co,c,s,ite
            endif
          elseif(field2(j).eq.ch(ipt))then
              write(unitout,20)ch(1),el,rf,ch(2),atm,ch(3),co,c,s,ite
          endif
      enddo
```

```
100   continue
      enddo
150   continue
200   continue
      close(unit=unitout)
      close(unit=unitin)
      return
      end
      subroutine sort(n,ra,rb,rc)
      character*48 ra(n),rra
      character*14 rc(n),rrc
      dimension rb(n)
      l=n/2+1
      ir=n
   10 continue
      if (l.gt.1)then
      l=l-1
      rra=ra(l)
      rrb=rb(l)
      rrc=rc(l)
      else
      rra=ra(ir)
      rrb=rb(ir)
      rrc=rc(ir)
      ra(ir)=ra(1)
      rb(ir)=rb(1)
      rc(ir)=rc(1)
      ir=ir-1
      if (ir.eq.1) then
      ra(1)=rra
      rb(1)=rrb
      rc(1)=rrc
      return
      endif
      endif
      i=l
      j=l+1
   20 if (j.le.ir)then
      if (j.lt.ir)then
      if (rb(j).lt.rb(j+1))j=j+1
      endif
      if (rrb.lt.rb(j))then
      ra(i)=ra(j)
      rb(i)=rb(j)
      rc(i)=rc(j)
      i=j
      j=j+j
      else
      j=ir+1
      endif
      go to 20
      endif
      ra(i)=rra
      rb(i)=rrb
      rc(i)=rrc
```

```
go to 10
end
```

Table B-II

Subroutine AN

```
      PROGRAM ANALYSIS

*************************************************************************
*                                                                       *
*       Algorithm by: Hector R. Fuentes                                 *
*       Program by: Jan Gorlitz and Bernie Lauctes                      *
*                                                                       *
*       Program ANALYSIS.FOR uses sorption data and performs a linear   *
*       least squares analysis on four linear isotherm models to produce *
*       model constants, regression parameters, and the following sets of *
*       (x,y) data for plotting:                                        *
*                                                                       *
*                                (i) C vs S                             *
*                               (ii) log(C) vs log(S)                   *
*                              (iii) S vs Scalc                         *
*                               (iv) log(S) vs log(Scalc)               *
*                                                                       *
*       where S is the amount of solute adsorbed onto soil particles and *
*       C is the amount of solute in solution .  The four linear models are *
*       LINEAR, LANGMUIR, FREUNDLICH, and  MODIFIED FREUNDLICH.         *
*                                                                       *
*                                                                       *
*        ---------------------- INPUT INFORMATION ----------------------*
*                                                                       *
*        A typical line of input data is sorted by the GET.FOR program: *
*                                                                       *
*        SAMPLE ELEMENT RD     TI ATM  PART    INIT CONC      C         S *
*                                                                       *
*        ja-18    sr  19000.0  14 air 355-500   1.00E-06  2.10E-06  4.00E-02 *
*                                                                       *
*        where RD is the distribution coefficient, TI is contact time, ATM *
*        is atmospheric conditions, PART is particle size range, INIT CONC *
*        is the initial concentration.  Also needed is the cation exchange *
*        capacity for each mineral type.                                *
*                                                                       *
*                                                                       *
*        ---------------------- OUTPUT INFORMATION ---------------------*
*                                                                       *
*        Statistical information is in the STAT.DAT output file.        *
*                                                                       *
*        Mapper output is in the files out1.out, out2.out, out3.out, out4.out. *
*        They correspond to the four sets of (x,y) data shown above.    *
*                                                                       *
*************************************************************************

      character*1 ans
      character*2 el(nop)
      character*3 t(nop),atm(nop)
      character*7 size(nop),part(nop)
      character*8 samp(nop),sname(nop), filenm(4)
      dimension rf(nop),co(nop),c(nop),s(nop),cec(nop),cds(nop),a(nop)
      dimension xlgc(nop),xlgs(nop),q(nop),xlgcds(nop),xlgq(nop)
      dimension xlgscal(nop),xlgscl(nop),scalc(nop)
      dimension slcalc(nop),xlgscal(nop),logscl(nop),logscal(nop)
      data filenm/'out1.out','out2.out','out3.out','out4.out'/
      open(30,file='stat.dat')
```

```
c
c
c     ----- READ SORTED INPUT DATA -----
c
      call rddata(samp,el,rf,t,atm,size,co,c,s,kounter)
c
c
c     ----- TEST FOR LESS THAN (3) DATA LINES -----
c
      if(kounter.lt.3) then
         write(6,55)kounter
         go to 999
      endif
c
c
c     ----- CHOOSE AN AVERAGE CEC VALUE OR MINERAL-SPECIFIC CEC -----
c
    3 write(6,110)
      read(5,303)ans
      if(ans.eq.'a'.or.ans.eq.'A') then
        write(6,120)
        read(5,*)avgcec
         do 65 i=1,kounter
           cec(i)=avgcec
   65    continue
        go to 20
      elseif(ans.eq.'b'.or.ans.eq.'B') then
        continue
      else
        go to 3
      endif
c
c
c     ----- INITIALIZE MINERAL-SPECIFIC  CEC VALUES -----
c

      call addval(samp,size,s,kounter,cec,test)
      if(test.eq.1) go to 999
c
c
c     ----- CALCULATE NEEDED PARAMETERS -----
c
   20 call calcl(c,s,kounter,xlgc,xlgs,q,xlgcds,xlgq,cds,cec)
c
c
c     ----- CALCULATE MEANS OF NEEDED PARAMETERS -----
c
      call calcmn(cmean,smean,cdsm,xlgcm,xlgsm,qmean,xlgcdsm,xlgqm,
     1c,s,cds,xlgc,xlgs,q,xlgcds,xlgq,kounter)
c
c
c     ----- INITIALIZE OUTPUT FILES -----
c
      do i= 1,4
        unum = i+19
        open(unit=unum,file=filenm(i),status='new')
```

```
      enddo
c
c
c     ----- CREATE HEADING FOR STAT.DAT OUTPUT FILE -----
c
      write(30,250)el(1),samp(1),t(1),avgcec,size(1)
      write(30,260)
c
c
c     ----- WRITE RAW C AND S DATA TO THE (4) OUTPUT FILES -----
c
      do 10 i = 1,4
        unum = i + 19
        write(unum,*)kounter
   10   continue
        do 11  j = 1,kounter
           write(20,*)c(j),s(j)
            write(21,*)xlgc(j),xlgs(j)
            write(22,*)s(j),s(j)
            write(23,*)xlgs(j),xlgs(j)
   11   continue
c
c
c     ----- LINEAR LEAST SQUARES ANALYSIS ON THE (4) LINEAR MODELS -----
c
      do 200 i = 1,4
        if(i.eq.1)then
          call prompt1(cmean,smean,xp,yp)
        else
          call prompt2(xp,yp,i,cmean,cdsm,smean,xlgc,xlgs,q,
     1    xlgcm,xlgsm,xlgqm)
        endif
        if(i.eq.1)then
          call lstsq(s,c,xp,yp,kounter,alpha,beta,rsq,see)
          xkd = beta
          write(30,100)kounter,alpha,beta,rsq,see,xkd
         write(*,*)xkd,beta
          do 400 j = 1,kounter
            scalc(j) = xkd*c(j) + alpha
            xlgscal(j) = alog10(scalc(j))
            write(20,*)c(j),scalc(j)
            write(21,*)xlgc(j),xlgscal(j)
            write(22,*)s(j),scalc(j)
            write(23,*)xlgs(j),xlgscal(j)
  400     continue
        else if (i.eq.2)then
          call lstsq(cds,c,xp,yp,kounter,alpha,beta,rsq,see)
          b = 1/beta
          xk = 1/(alpha*b)
          write(30,210)kounter,alpha,beta,rsq,see,b,xk
          write(*,*)b,xk
          do 500 j = 1,kounter
            slcalc(j) = (xk*b*c(j))/(1+xk*c(j))
            xlgscal(j) = alog10(slcalc(j))
            write(20,*)c(j),slcalc(j)
            write(21,*)xlgc(j),xlgscal(j)
```

```
          write(22,*)s(j),slcalc(j)
          write(23,*)xlgs(j),xlgscal(j)
 500      continue
        else if (i.eq.3)then
          call lstsq(xlgs,xlgc,xp,yp,kounter,alpha,beta,rsq,see)
          xn = beta
          xk = 10.**alpha
          write(30,220)kounter,alpha,beta,rsq,see,xk,xn
       write(*,*)xn,xk
          do 600 j=1,kounter
            slcalc(j) = xk*(c(j)**xn)
            xlgscal(j) = alog10(slcalc(j))
            write(20,*)c(j),slcalc(j)
            write(21,*)xlgc(j),xlgscal(j)
            write(22,*)s(j),slcalc(j)
            write(23,*)xlgs(j),xlgscal(j)
 599      continue
 600      continue
        elseif (i.eq.4)then
          call lstsq(xlgq,xlgc,xp,yp,kounter,alpha,beta,rsq,see)
          b = beta
      do 12 ii=1,kounter
          a(ii) =cec(ii)*(10.**alpha)
  12 continue
          xkd = (10**alpha)**(1/b)
          write(30,230)kounter,alpha,beta,rsq,see,a(1),b,xkd
          do 700 j=1,kounter
           slcalc(j) = (a(j)*c(j)**b)/(1+(a(j)*c(j)**b/cec(j)))
            xlgscal(j) = alog10(slcalc(j))
            write(20,*)c(j),slcalc(j)
            write(21,*)xlgc(j),xlgscal(j)
            write(22,*)s(j),slcalc(j)
            write(23,*)xlgs(j),xlgscal(j)
 700      continue
        endif
 200 continue
c
c
 250 format(///,35x,'ELEMENT    = ',A2,/,
    135x,'SAMPLE     = ',a8,/,
    235x,'TIME       =',A3,' days',/
    335x,'ATMOS      = Air',/
    435X,'CEC        =',f6.0,' micromol (p+)/g',/,
    435x,'SIZE       = ',a7,'microns',/)
 260 format(7x,'=================================================
    1================',/,
    17x,' ISOTHERM',7X,'n',10X,'ALPHA',9X,'BETA',8X,'R**2',6X,
    1'SSE',/,
    17x,'=================================================
    2=========',//)
 280 format(7x,'=================================================
    1================')
 100 format(7x,' LINEAR     ',I6,3X,2F14.7,f9.4,1x,F12.8,//,
    17x,' Kd = ',f16.8,///)
 210 format(7x,' LANGMUIR   ',I6,3X,2F14.7,f9.4,1x,F12.8,//,
    17x,'  b = ',f16.8,/,
```

```
   27x,'  k = ',f16.8,///)
220 format(7x,' FREUNDLICH',I6,3X,2F14.7,f9.4,1x,F12.8,//,
   17x,'  K = ',f16.8,/,
   27x,'  N = ',f16.8,//)
230 format(7x,' MODIFIED  ',I6,3X,2F14.7,f9.4,1x,F12.8,/,
   17x,' FREUNDLICH',//,
   27x,'  A = ',f16.8,/,
   37x,'  B = ',f16.8,/,
   47x,' KD = ',f16.8,//)
    write(30,280)
    write(30,290)
290 format(7x,' n = the number of experimental points',/,
   17x,' ALPHA and BETA are respectively the intercept and slope
   1 from',/,8x,' the linear regression analysis',/,
   17x,' R**2 = correlation coefficient',/
   27x,' SSE  = standard error',/,
   37x,' Kd in mL/g',/,
   47x,' b in micromol(p+)/g and k in mL/micromol(p+) ',/,
   57x,' K,N,A,B and KD in units corresponding to solute adsorbed
   6 S in',/,
   67x,'  micromol(p+)/g and solute in solution C in micro
   7mol(p+)/mL.')
 55 format(9x,'**********',//,'  THERE ARE ONLY',I2,' DATA POINTS',//,
   1'   A MINIMUM OF 3 IS REQUIRED ',//,9X,'**********')
110 format(///,' CATION EXCHANGE CAPACITY :',//,10x,
   1' (A)  DO YOU WANT TO USE AN AVERAGE CEC FOR ALL OF THE DATA',//,
   210X,' (B)  OR USE THE CEC UNIQUE TO EACH MINERAL AND SIZE RANGE?',
   3//,'   A or B',//)
120 format(' ENTER AVERAGE CEC VALUE :',//)
303 format(al)
999 end
    subroutine rddata(samp,el,rf,t,atm,size,co,c,s,kounter)
    dimension rf(*),co(*),c(*),s(*)
    character*(*) samp(*),t(*),atm(*),size(*)
    character*(*) el(*)
    open(unit=7,file = 'data6.dat',status='old')
    i=1
    do 11 i = 1,2000
      read(7,10,end=200)samp(i),el(i),rf(i),t(i),
   1  atm(i),size(i),co(i),c(i),s(i)
 10   format(a9,1x,a2,1x,f8.1,1x,a3,1x,a3,1x,a7,1x,1pe10.2,
   1  e10.2,e10.2)
 11  continue
200 continue
    kounter = i -1
    return
    end
    subroutine addval(samp,size,s,kounter,cec,test)
    character*8 sname(2000),tsamp
    character*(*) samp(*)
    character*7 part(2000),tsize
    character*(*) size(*)
    character*1 ans
    dimension s(*)
    dimension cec(kounter),val(2000)
    itest=kounter
```

```
      open(unit=8,file='cec.dat',status='old')
      read(8,*) ncec
      do 20 i = 1,ncec
        read(8,10)sname(i),part(i),val(i)
 10     format(a8,a7,f10.2)
 20   continue
      do 30 j=1,kounter
      do 40 k=1,ncec
      if(sname(k).eq.samp(j)) go to 2
 40   continue
  2   if(part(k).eq.size(j)) cec(j)=val(k)
 30   continue
      do 50 i = 1,kounter
        if(cec(i).eq.0.0)then
          write(6,300)samp(i),size(i),s(i)
          read(5,303)ans
             if(ans.eq.'y'.or.ans.eq.'Y') then
                 write(6,*)' ENTER CEC VALUE NOW:'
                 read(5,*)cec(i)
             else
               test=1
               go to 66
             endif
        elseif (cec(i).lt.s(i))then
          write(6,301)samp(i),size(i),s(i)
          read(5,303)ans
            if(ans.eq.'y'.or.ans.eq.'Y')then
              write(6,*)' ENTER CEC VALUE NOW:'
              read(5,*)cec(i)
              write(6,304)
              read(5,303)ans
                if(ans.eq.'y'.or.ans.eq.'Y') then
                  tcec=cec(i)
                  tsamp=samp(i)
                  tsize=size(i)
                  call newcec(samp,size,tcec,tsamp,tsize,itest,cec)
                else
                   continue
                 endif
           else
             test=1
             go to 66
            endif
        else
          continue
        endif
 50   continue
300     format(///' NO CATION EXCHANGE CAPACITY (CEC) FOR :',//,
   12x,a8,a7,' S =',1pe10.2,//,' IN THE FILE: CEC.DAT',//,
   2'  DO YOU WANT TO ENTER A CEC VALUE?')
301     format(///,' THE CATION EXCHANGE CAPACITY (CEC) FOR: ',//,
   12X,A8,A7,7x,'S =',1pe10.2,//,
   2' IS LESS THAN THE AMOUNT SORBED ON THE SOIL.',//,
   4' DO YOU WANT TO ENTER A CEC VALUE?')
303     format(a1)
304 format(' DO YOU WANT ALL OF THE CEC"S FOR THIS PARTICULAR',/,
```

```
  1' MINERAL AND SIZE TO BE CHANGED TO THE NEW CEC?')
66 return
   end
   subroutine calcl(c,s,n,xlgc,xlgs,q,xlgcds,xlgq,cds,cec)
   dimension c(*),s(*),xlgc(*),xlgs(*),q(*),xlgcds(*),xlgq(*),
  1cec(*),cds(*)
   do 10 i = 1,n
     cds(i)= c(i)/s(i)
     xlgc(i) = alog10(c(i))
     xlgs(i) = alog10(s(i))
     xlgcds(i) = alog10(cds(i))
     q(i) = s(i)/(cec(i)-s(i))
     xlgq(i) = alog10(q(i))
10 continue
   return
   end
   subroutine calcmn(cmean,smean,cdsm,xlgcm,xlgsm,qmean,
  1xlgcdsm,xlgqm,c,s,cds,xlgc,xlgs,q,xlgcds,xlgq,kounter)
   cmean = amean(c,kounter)
   smean =amean(s,kounter)
   cdsm =amean(cds,kounter)
   xlgcm =amean(xlgc,kounter)
   xlgsm =amean(xlgs,kounter)
   qmean =amean(q,kounter)
   xlgcdsm =amean(xlgcds,kounter)
   xlgqm =amean(xlgq,kounter)
   return
   end
   subroutine promptl(cmean,smean,xp,yp)
   character*1 answer
 1 write(6,11)
11 format(//,'    1.  PERFORM A NORMAL LEAST SQUARES FIT FOR THE'/
  1'        LINEAR MODEL, THROUGH THE ORIGIN (ALPHA = 0)?'//
  1'    2.  FORCE THE FIT THROUGH A POINT OTHER'/
  1'        THAN (0,0)? (ALPHA <> 0)'//
  1'    3.  FORCE THE FIT THROUGH AN ARBITRARY C AND S?')
   read(5,10)answer
10 format(a1)
   if(answer.eq.'1')then
     xp = 0.0
     yp = 0.0
   else if(answer.eq.'2')then
     write(6,22)
22   format(//' ENTER X:')
     read(5,*)xp
     write(6,*)' ENTER Y: '
     read(5,*)yp
   else if(answer.eq.'3')then
     xp = cmean
     yp = smean
    else
      go to 1
   endif
    return
   end
```

```
      subroutine prompt2(xp,yp,i,cmean,cdsm,smean,xlgc,xlgs,q,
     1xlgcm,xlgsm,xlgqm)
      character*1 ans
    1 if(i.eq.2) write(6,*)'                    LANGMUIR MODEL'
      if(i.eq.3)write(6,*)'                 FREUNDLICH MODEL'
      if(i.eq.4)write(6,*)'                 MODIFIED FREUNDLICH'
      write(6,10)
   10 format(//,'    1.  NORMAL FIT THROUGH THE THROUGH THE MEAN OF S AND
     1 AND C?'//
     1'    2.  DO YOU WANT TO FORCE THE FIT THROUGH AN ARBITRARY POINT
     1 (C,S)?')
      read(5,11)ans
   11 format(a1)
      if(ans.eq.'1')then
        if(i.eq.2)then
          xp = cmean
          yp = cdsm
        else if(i.eq.3)then
          xp = xlgcm
          yp = xlgsm
        else if(i.eq.4)then
          xp = xlgcm
          yp = xlgqm
        write(*,*)xp,yp
        endif
      else if(ans.eq.'2')then
        write(6,20)
   20   format(//,' ENTER X-VALUE:')
        read(5,*)xp
        write(6,22)
   20  format(//,' ENTER Y-VALUE:')
        read(5,*)yp
      else
        go to 1
      endif
      return
      end
      subroutine lstsq(y,x,xp,yp,n,alpha,beta,rsq,see)
      dimension x(2000),y(2000)
      sumxy = 0.0
      sumx2 = 0.0
      sumy2 = 0.0
      sumse = 0.0
      do 4 i = 1,n
        sumxy = sumxy+(x(i)*y(i))
        sumx2 = sumx2 + x(i)**2.
        sumy2 = sumy2+y(i)**2.
    4 continue
      b1 = (sumxy) - (n*xp*yp)
      b2 = (sumx2) - (n*xp**2)
      beta = b1/b2
      alpha = yp - beta*xp
      r1 = sumxy - (xp*yp*n)
      r2 = sumx2 - (n*xp**2)
      r3 = sumy2 - (n*yp**2)
      r=r1/((r2*r3)**.5)
```

```
      rsq=r**2
         write(*,*)r,rsq
      s1 = sumy2 - n*yp**2.
      s2 = sumxy - n*xp*yp
      see =(((s1-beta*s2)/(n-2.))**.5)
      return
      end
      function amean(a,n)
      dimension a(*)
      asum = 0.0
      do 10 i=1,n
        asum = asum+a(i)
   10 continue
      amean = asum/n
      return
      end
      subroutine newcec(samp,size,tcec,tsamp,tsize,itest,cec)
      character*7 size(2000),tsize
      character*8 samp(2000),tsamp
      dimension cec(2000)
      do 60 l=1,itest
       if(samp(l).eq.tsamp) then
            go to 2
         else
           go to 60
                 endif
    2  if(size(l).eq.tsize) then
             cec(l)=tcec
       else
         go to 60
         endif
   60 continue
      return
      end
```

Table B-III

Subroutine MAP

```
      PROGRAM MAPPER

*****************************************************************************
*                                                                           *
*     Algorithm by Hector R. Fuentes                                        *
*     Program by Bernie Lauctes                                             *
*                                                                           *
*     This program accepts four output files generated by ANALYSIS.FOR and  *
*     creates four MAPPER files which use DISSPLA.                          *
*                                                                           *
*****************************************************************************

      DIMENSION C(2000),S(2000)
      CHARACTER*7 TITLE
      CHARACTER*72 T1,T2

      OPEN(10,FILE='OUT1.OUT',STATUS='OLD')
      OPEN(11,FILE='OUT2.OUT',STATUS='OLD')
      OPEN(12,FILE='OUT3.OUT',STATUS='OLD')
      OPEN(13,FILE='OUT4.OUT',STATUS='OLD')

      OPEN(14,FILE='OUT1.MAP',STATUS='NEW')
      OPEN(15,FILE='OUT2.MAP',STATUS='NEW')
      OPEN(16,FILE='OUT3.MAP',STATUS='NEW')
      OPEN(17,FILE='OUT4.MAP',STATUS='NEW')

      XMIN=-10.0
      IXTIC=2
      IXMAX=2
      YMIN=-10.0
      IYTIC=2
      IYMAX=2
      IPARAM=-1

      WRITE(6,*)' Enter mapper file title(up to 7 chars in length):'
      READ(5,100)TITLE
 100  FORMAT(A70)

      N=13

      DO 10 M=10,13

      READ(M,*)NOB
      N=N+1

      WRITE(N,110)TITLE
 110  FORMAT('NO DRAW',/
     1 'START',10X,A7,/,
     2 '0,100,5,110',/,
     3 'DUPLX',/,
     4 'NO DRAW',/,
     5 'BOX(50,65,70,70',/,
     6 'DRAW')


      IF(M.EQ.10.OR.M.EQ.12) THEN
         XMIN=0.0000001
```

```
        IXTIC=0
        IXMAX=9
        YMIN=0.0000001
        IYTIC=0
        IPARAM=1
        IYMAX=9
        GO TO 111
     ELSEIF(M.EQ.11.OR.M.EQ.13) THEN
         XMIN=-10.0
         IXTIC=2
         IXMAX=2
         YMIN=-10.0
         IYTIC=2
         IYMAX=2
         IPARAM=-1

          GO TO 111
      ENDIF
111   WRITE(N,120)XMIN,IXTIC,IXMAX,IPARAM
120   FORMAT('X-AXIS(',F14.9,',',I5,',',I15,',0,2.5,1,',I5,',2')
      WRITE(N,130)YMIN,IYTIC,IYMAX,IPARAM
130   FORMAT('Y-AXIS(',F14.9,',',I5,',',I15,',0,2.5,1,',I5,',2')

      IF(M.EQ.12) GO TO 20

      DO 30 J=1,5
      IF(J.EQ.1) THEN
        GO TO 1
      ELSE IF(J.EQ.2) THEN
        GO TO 2
      ELSE IF(J.EQ.3) THEN
        GO TO 3
      ELSE IF(J.EQ.4) THEN
        GO TO 4
      ELSE
        GO TO 5
      ENDIF

    1 WRITE(N,140)NOB
      GO TO 6
    2 WRITE(N,141)NOB
      GO TO 6
    3 WRITE(N,142)NOB
      GO TO 6
    4 WRITE(N,143)NOB
      GO TO 6
    5 WRITE(N,144)NOB

  140  FORMAT('PLOTIT(',I15,',-1,15')
  141  FORMAT('PATTERN(.5,.1',/,
     1 'PLOTIT(',I15)
  142  FORMAT('PATTERN(.1,.05',/,
     1 'PLOTIT(',I15)
  143  FORMAT('PATTERN(.5,.05,.1,.05,.1,.05,.1,.05',/,
     1 'PLOTIT(',I15)
  144  FORMAT('PATTERN(-.8,-.1,-.1,-.1,-.1,-.1',/,
```

```
     1 'PLOTIT(',I15)

   6  DO 40 I=1,NOB
      READ(M,*)C(I),S(I)
      WRITE(N,150)C(I),S(I)
 150  FORMAT(F20.10,',',F20.10)
  40  CONTINUE
  30  CONTINUE
      GO TO 10

  20  DO 35 J=1,5
      IF(J.EQ.1) THEN
        GO TO 11
      ELSE IF(J.EQ.2) THEN
        GO TO 22
      ELSE IF(J.EQ.3) THEN
        GO TO 33
      ELSE IF(J.EQ.4) THEN
        GO TO 44
      ELSE
        GO TO 55
      ENDIF

  11  WRITE(N,240)NOB
      GO TO 66
  22  WRITE(N,241)NOB
      GO TO 66
  33  WRITE(N,242)NOB
      GO TO 66
  44  WRITE(N,243)NOB
      GO TO 66
  55  WRITE(N,244)NOB

 240  FORMAT('*PLOTIT(',I15,',-1,15')
 241  FORMAT('*PATTERN(.5,.1',/,
     1 'PLOTIT(',I15,',-1,0')
 242  FORMAT('*PATTERN(.1,.05',/,
     1 'PLOTIT(',I15,',-1,1')
 243  FORMAT('*PATTERN(.5,.05,.1,.05,.1,.05,.1,.05',/,
     1 'PLOTIT(',I15,',-1,2')
 244  FORMAT('*PATTERN(-.8,-.1,-.1,-.1,-.1,-.1',/,
     1 'PLOTIT(',I15,',-1,3')

  66  DO 45 I=1,NOB
      READ(M,*)C(I),S(I)
      WRITE(N,250)C(I),S(I)
 250  FORMAT(F20.10,',',F20.10)
  45  CONTINUE
  35  CONTINUE
  10  CONTINUE

      WRITE(14,160)
 160  FORMAT('REVERT',/,
     1 'LABEL(1,2.6,50,17.5',/,
     2 'C (#M><EQ ML[+-1])>',/,
     3 'LABEL(1,2.6,1.78,65,,,90',/,
```

```
    4 'S (#M><EQ G[+-1]>)')


     WRITE(15,170)
170  FORMAT('REVERT',/,
    1 'LABEL(1,2.5,50,20',/,
    2 'C (<LOG >#M><EQ ML[+-1]>)',/,
    3 'LABEL(1,2.5,3,65,,,90',/,
    4 'S (<LOG >#M><EQ G[+-1]>)')


     WRITE(16,180)
180  FORMAT('REVERT',/,
    1 'LABEL(1,2.6,50,17.5',/,
    2 'S[-OBS] (#M><EQ G[+-1]>)',/,
    3 'LABEL(1,2.6,1.78,65,,,90',/,
    4 'S[-CALC] (#M><EQ G[+-1]>)')

     WRITE(17,190)
190  FORMAT('REVERT',/,
    1 'LABEL(1,2.5,50,20',/,
    2 'S[-OBS] (<LOG >#M><EQ G[+-1]>)',/,
    3 'LABEL(1,2.5,3,65,,,90',/,
    4 'S[-CALC] (<LOG >#M><EQ G[+-1]>)')

     DO 50 N=14,17

     IF(N.EQ.16) GO TO 60

     write(N,500)
500  FORMAT('LLABEL(1,-1.000,64.00,42.00,,,0.00',/,
    1'L<INEAR',/,
    1'LLABEL(1,-1.000,64.00,39.50,,,0.00',/,
    2'L<ANGMUIR',/,
    3'LLABEL(1,-1.000,64.00,37.00,,,0.00',/,
    4'F<REUNDLICH',/,
    5'LLABEL(1,-1.000,64.00,34.50,,,0.00',/,
    6'M<ODIFIED> F<REUNDLICH',/,
    7'PATTERN(.5,.1',/,
    8'LINE(51.052,46.559,1',/,
    9'61.820,46.559,1',/,
    2'50.913,46.559,2',/,
    3'PATTERN(.1,.05',/,
    4'LINE(50.913,43.819,1',/,
    5'61.682,43.819,2',/,
    5'PATTERN(.5,.05,.1,.05,.1,.05,.1,.05',/,
    6'LINE(61.682,41.217,1',/,
    7'50.913,41.217,2',/,
    8'PATTERN(-.8,-.1,-.1,-.1,-.1,-.1',/,
    9'LINE(50.913,38.612,1',/,
    1'61.820,38.612,2')


     GO TO 50

  60 WRITE(16,600)
```

```
600 FORMAT('LINE(77.084,92.188,1',/,
   1'15.013,29.843,2',/,
   2'PLOTIT(1,-1,0',/,
   3'61.45,42.0',/,
   4'PLOTIT(1,-1,1',/,
   5'61.45,39.5',/,
   6'PLOTIT(1,-1,2',/,
   7'61.45,37.0',/,
   8'PLOTIT(1,-1,3',/,
   9'61.45,34.5',/,
   2'LLABEL(1,-1.000,64.00,42.00,,,0.00',/,
   1'L<INEAR',/,
   1'LLABEL(1,-1.000,64.00,39.50,,,0.00',/,
   2'L<ANGMUIR',/,
   3'LLABEL(1,-1.000,64.00,37.00,,,0.00',/,
   4'F<REUNDLICH',/,
   5'LLABEL(1,-1.000,64.00,34.50,,,0.00',/,
   6'M<ODIFIED> F<REUNDLICH')
50   CONTINUE

    WRITE(6,*)'ENTER TITLE (2 LINES) :'
    READ(5,666)T1,T2
666 FORMAT(A72,/,A72)

    N=13

    DO 70 I=1,4
    N=N+1
    WRITE(N,67)T1,T2
 67 FORMAT('CLABEL(2,1.75,50.00,104.52',/,
   1A,/,A,/,
   2'END')
 70 CONTINUE
    END
```

Appendix C

Isotherms Modeling: Case 1

Appendix C is a compilation of modeling efforts for case 1. Results from this case are summarized in Tables V and VI in the main body of this report. The information for each data set is sequentially organized as follows:

1. A table with estimated constants and statistical parameters for each isotherm.
2. Curves of adsorbed concentration S [μmol(p+)/g] versus concentration in solution [μmol(p+)/mL] in a logarithmic scale. Both raw data and predictions by isotherms are included.
3. A graph with the calculated S-values versus observed S-values for all tested isotherms.

Tables and figures for the same data set are identified by the conditions defined in the table heading, which are also included in each figure in the same order but without units.

Units for constants are as follows: K_d in mL/g; b in μmol(p+)/g and k in mL/μmol(p+); K, N, A, β, and K_D have units corresponding to S in μmol(p+)/g and C in μmol/(p+)/mL.

The following table of contents serves as a guide to locate the sample, e.g., YM-22, and respective experimental conditions, e.g., 14 micromol (p+)/g for particle sizes less than 75 microns, that identify the set used for isotherm modeling.

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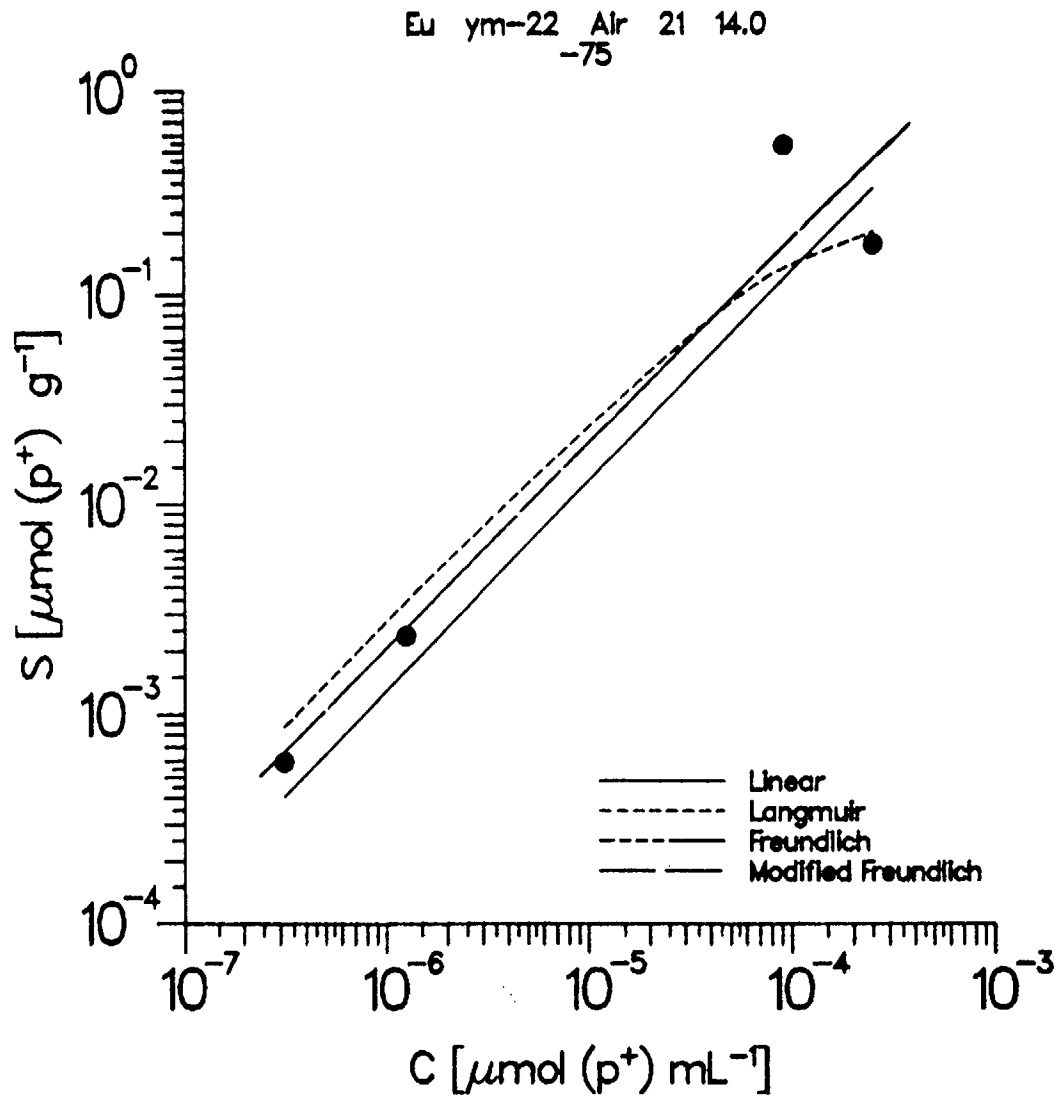
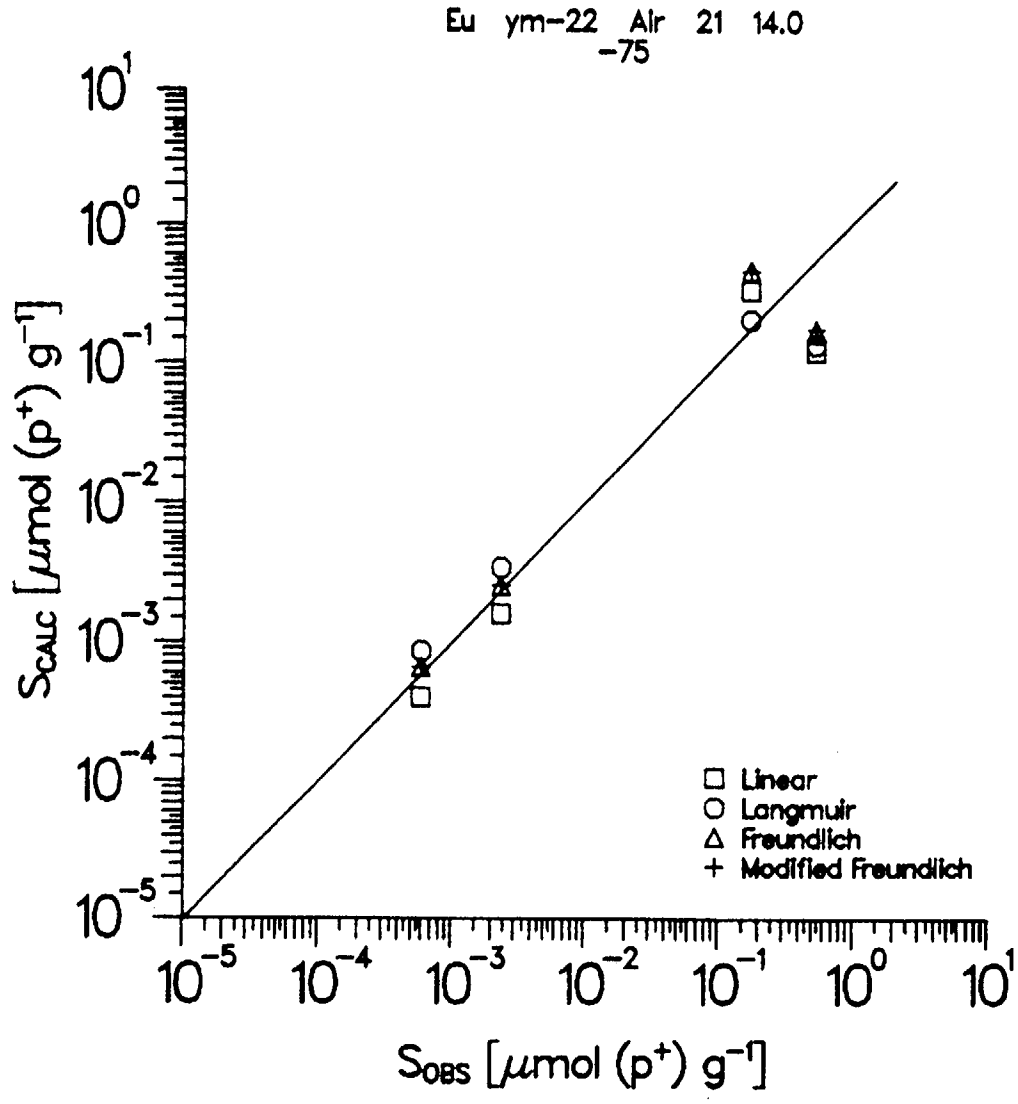
ELEMENT = Eu
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 14 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	1290.5809326	0.3805	0.31485751
Kd =	1290.58093262				
LANGMUIR	4	0.0003590	3.5612335	0.6034	0.00042234
b =	0.28080159				
k =	9919.87207031				
FREUNDLICH	4	3.1641402	0.9749284	0.9306	0.46074066
K =	1459.28540039				
N =	0.97492844				
MODIFIED FREUNDLICH	4	2.0439265	0.9789752	0.9293	0.46747187
A =	1549.01110840				
B =	0.97897518				
KD =	122.41162109				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

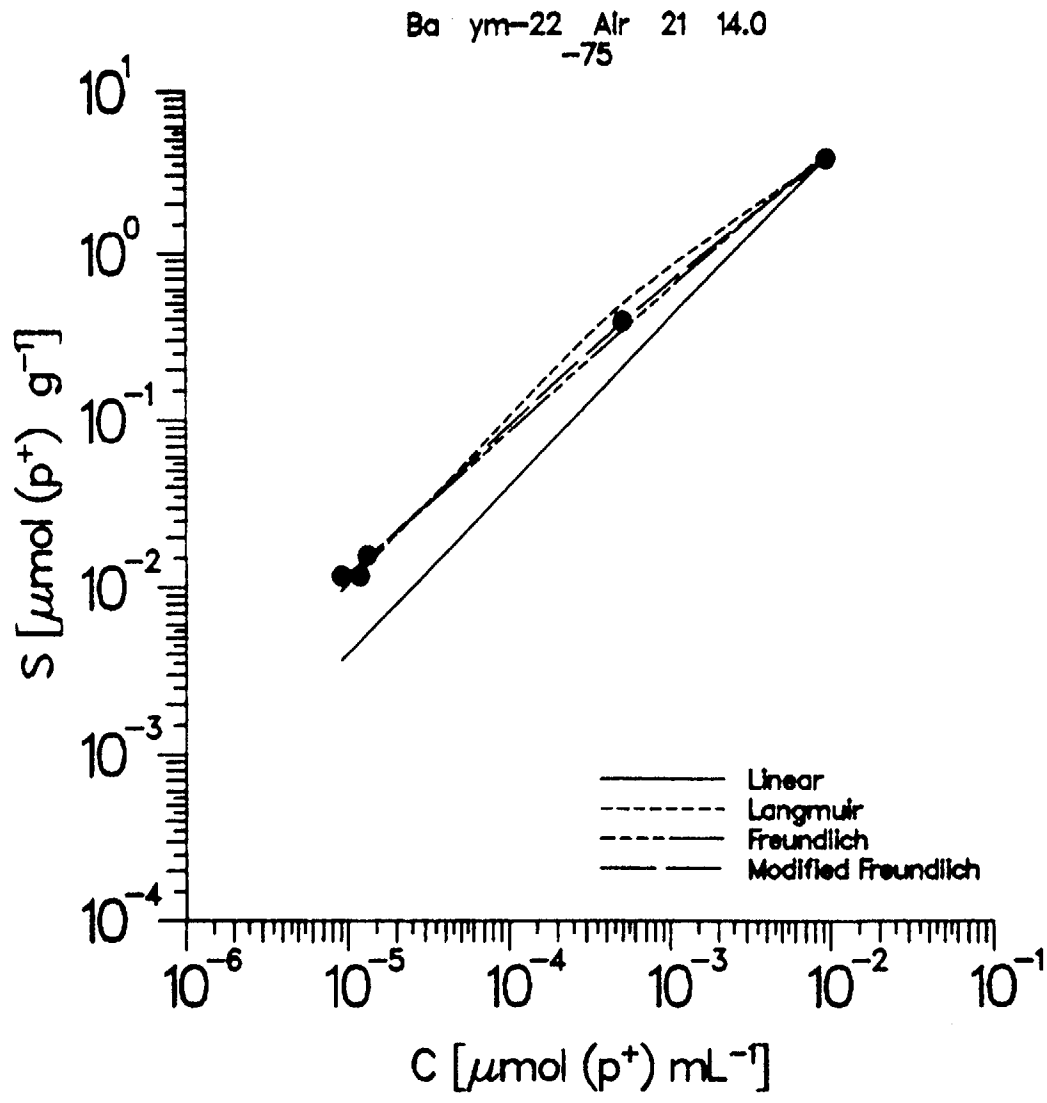

Eu ym-22 Air 21 14.0
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

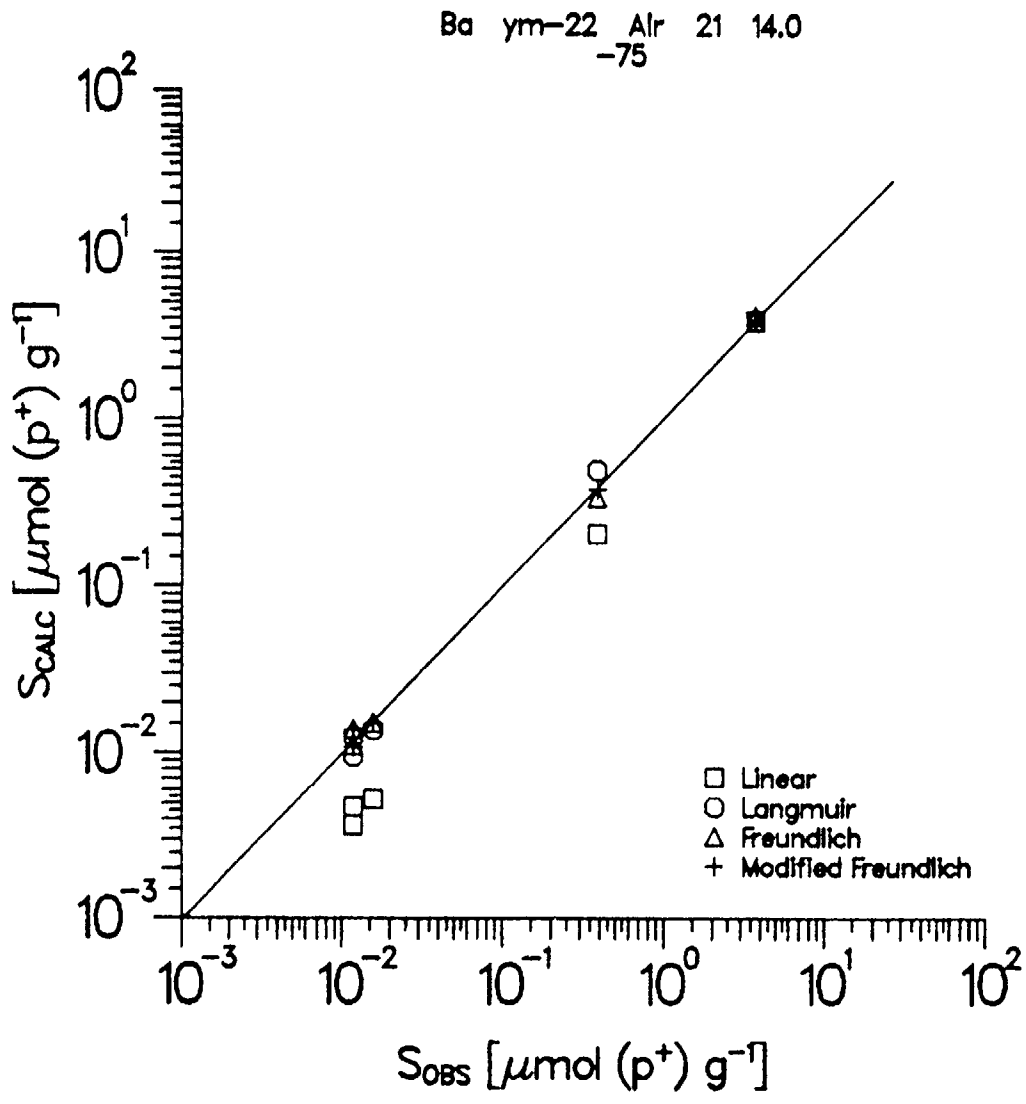

Eu ym-22 Air 21 14.0
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 14 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	401.2557068	0.9977	0.10683136
Kd =	401.25570679				
LANGMUIR	5	0.0009540	0.1638004	0.9366	0.00020671
b =	6.10499144				
k =	171.70465088				
FREUNDLICH	5	2.3308990	0.8501906	0.9981	0.05784982
K =	214.23922729				
N =	0.85019058				
MODIFIED FREUNDLICH	5	1.3763185	0.8901783	0.9990	0.04449347
A =	333.00170898				
B =	0.89017826				
KD =	35.16540146				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

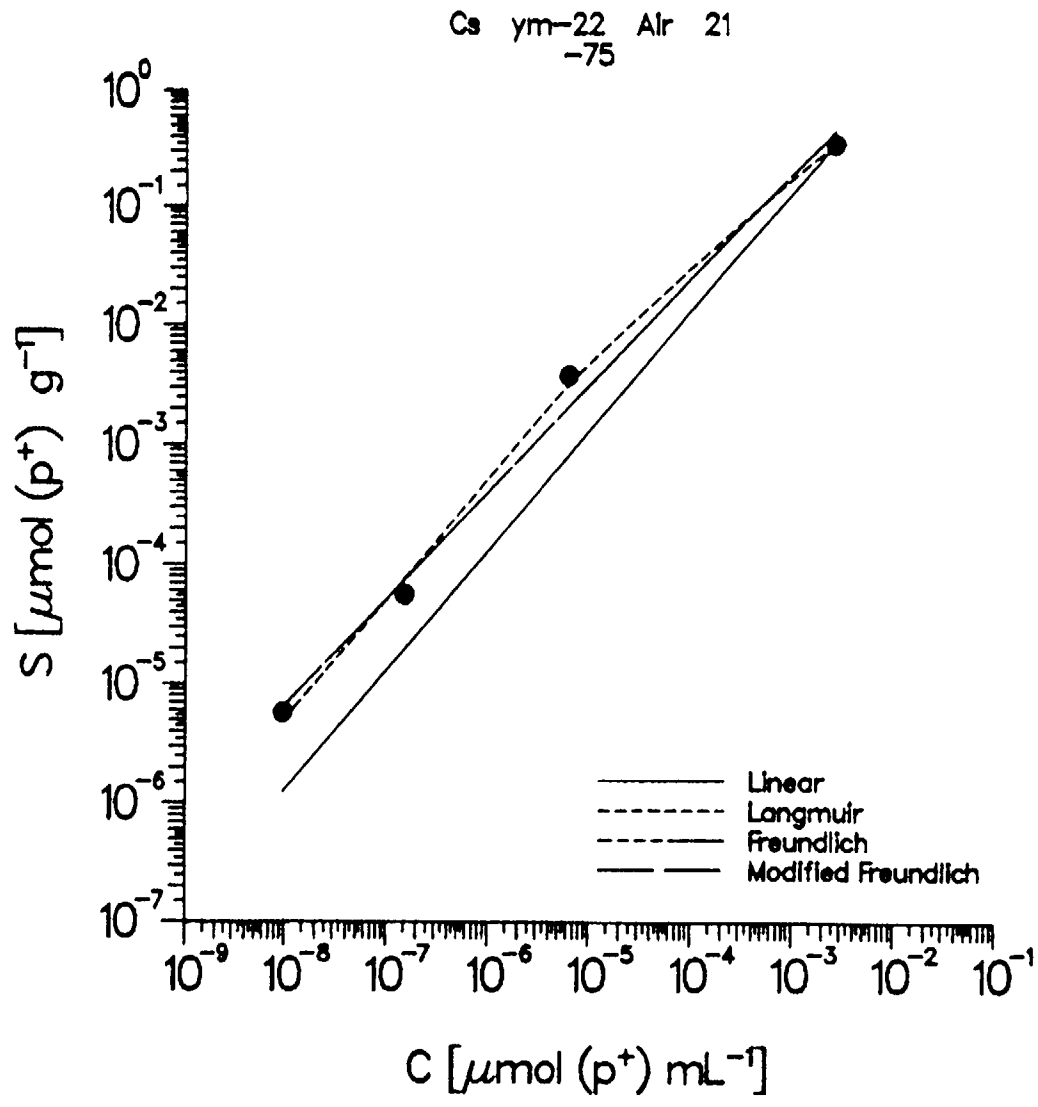

Ba ym-22 Air 21 14.0
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

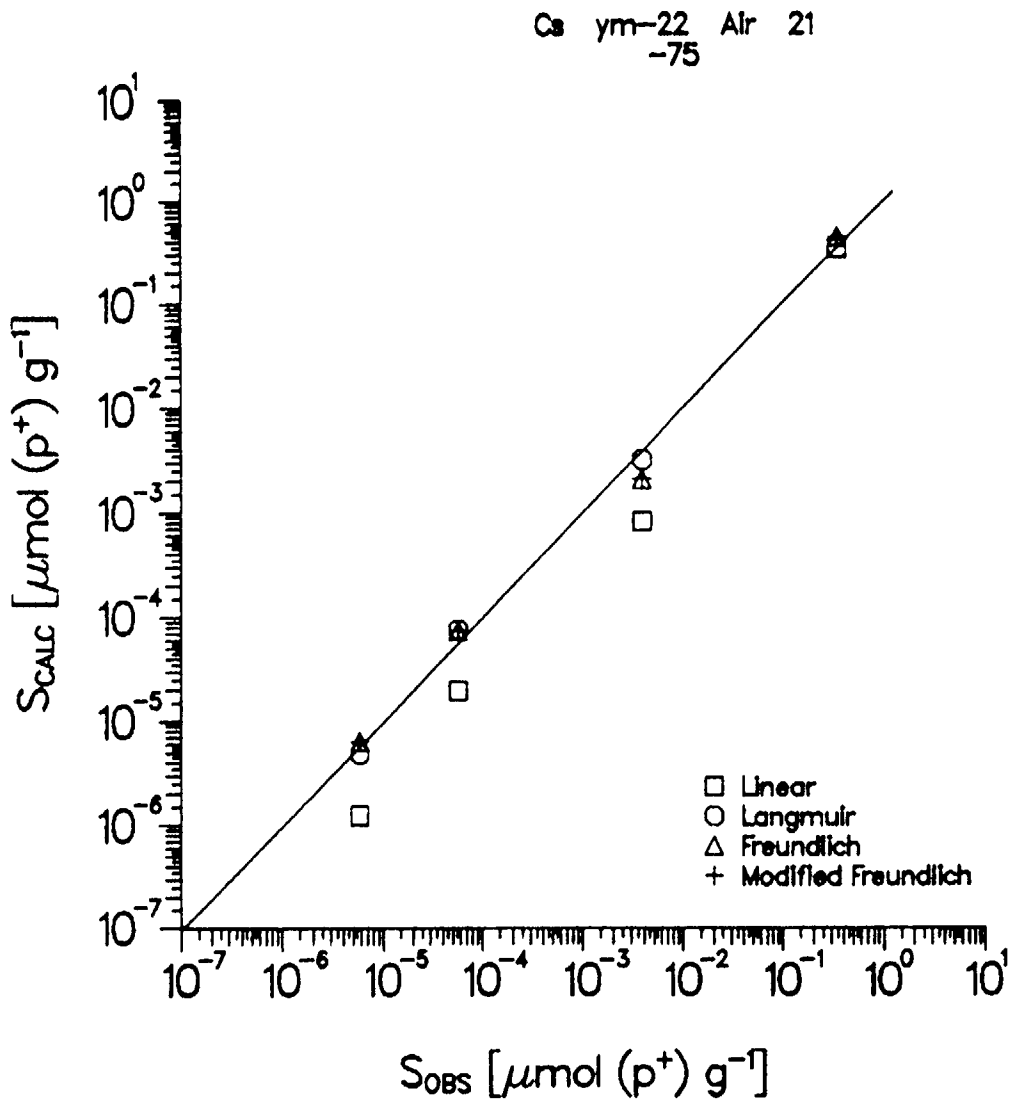

Ba ym-22 Air 21 14.0
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 14 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	129.9652557	0.9999	0.00215360
Kd =	129.96525574				
LANGMUIR	4	0.0019659	2.1452558	0.9737	0.00057645
b =	0.46614489				
k =	1091.22119141				
FREUNDLICH	4	1.9457891	0.8903023	0.9925	0.22379588
K =	88.26511383				
N =	0.89030230				
MODIFIED FREUNDLICH	4	0.8138189	0.8923191	0.9927	0.22110786
A =	91.18994904				
B =	0.89231908				
KD =	8.16632748				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

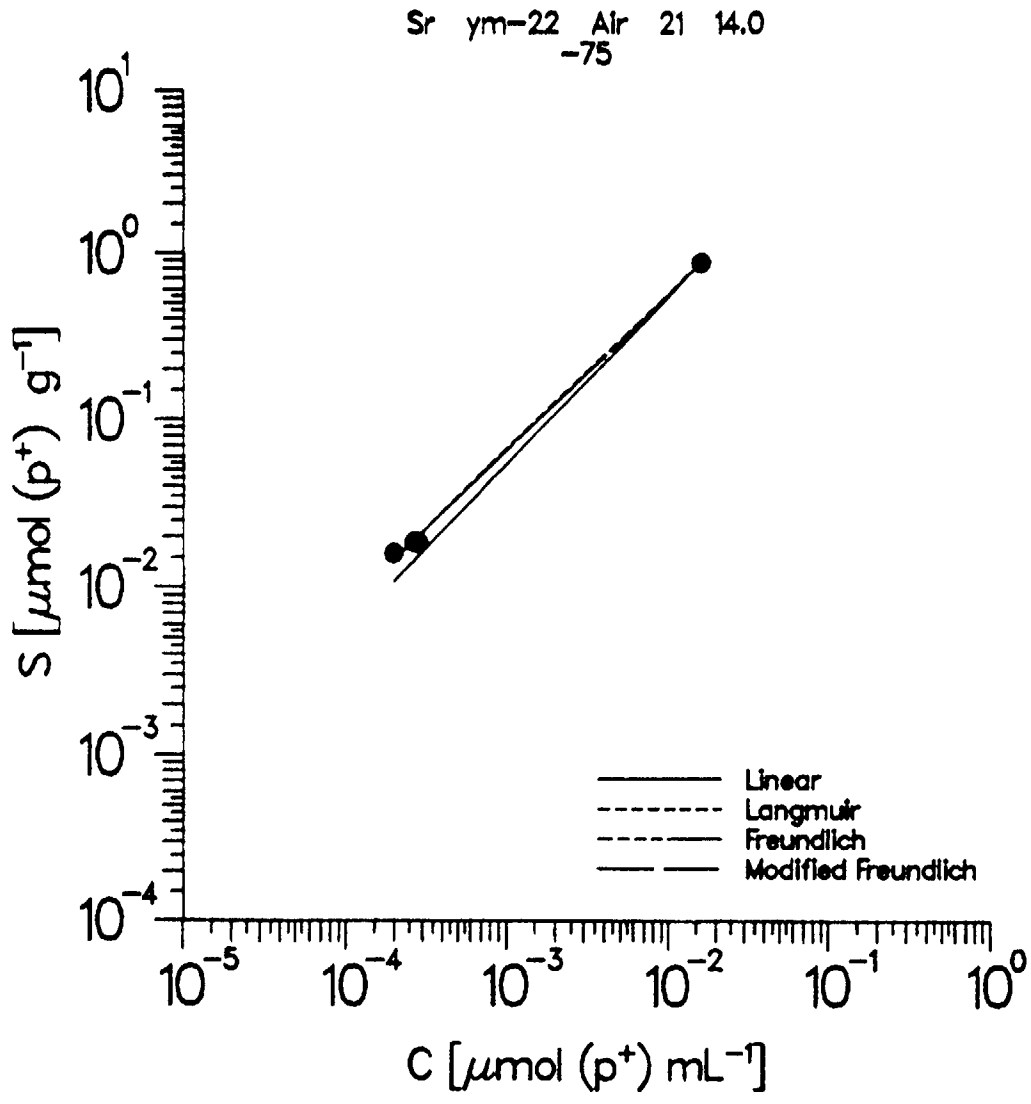

Cs ym-22 Air 21
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

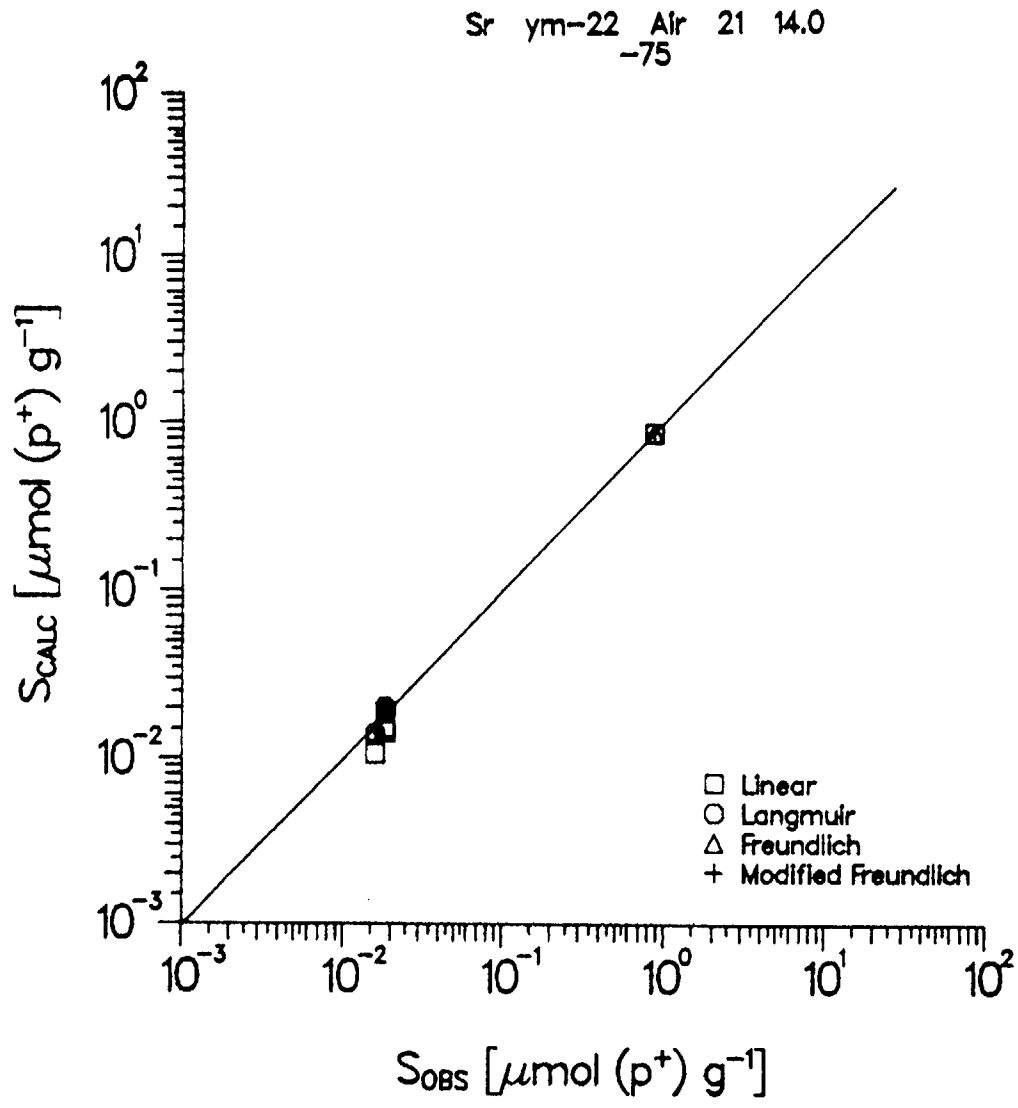

Cs ym-22 Air 21
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 14 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	54.0857773	0.9999	0.00529847
Kd =	54.08577728				
LANGMUIR	4	0.0139199	0.2828040	0.7761	0.00148362
b =	3.53601766				
k =	20.31651306				
FREUNDLICH	4	1.6035200	0.9297567	0.9984	0.04173877
K =	40.13470078				
N =	0.92975670				
MODIFIED FREUNDLICH	4	0.5122929	0.9448073	0.9983	0.04290767
A =	45.54292297				
B =	0.94480729				
KD =	3.48513317				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

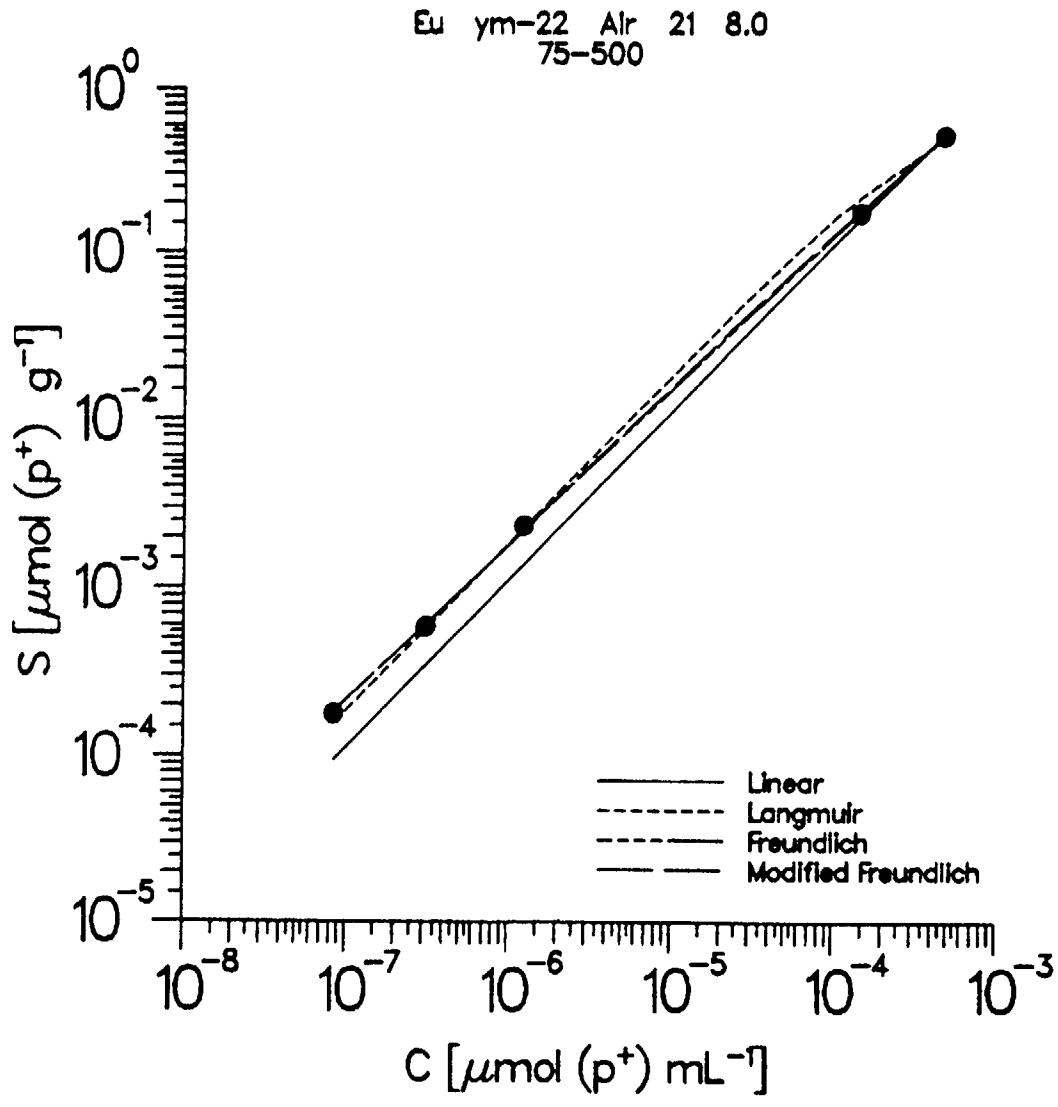

Sr ym-22 Air 21 14.0
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

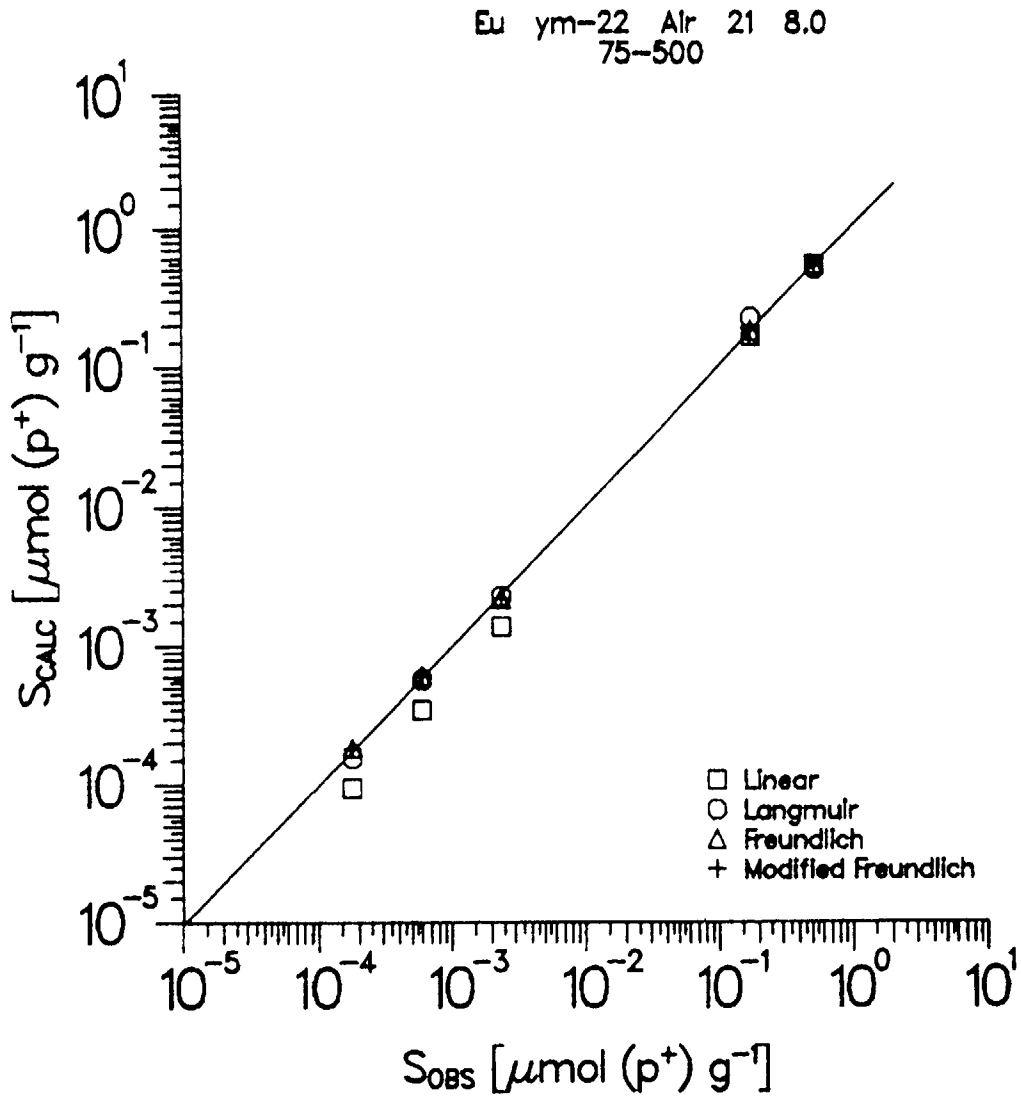

Sr ym-22 Air 21 14.0
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 8 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	1107.8924561	0.9994	0.00789409
Kd =	1107.89245605				
LANGMUIR	5	0.0005470	0.8553579	0.7860	0.00010761
b =	1.16910124				
k =	1563.75231934				
FREUNDLICH	5	2.7883842	0.9227842	0.9998	0.02225477
K =	614.30523682				
N =	0.92278421				
MODIFIED FREUNDLICH	5	1.9289954	0.9295011	0.9999	0.02113380
A =	679.33715820				
B =	0.92950112				
KD =	118.93286896				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

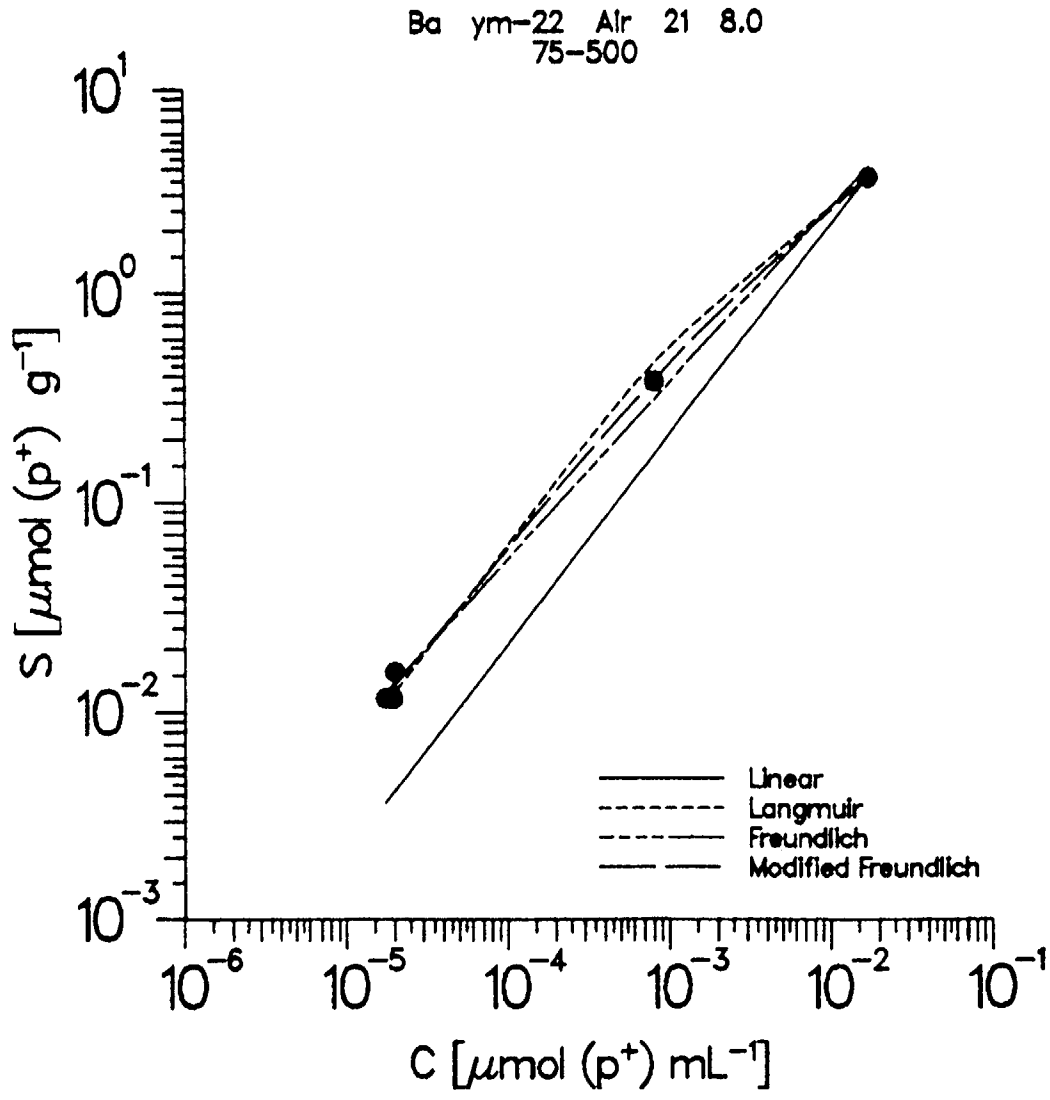

Eu ym-22 Air 21 8.0
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

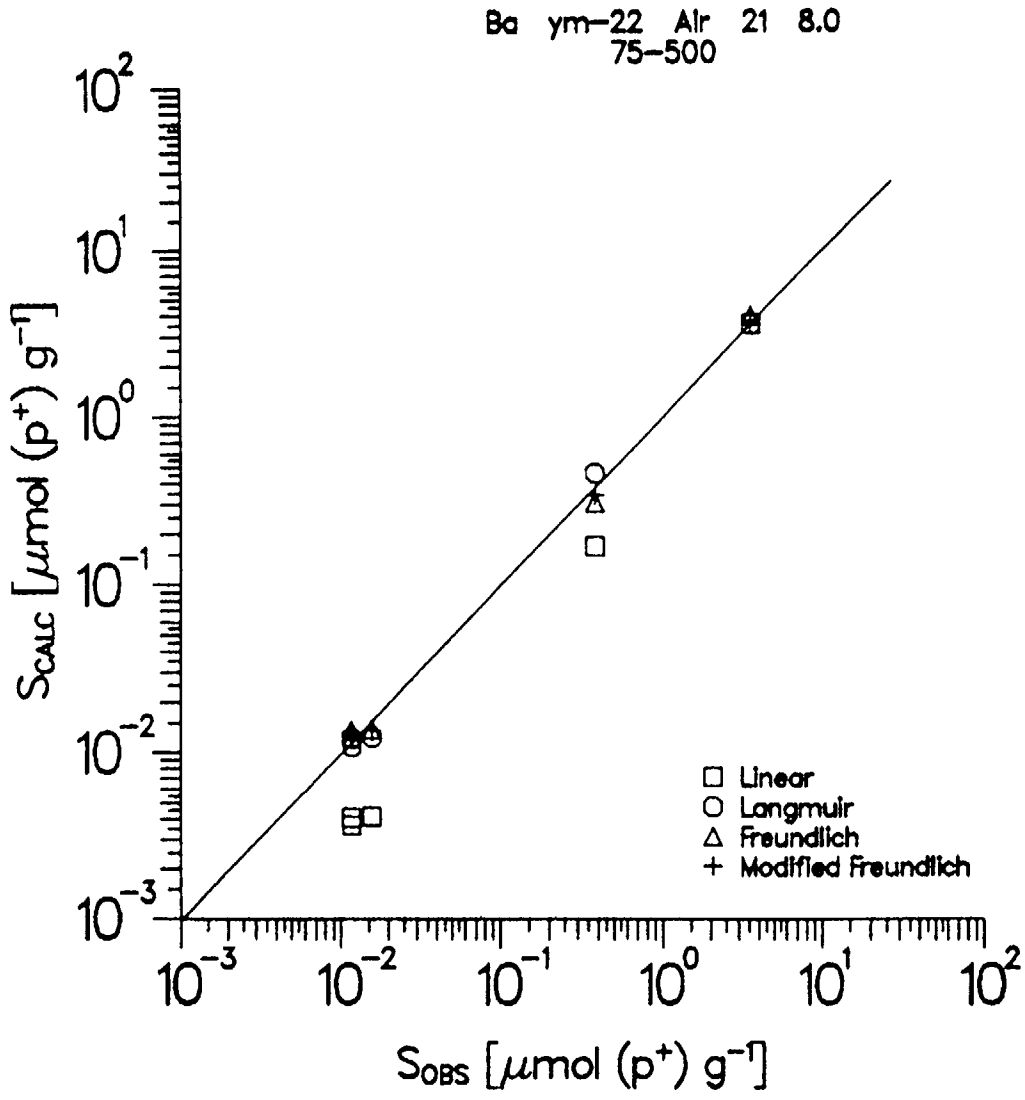

Eu ym-22 Air 21 8.0
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 8 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	210.3441467	0.9966	0.12308562
Kd =	210.34414673				
LANGMUIR	5	0.0015941	0.1833631	0.9670	0.00030072
b =	5.45365858				
k =	115.02719116				
FREUNDLICH	5	2.0887375	0.8395894	0.9964	0.07813212
K =	122.66975403				
N =	0.83958936				
MODIFIED FREUNDLICH	5	1.5346854	0.9161878	0.9988	0.04973922
A =	274.01565552				
B =	0.91618782				
KD =	47.32355118				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

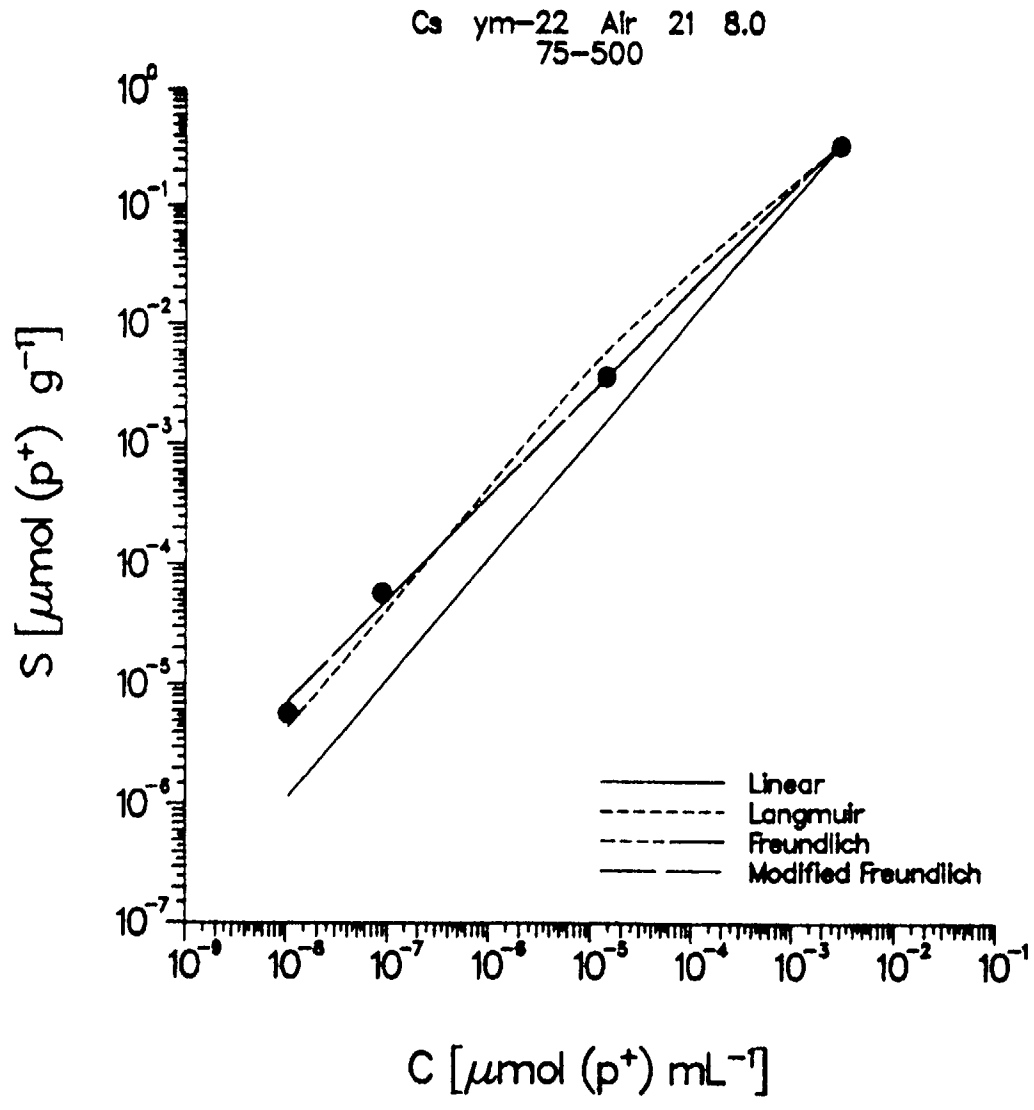

Ba ym-22 Air 21 8.0
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

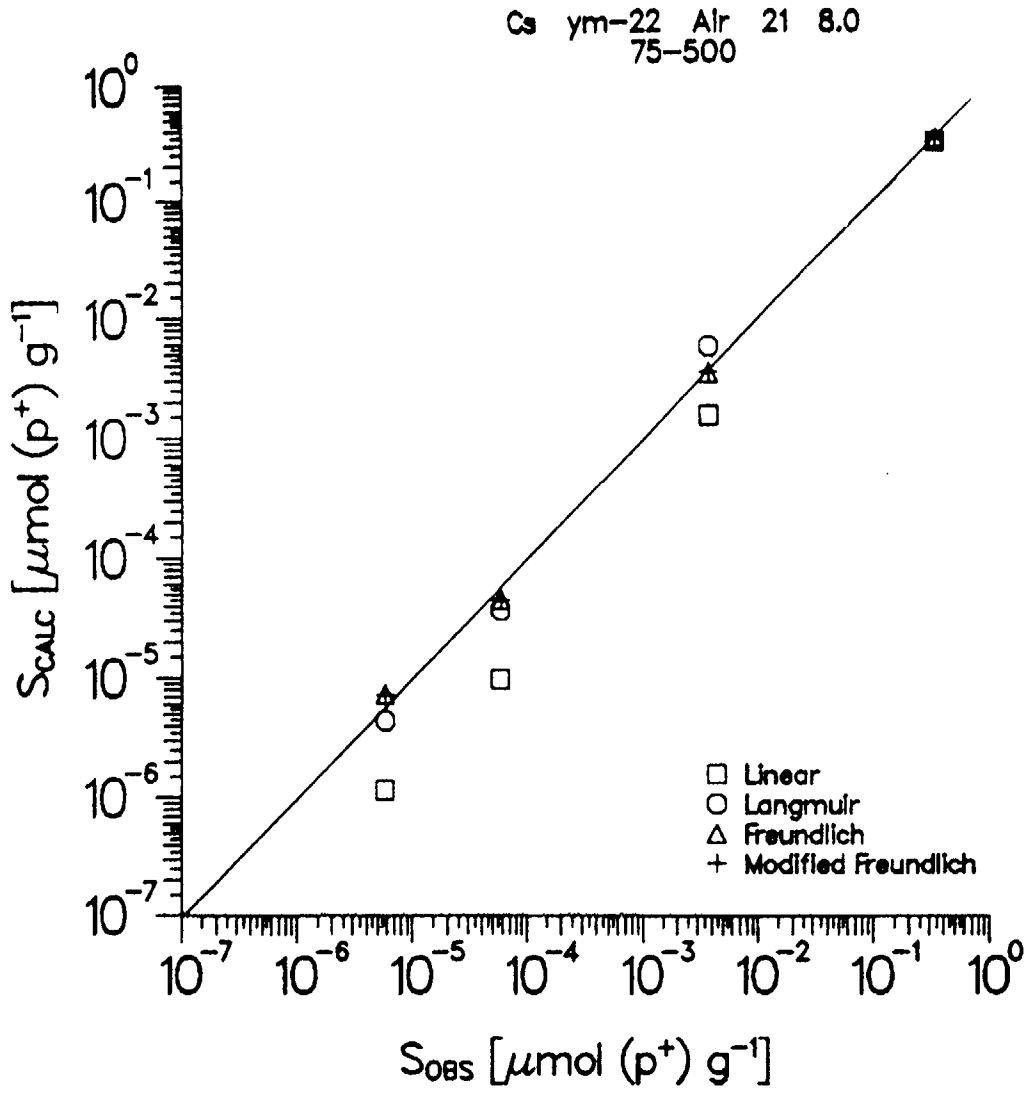

Ba ym-22 Air 21 8.0
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 8 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	109.7434845	1.0000	0.00151485
Kd =	109.74348450				
LANGMUIR	4	0.0023817	2.1874518	0.9150	0.00125528
b =	0.45715293				
k =	918.42578125				
FREUNDLICH	4	1.7139728	0.8588864	0.9983	0.10684326
K =	51.75744247				
N =	0.85888642				
MODIFIED FREUNDLICH	4	0.8337708	0.8621290	0.9984	0.10457885
A =	54.55828857				
B =	0.86212903				
KD =	9.27057457				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

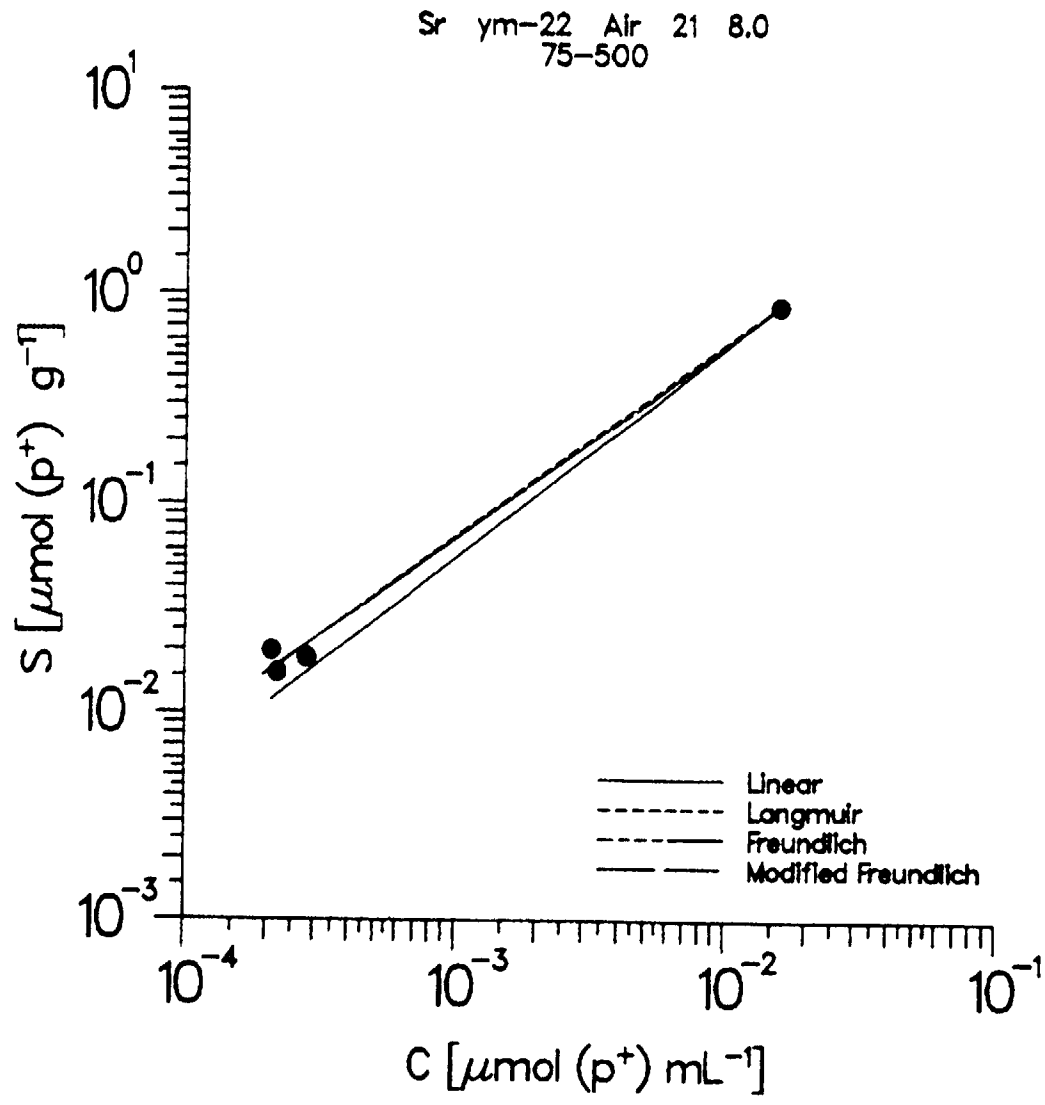

Cs ym-22 Air 21 8.0
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

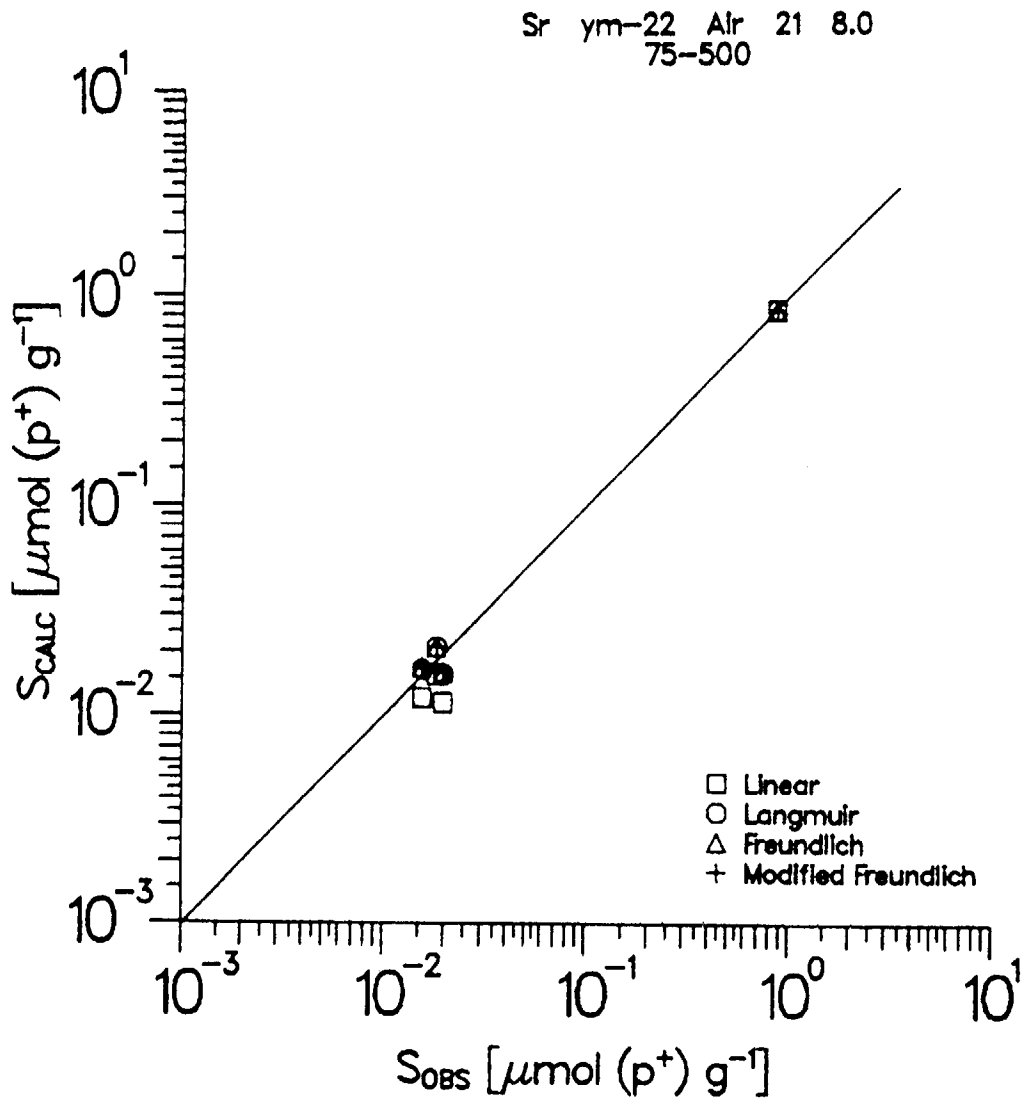

Cs ym-22 Air 21 8.0
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 8 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	55.0129623	0.9999	0.00668829
Kd =	55.01296234				
LANGMUIR	4	0.0132517	0.3087437	0.5932	0.00246819
b =	3.23893285				
k =	23.29850197				
FREUNDLICH	4	1.5923141	0.9201378	0.9939	0.08082124
K =	39.11236954				
N =	0.92013782				
MODIFIED FREUNDLICH	4	0.7881284	0.9471096	0.9941	0.08233441
A =	49.11547852				
B =	0.94710958				
KD =	6.79423714				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

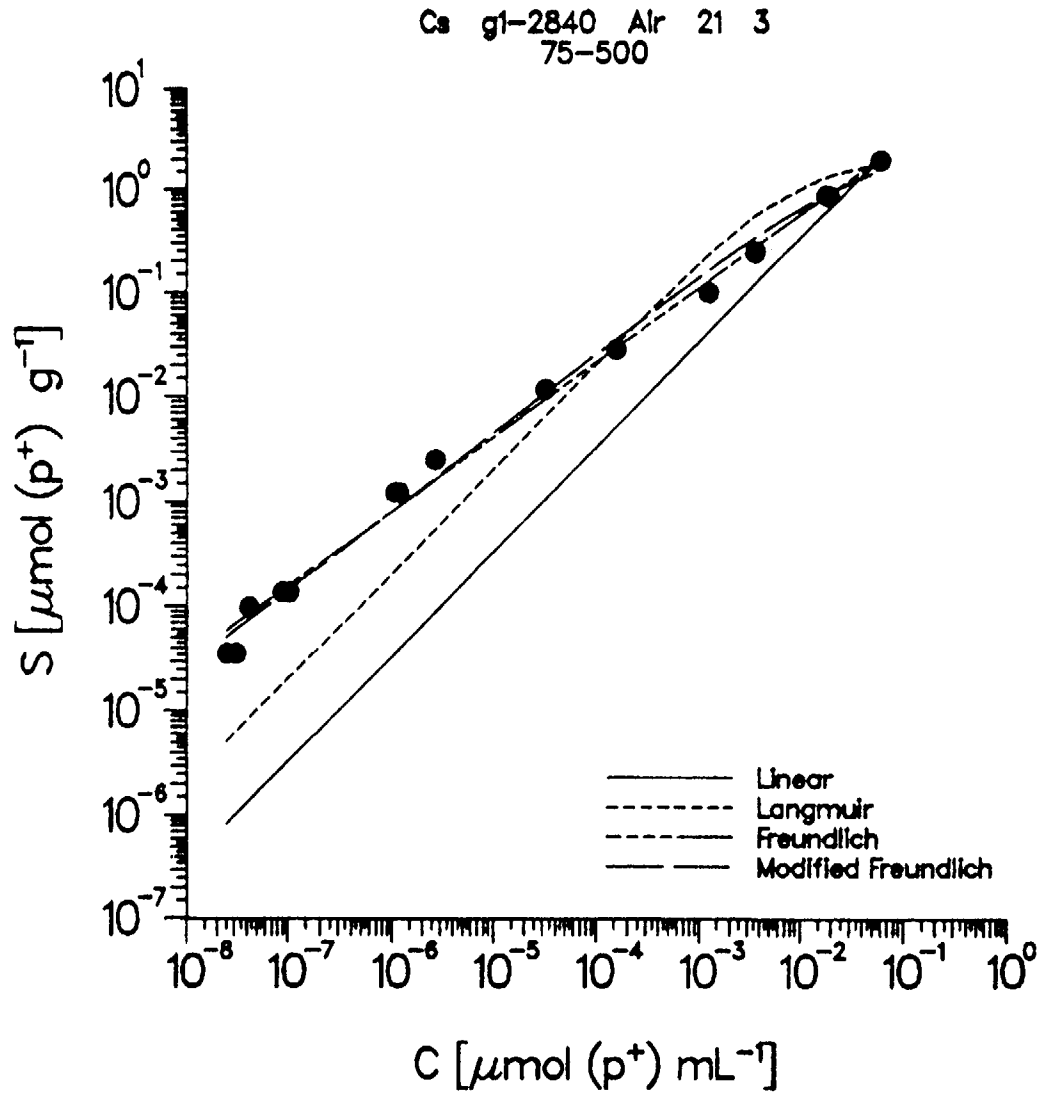

Sr ym-22 Air 21 8.0
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

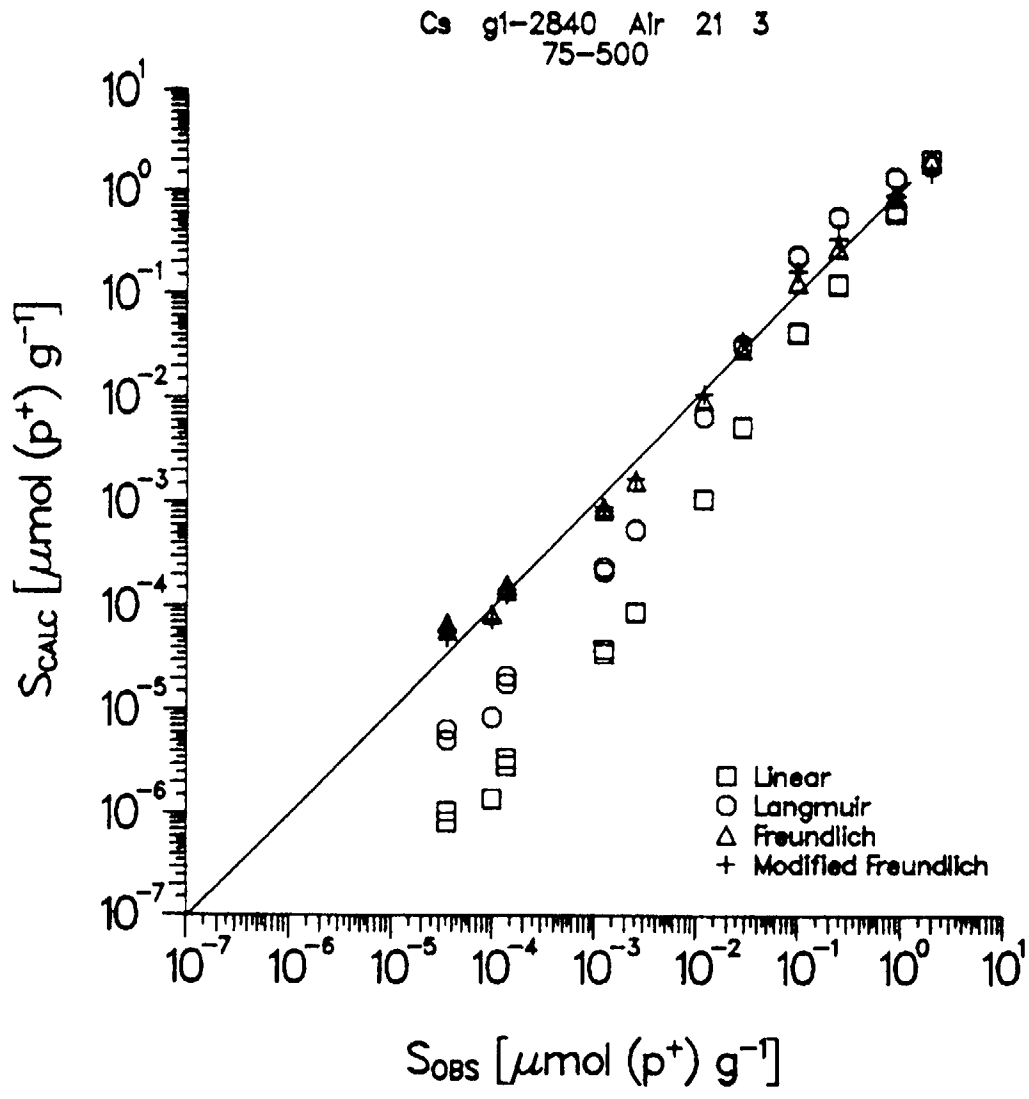

Sr ym-22 Air 21 8.0
75-500
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = gl-2840
TIME = 21 days
ATMOS = Air
CEC = 3 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	21	0.0000000	32.9728851	0.9792	0.10134283
Kd =	32.97288513				
LANGMUIR	21	0.0048967	0.4782462	0.7518	0.00529103
b =	2.09097314				
k =	97.66641998				
FREUNDLICH	21	1.1679314	0.7100860	0.9937	0.12864120
K =	14.72080040				
N =	0.71008605				
MODIFIED FREUNDLICH	21	0.9332447	0.7505561	0.9911	0.16156103
A =	25.72562599				
B =	0.75055605				
KD =	17.51476669				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

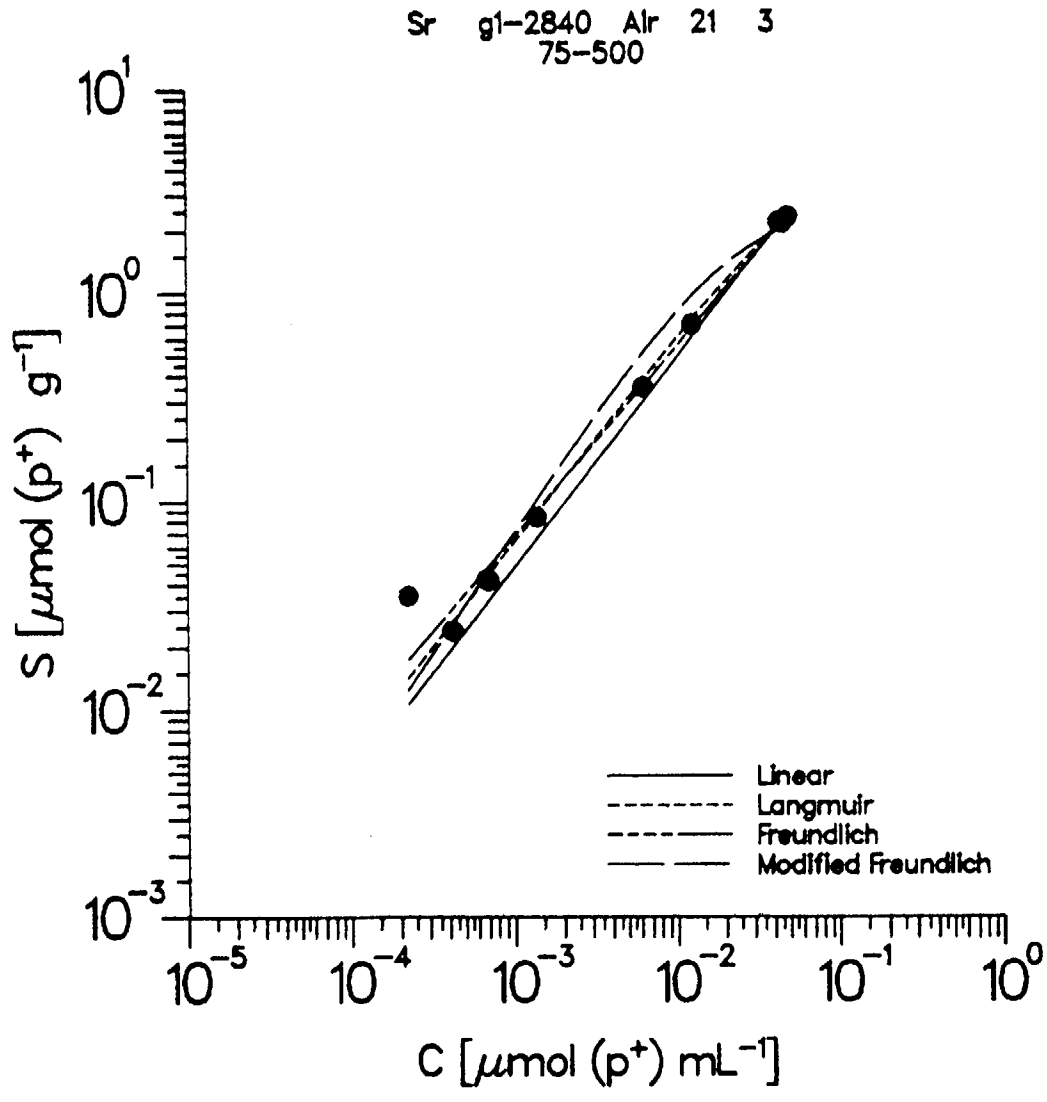

Cs g1-2840 Air 21 3
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

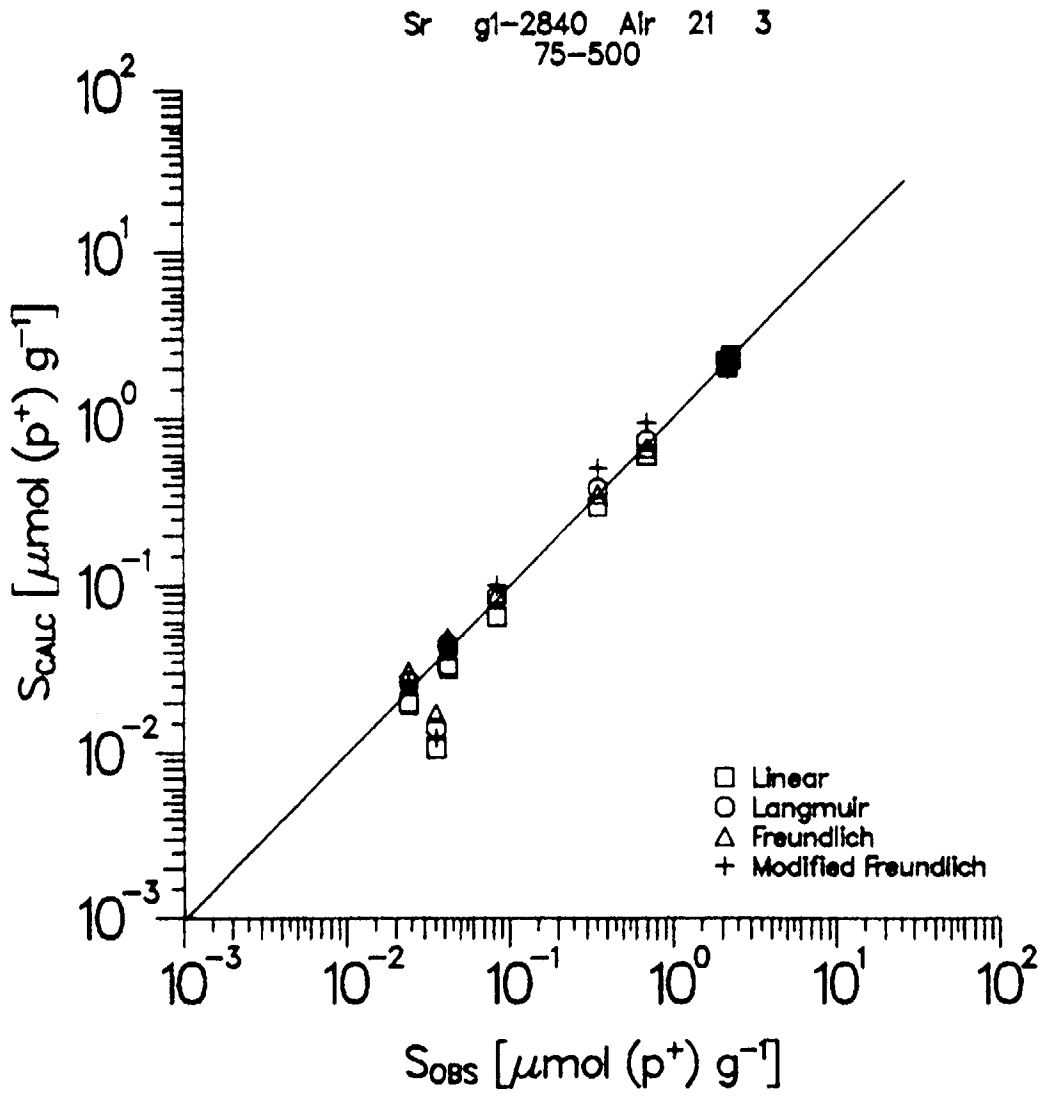

Cs g1-2840 Air 21 3
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = gl-2840
TIME = 21 days
ATMOS = Air
CEC = 3 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	15	0.0000000	48.1376190	0.9976	0.06328616
Kd =	48.13761902				
LANGMUIR	15	0.0155212	0.1188250	0.4455	0.00278620
b =	8.41573906				
k =	7.65567923				
FREUNDLICH	15	1.5421194	0.9032601	0.9848	0.09982640
K =	34.84330750				
N =	0.90326005				
MODIFIED FREUNDLICH	15	1.8852967	1.1668545	0.9685	0.18708089
A =	230.36576843				
B =	1.16685450				
KD =	41.27703094				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

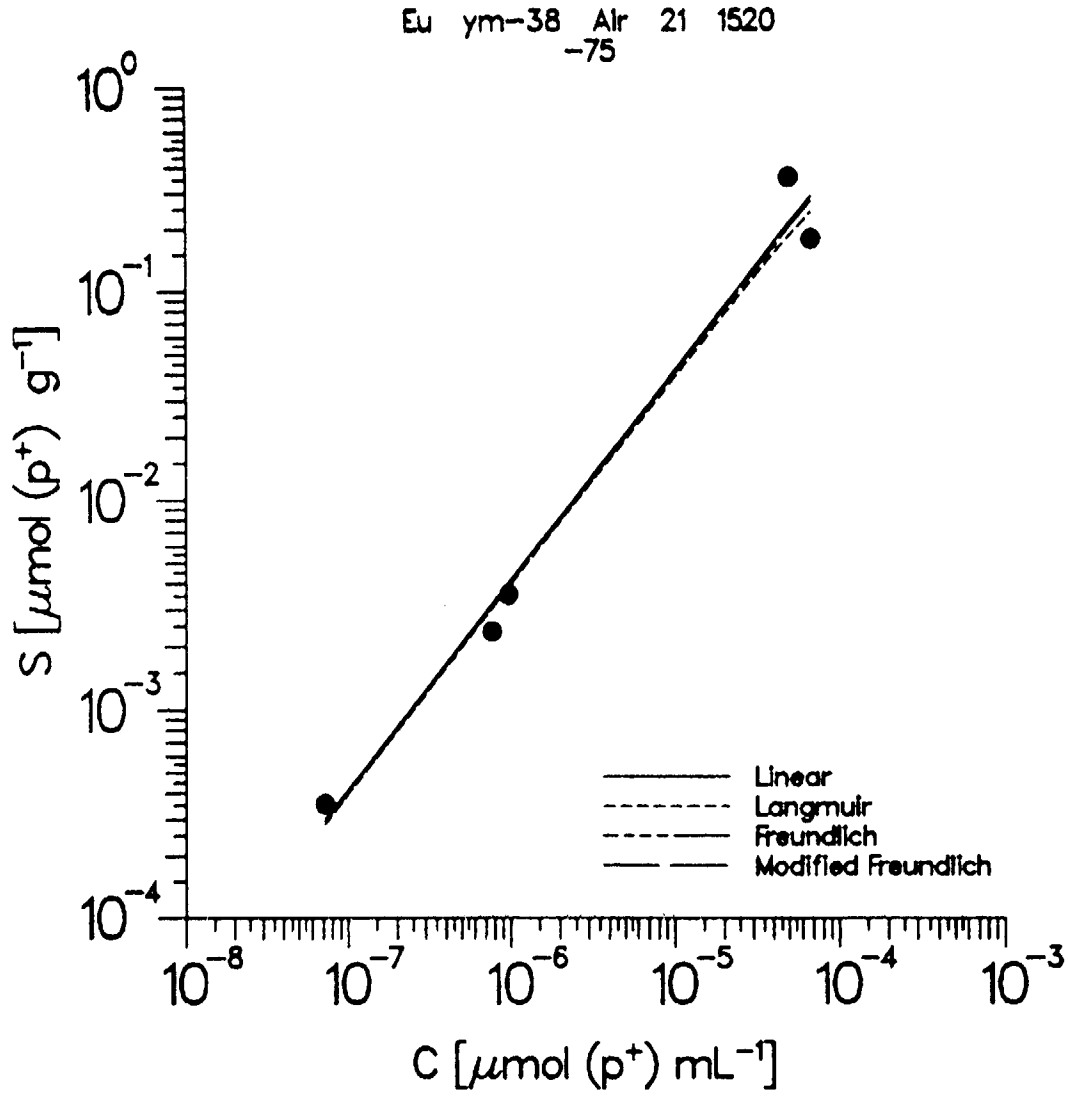

Sr g1-2840 Air 21 3
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

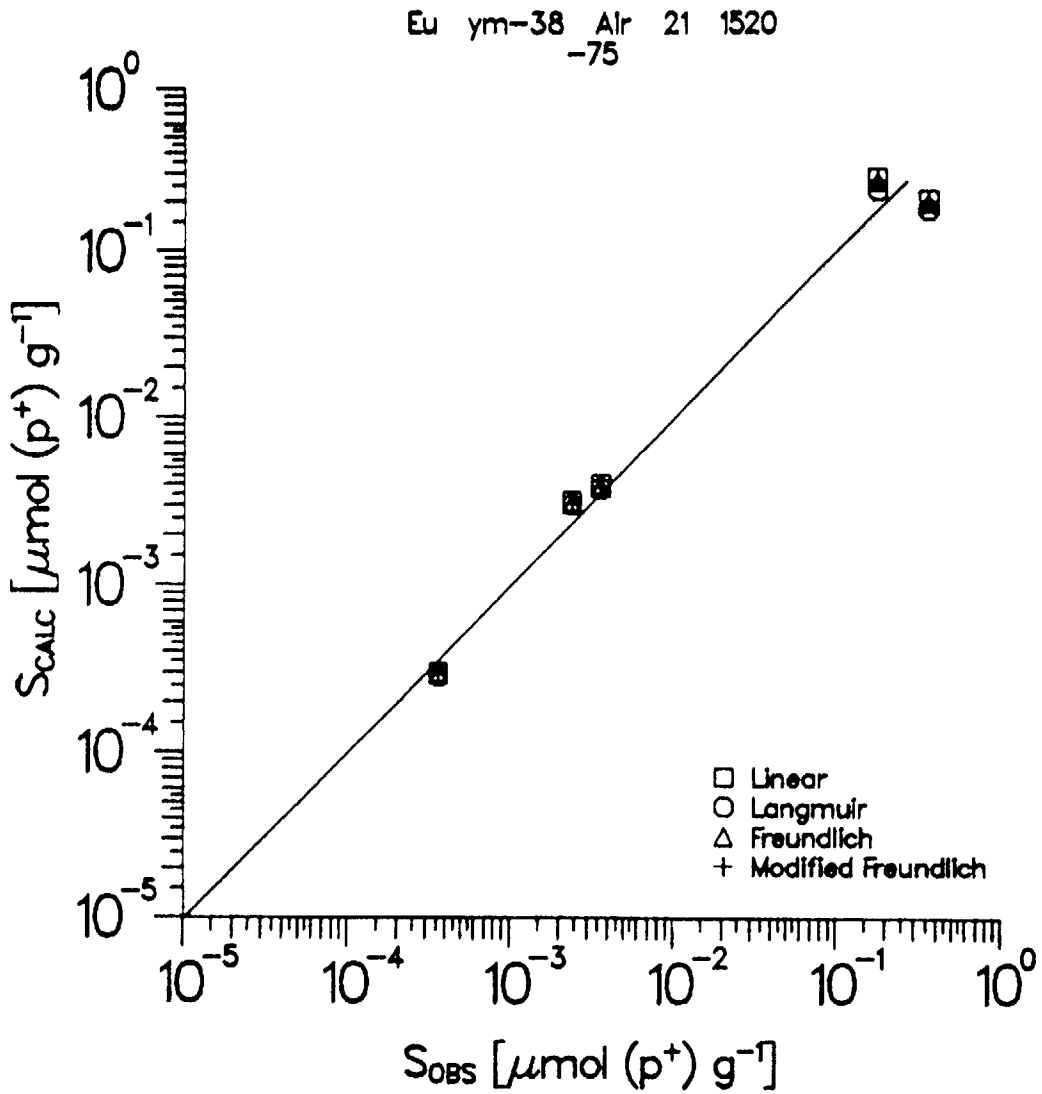

Sr g1-2840 Air 21 3
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	4184.2578125	0.7921	0.10560074
Kd =	4184.25781250				
LANGMUIR	5	0.0002519	0.4829596	0.0273	0.00010977
b =	2.07056642				
k =	1917.30212402				
FREUNDLICH	5	3.5856454	0.9965077	0.9820	0.19962683
K =	3851.63769531				
N =	0.99650770				
MODIFIED FREUNDLICH	5	0.4039907	0.9965361	0.9820	0.19966266
A =	3853.31347656				
B =	0.99653614				
KD =	2.54328489				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

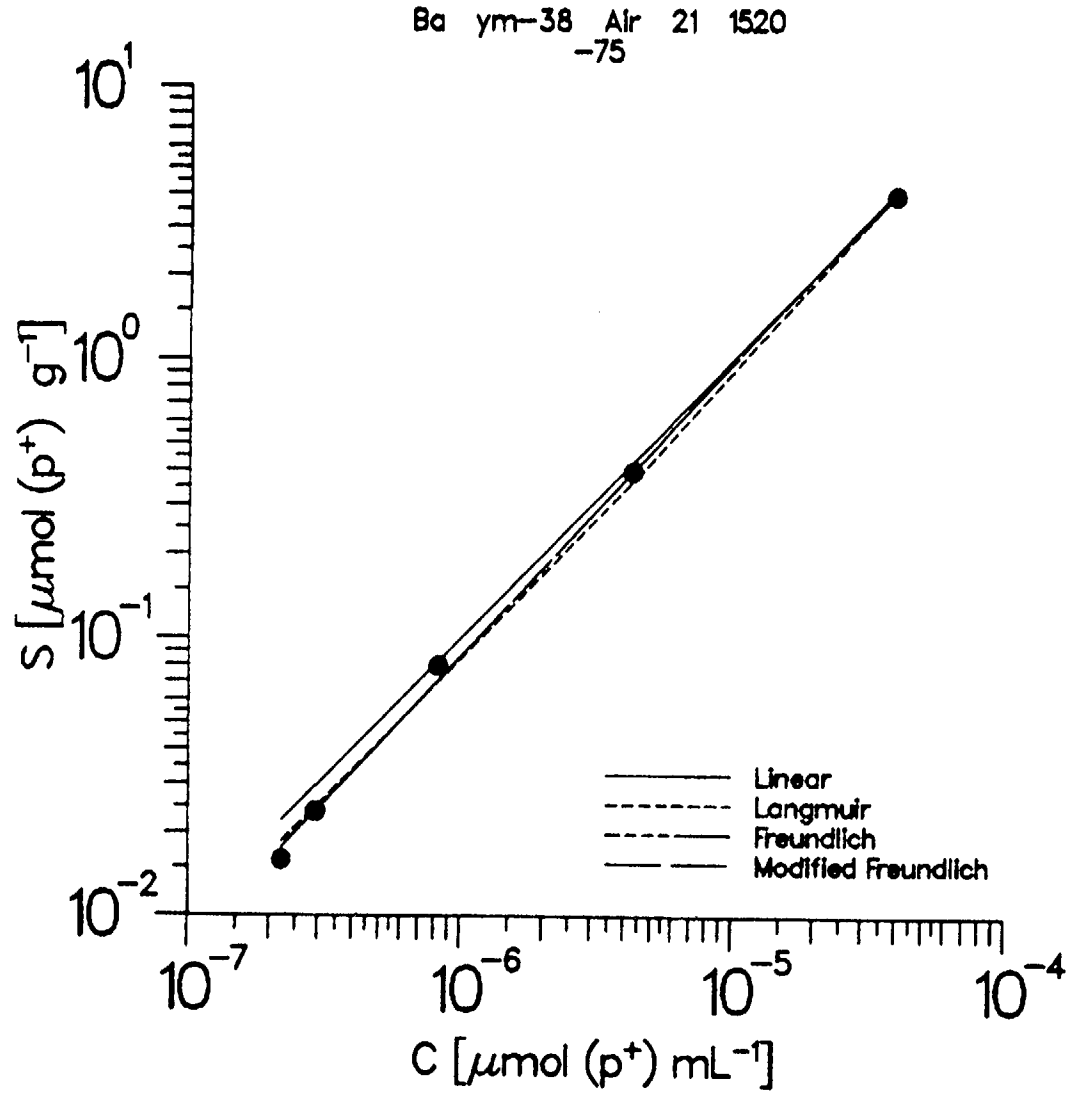

Eu ym-38 Air 21 1520
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

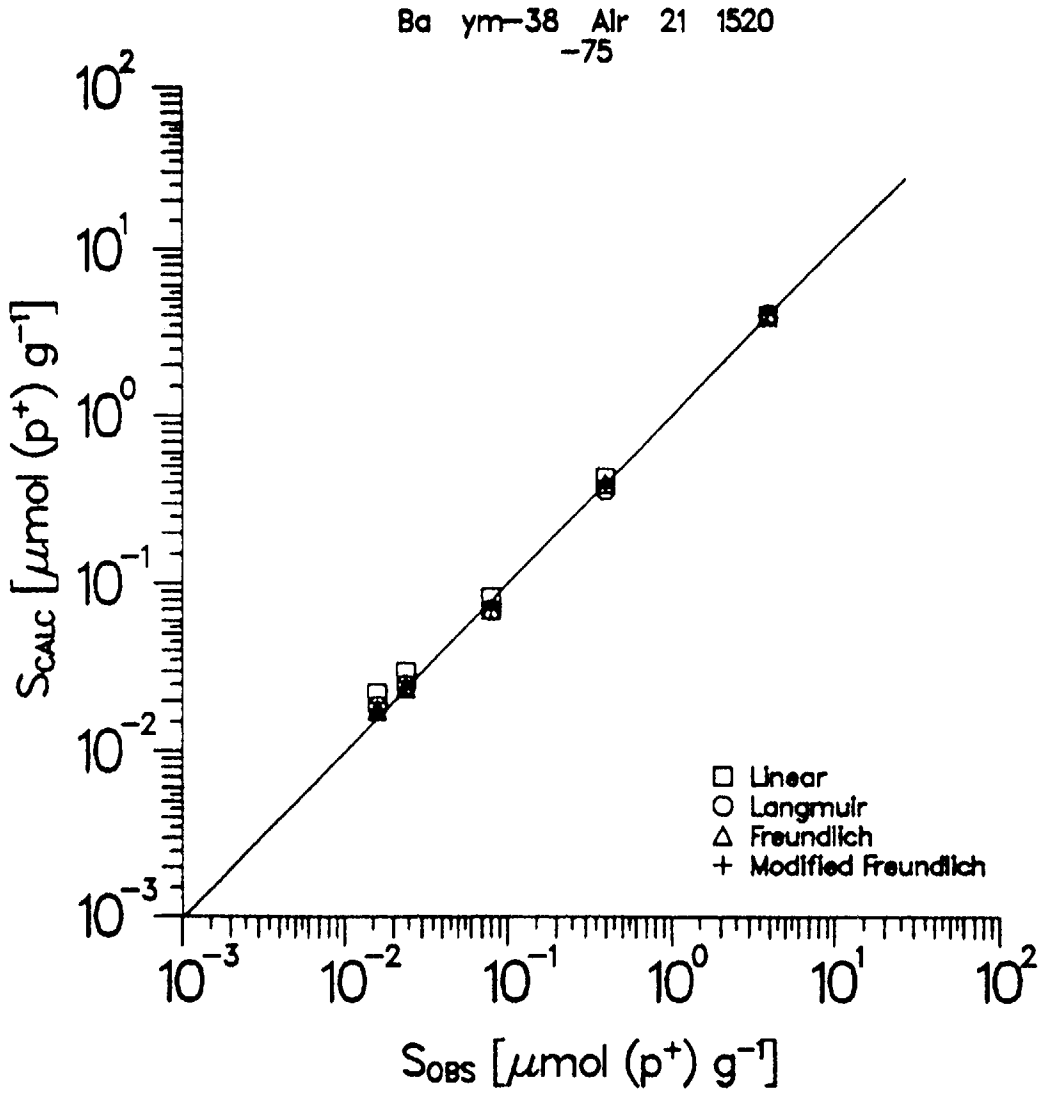

Eu ym-38 Air 21 1520
-75
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^0
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	99917.1875000	0.9999	0.01795388
Kd = 99917.18750000					
LANGMUIR	5	0.0000119	-0.0510031	0.2966	0.00000157
b = -19.60666275					
k = -4278.86962891					
FREUNDLICH	5	5.2373405	1.0504571	0.9986	0.04213389
K = 172719.14062500					
N = 1.05045712					
MODIFIED FREUNDLICH	5	2.0585070	1.0509310	0.9986	0.04192590
A = 173920.42187500					
B = 1.05093098					
KD = 90.93814087					

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

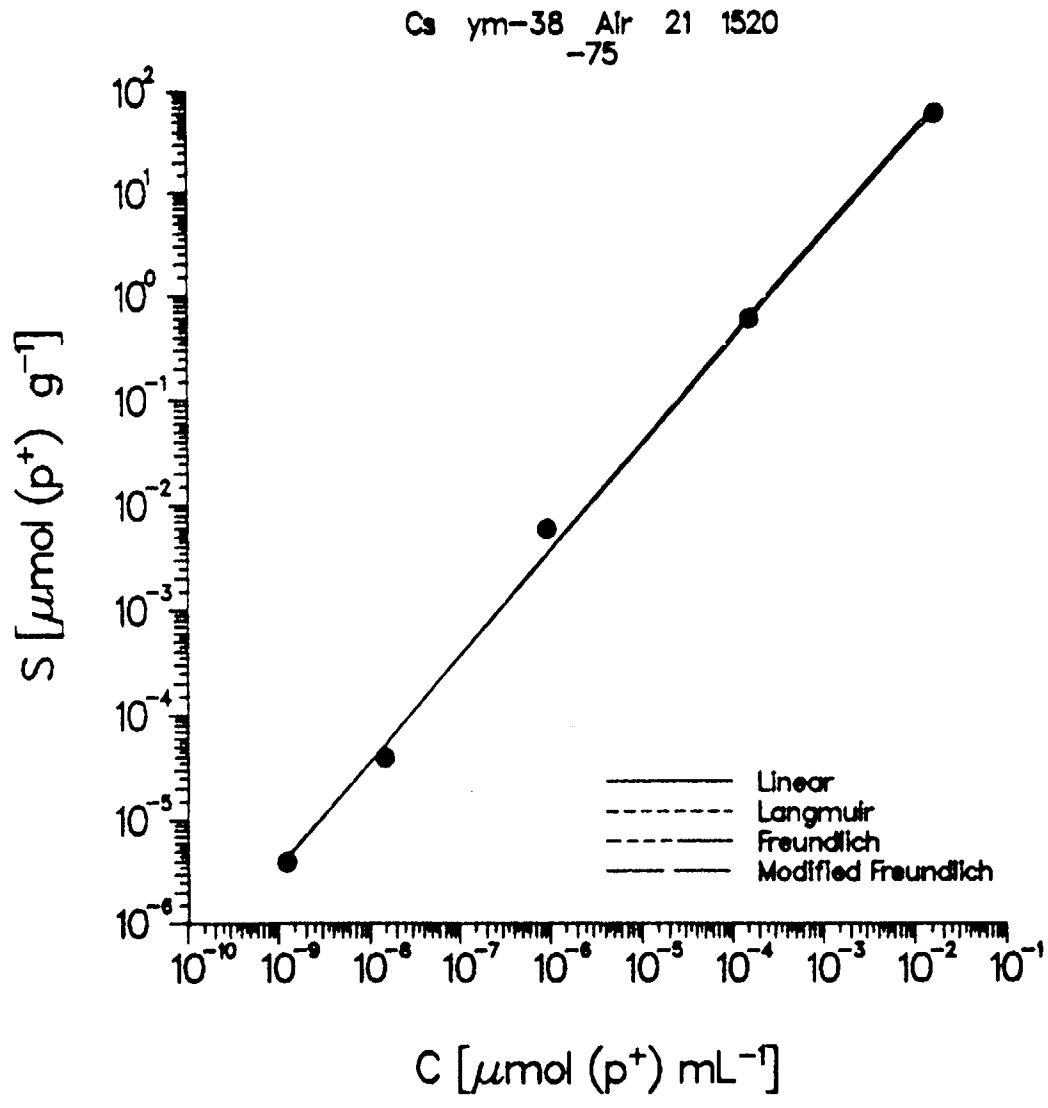

Ba ym-38 Air 21 1520
-75
10^1
10^0
10^{-1}
10^{-2}
S [μmol (p^+) g^{-1}]
10^{-7}
10^{-6}
10^{-5}
10^{-4}
C [μmol (p^+) mL^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

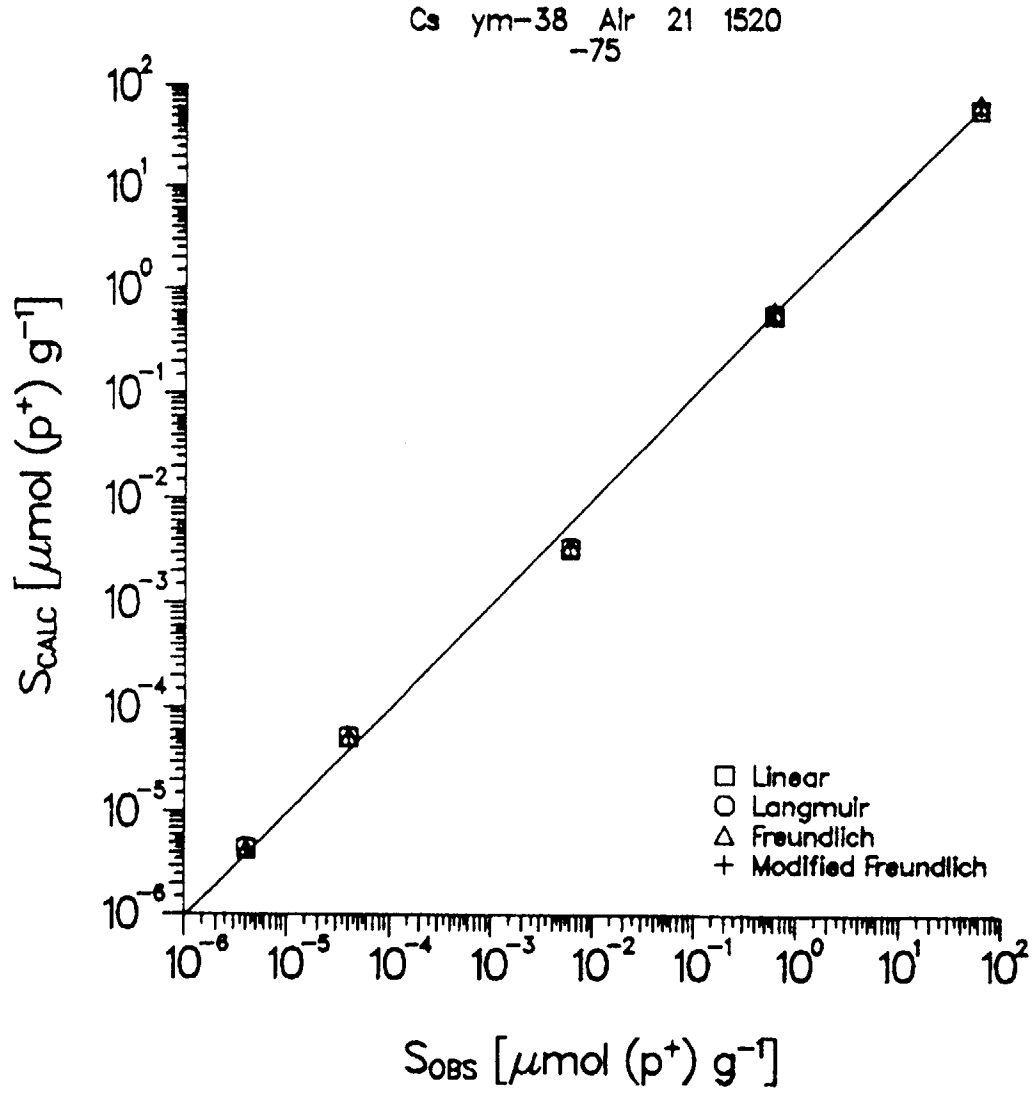

Ba ym-38 Air 21 1520
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	10	0.0000000	3511.7824707	1.0000	0.00781250
Kd =	3511.78247070				
LANGMUIR	10	0.0002776	0.0004188	0.0017	0.00007737
b =	2388.05200195				
k =	1.50870621				
FREUNDLICH	10	3.6249113	1.0096209	0.9979	0.13540806
K =	4216.10400391				
N =	1.00962090				
MODIFIED FREUNDLICH	10	0.4579196	1.0116223	0.9980	0.13352863
A =	4362.77832031				
B =	1.01162231				
KD =	2.83568931				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

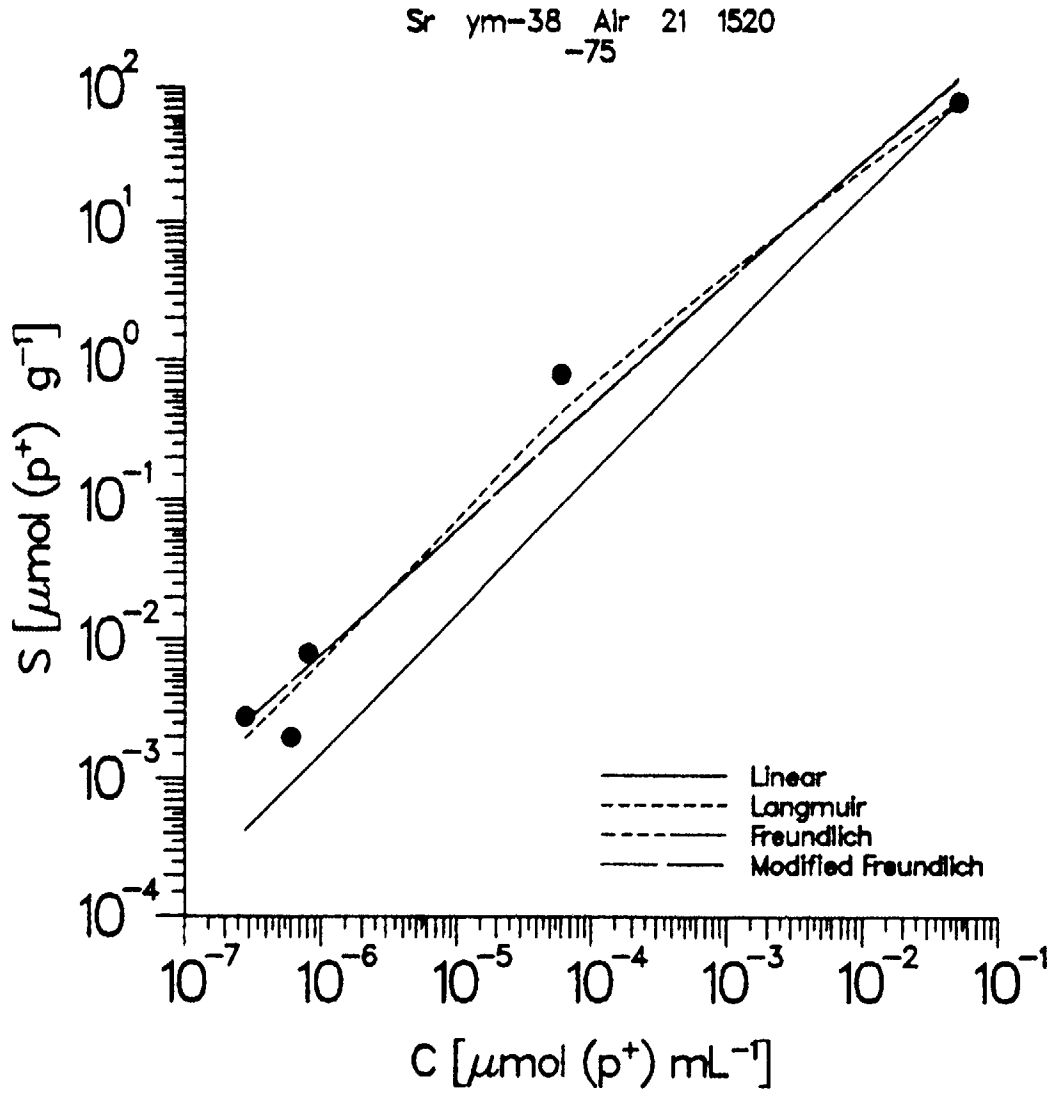

Cs ym-38 Air 21 1520
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

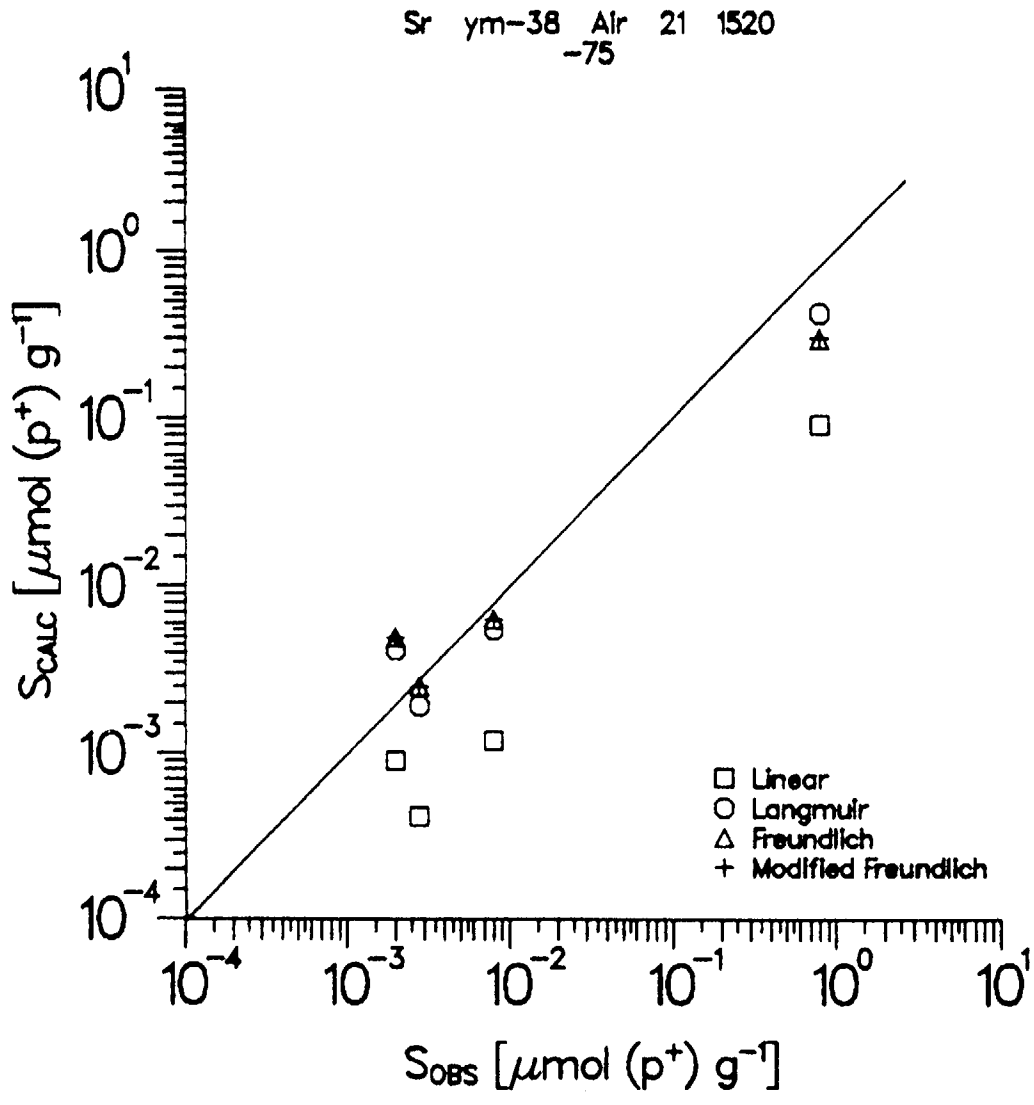

Cs ym-38 Air 21 1520
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	1500.0157471	0.9999	0.40804890
Kd =	1500.01574707				
LANGMUIR	5	0.0001447	0.0099218	0.8664	0.00010581
b =	100.78855133				
k =	68.56639862				
FREUNDLICH	5	3.2027719	0.8852442	0.9756	0.35726085
K =	1595.04113770				
N =	0.88524419				
MODIFIED FREUNDLICH	5	0.0464277	0.8895176	0.9763	0.35362667
A =	1691.49731445				
B =	0.88951761				
KD =	1.12770176				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

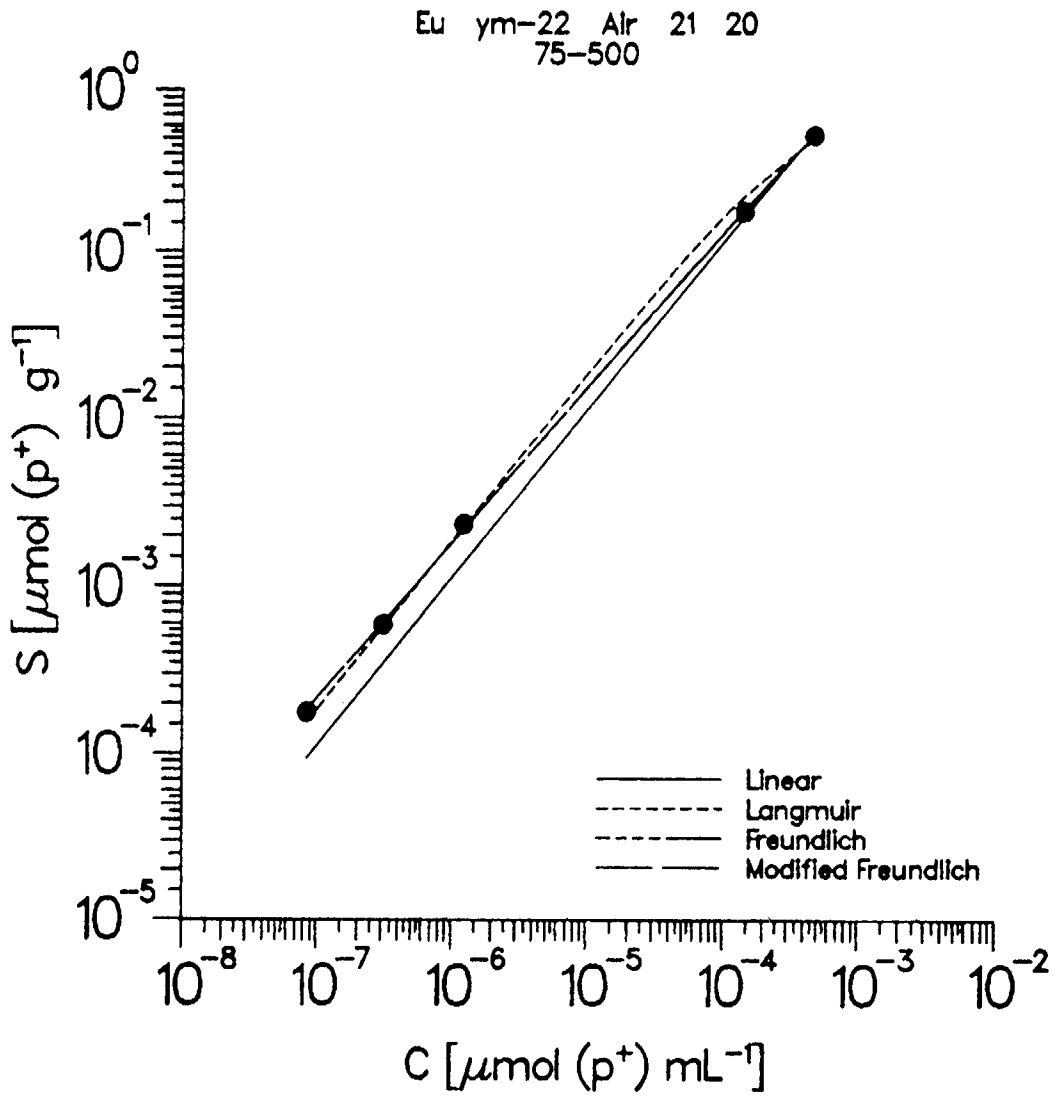

Sr ym-38 Air 21 1520
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

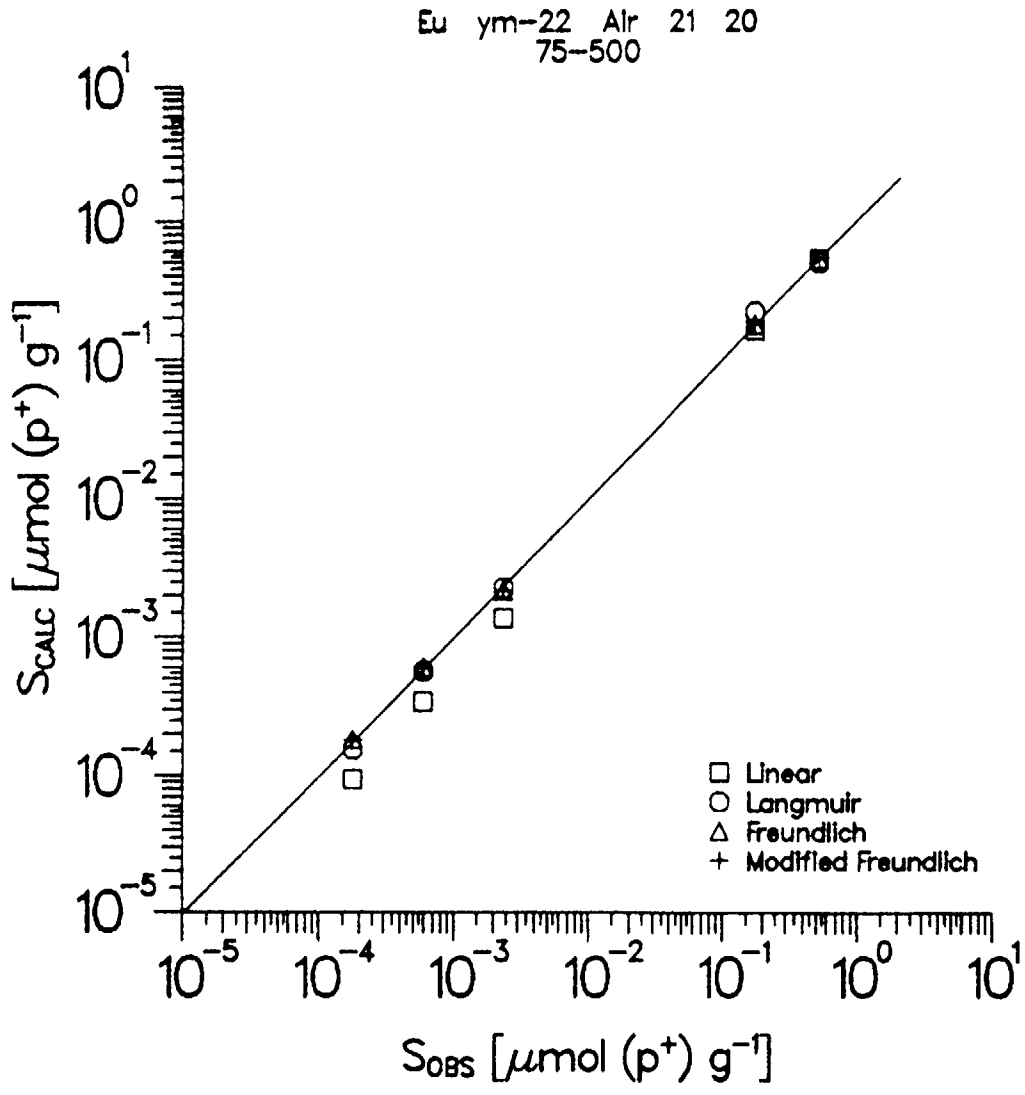

Sr ym-38 Air 21 1520
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	1107.8924561	0.9994	0.00789409
Kd =	1107.89245605				
LANGMUIR	5	0.0005470	0.8553579	0.7860	0.00010761
b =	1.16910124				
k =	1563.75231934				
FREUNDLICH	5	2.7883842	0.9227842	0.9998	0.02225477
K =	614.30523682				
N =	0.92278421				
MODIFIED FREUNDLICH	5	1.5045297	0.9254238	0.9999	0.02152133
A =	639.08660889				
B =	0.92542380				
KD =	42.24484253				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

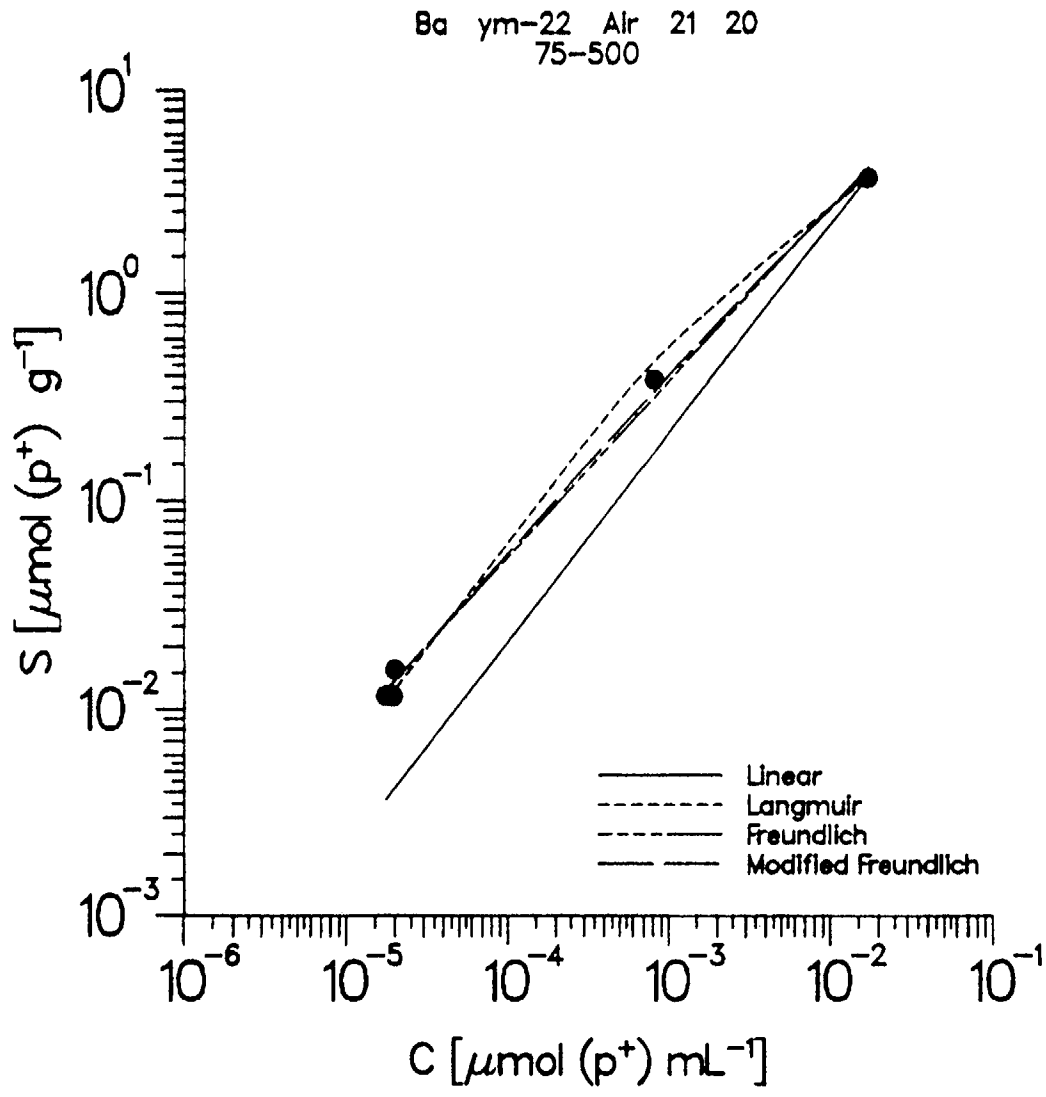

Eu ym-22 Air 21 20
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

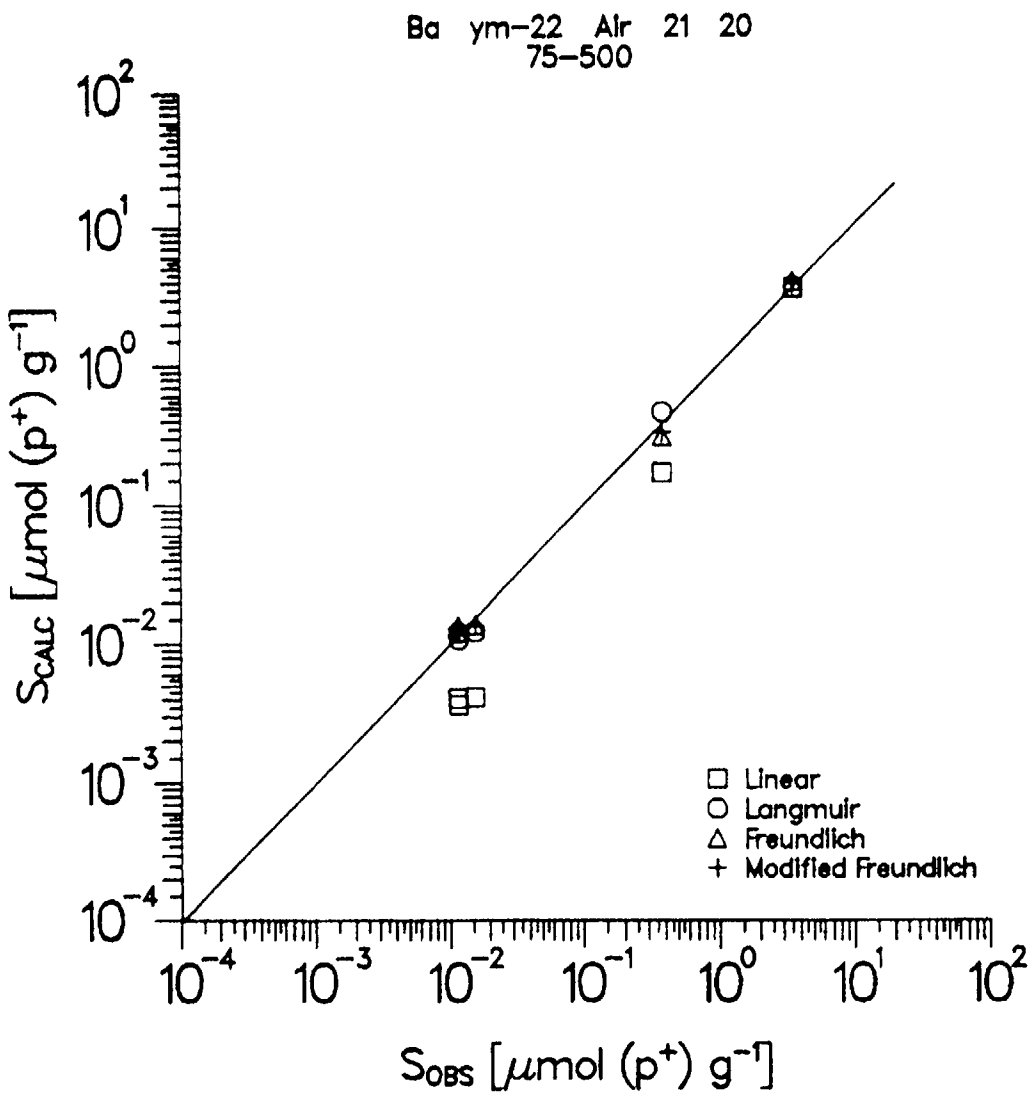

Eu ym-22 Air 21 20
75--500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	210.3441467	0.9966	0.12308562
Kd =	210.34414673				
LANGMUIR	5	0.0015941	0.1833631	0.9670	0.00030072
b =	5.45365858				
k =	115.02719116				
FREUNDLICH	5	2.0887375	0.8395894	0.9964	0.07813212
K =	122.66975403				
N =	0.83958936				
MODIFIED FREUNDLICH	5	0.9038846	0.8650384	0.9977	0.06415899
A =	160.29302979				
B =	0.86503839				
KD =	11.08937168				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

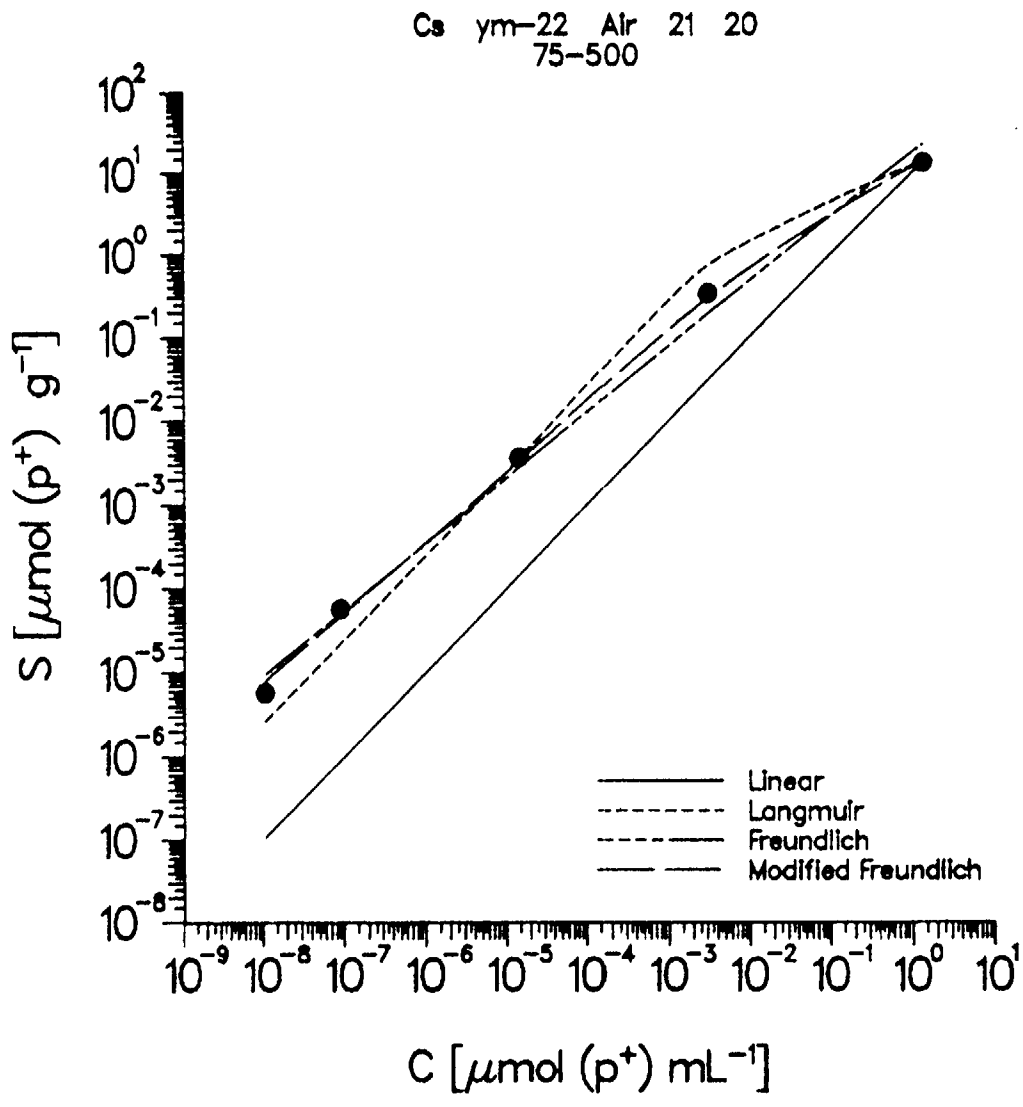

Ba ym-22 Air 21 20
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

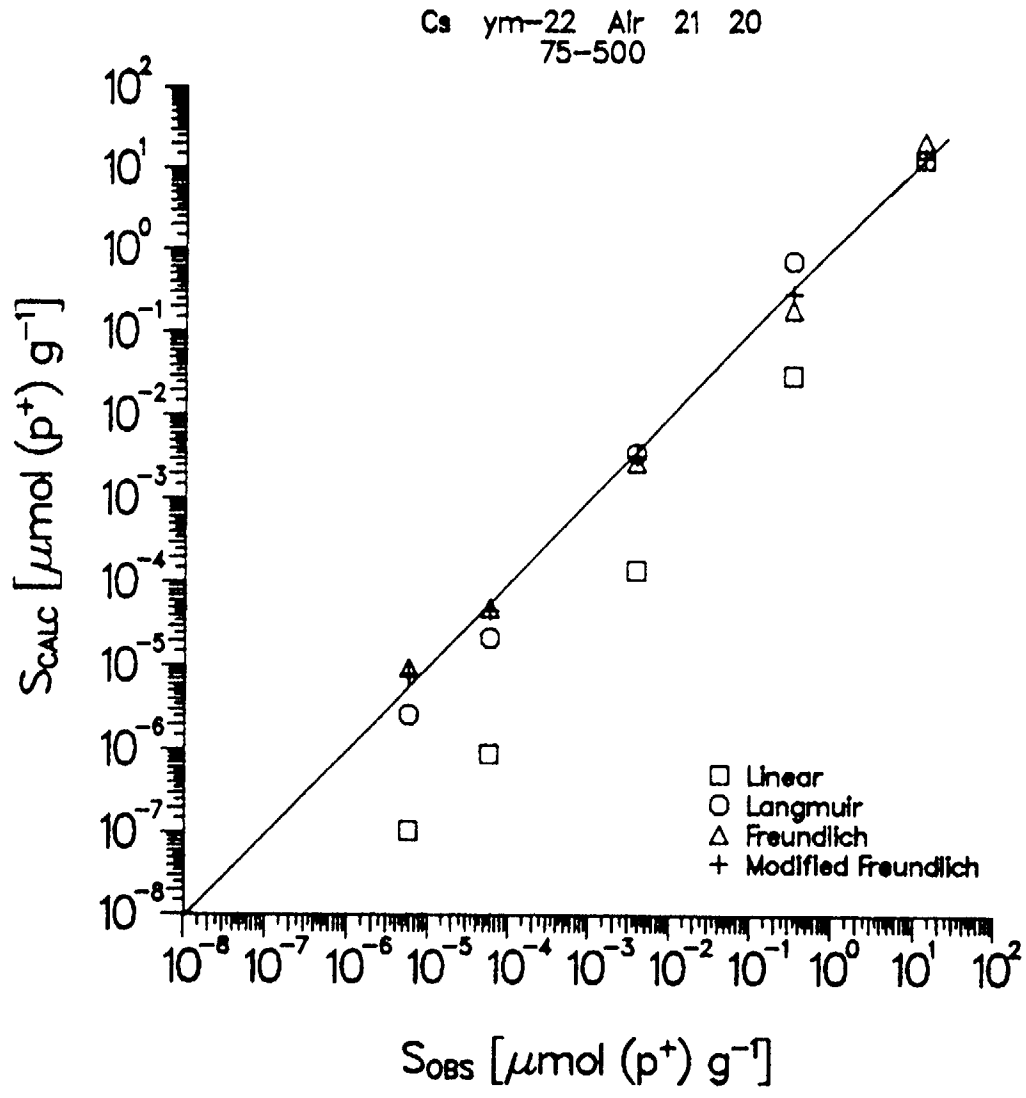

Ba ym-22 Air 21 20
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	10.0005350	0.9995	0.17735121
Kd =	10.00053501				
LANGMUIR	5	0.0040153	0.0721774	0.9953	0.00341029
b =	13.85474777				
k =	17.97561455				
FREUNDLICH	5	1.2525532	0.7865505	0.9934	0.24516323
K =	17.88764763				
N =	0.78655052				
MODIFIED FREUNDLICH	5	0.2691224	0.8362036	0.9987	0.11502729
A =	37.16656113				
B =	0.83620358				
KD =	2.09815860				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

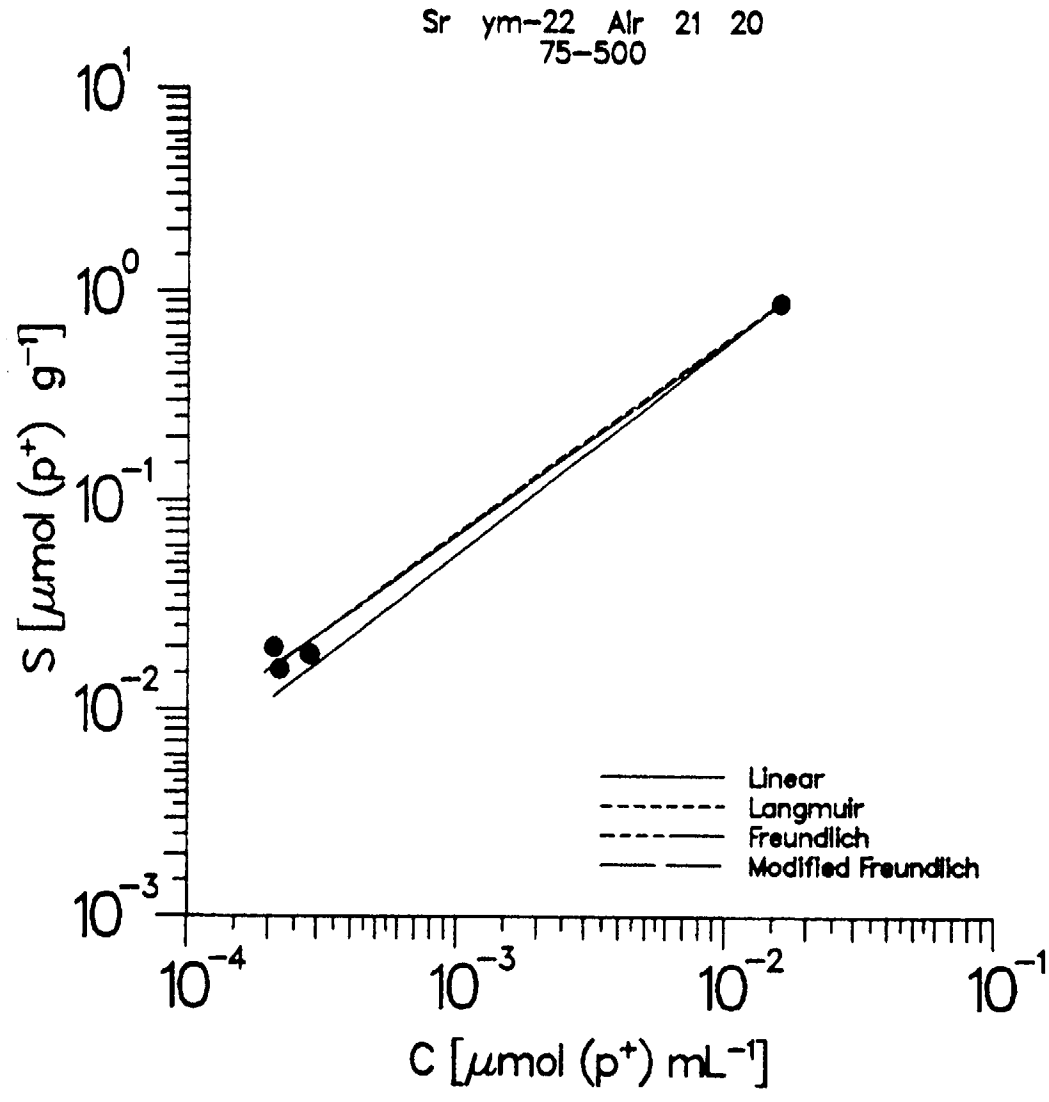

Cs ym-22 Air 21 20
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

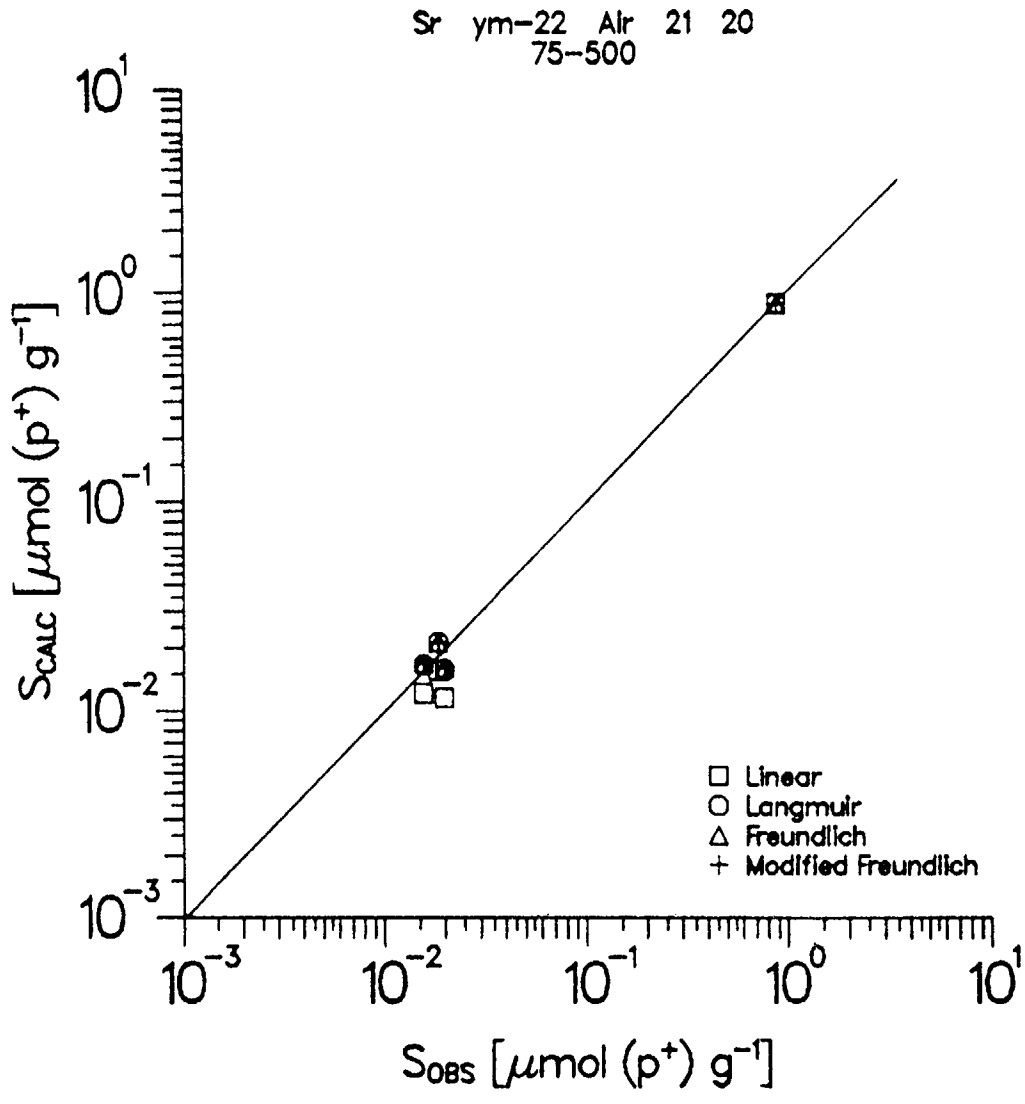

Cs ym-22 Air 21 20
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = 75-500 zomicrons

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	55.0129623	0.9999	0.00668829
Kd =	55.01296234				
LANGMUIR	4	0.0132517	0.3087437	0.5932	0.00246819
b =	3.23893285				
k =	23.29850197				
FREUNDLICH	4	1.5923141	0.9201378	0.9939	0.08082124
K =	39.11236954				
N =	0.92013782				
MODIFIED FREUNDLICH	4	0.3294551	0.9305434	0.9940	0.08142886
A =	42.70563126				
B =	0.93054342				
KD =	2.25967503				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

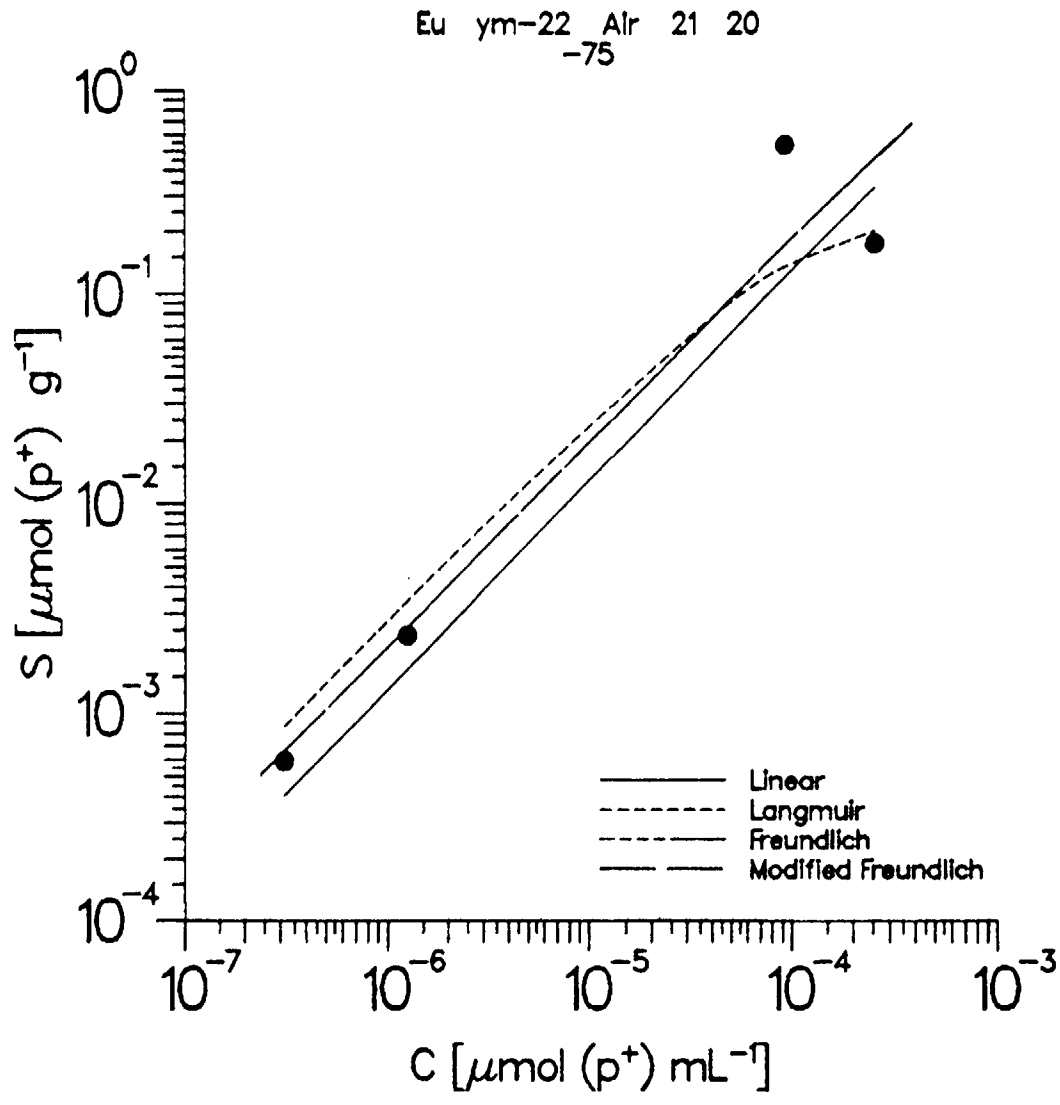

Sr ym-22 Air 21 20
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich


Sr ym-22 Air 21 20
75-500
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	1290.5809326	0.3805	0.31485751
Kd =	1290.58093262				
LANGMUIR	4	0.0003590	3.5612335	0.6034	0.00042234
b =	0.28080159				
k =	9919.87207031				
FREUNDLICH	4	3.1641402	0.9749284	0.9306	0.46074066
K =	1459.28540039				
N =	0.97492844				
MODIFIED FREUNDLICH	4	1.8811672	0.9777485	0.9297	0.46541631
A =	1521.23791504				
B =	0.97774845				
KD =	83.94184875				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.


Eu ym-22 Air 21 20
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
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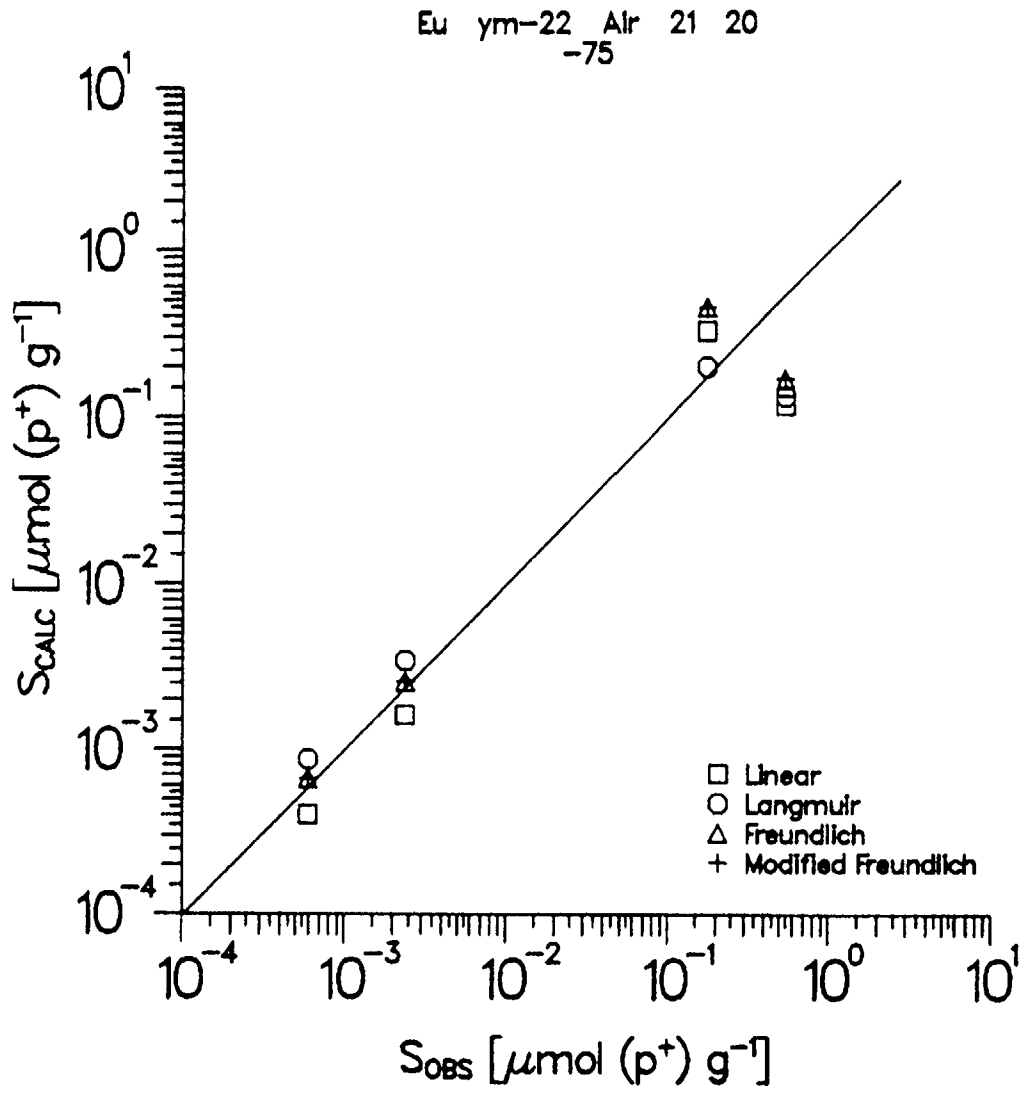
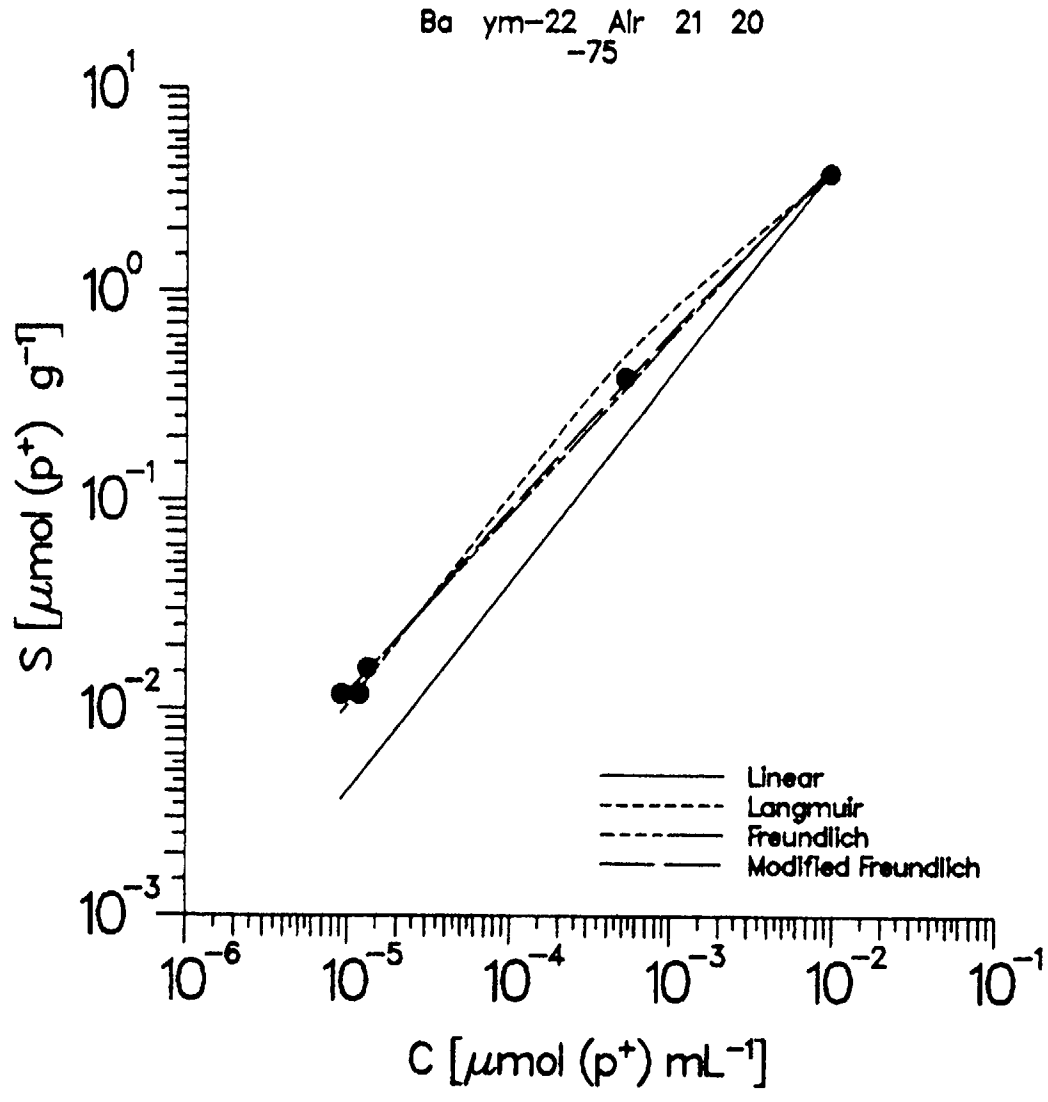
Modified Freundlich

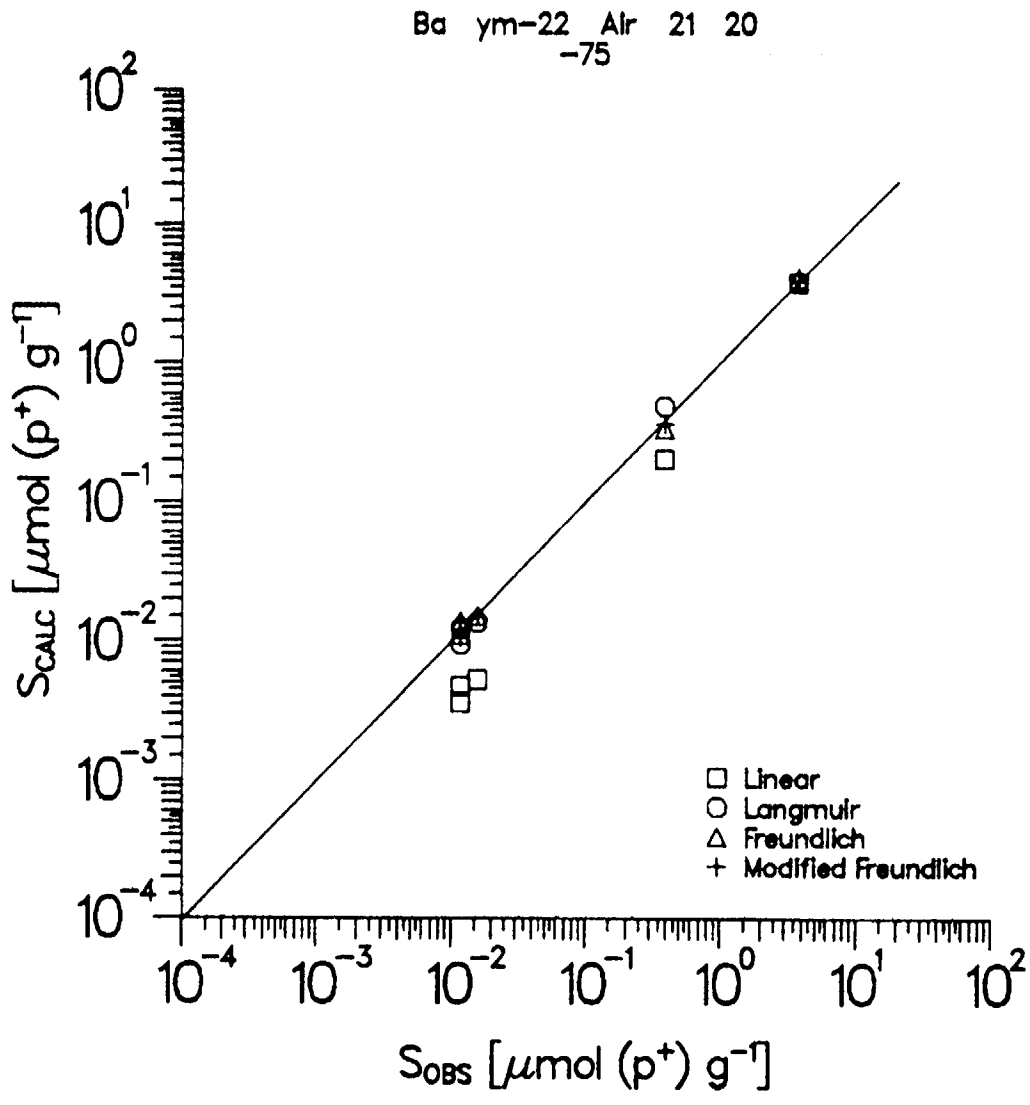

Eu ym-22 Air 21 20
-75
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	401.2557068	0.9977	0.10683136
Kd =	401.25570679				
LANGMUIR	5	0.0009540	0.1638004	0.9366	0.00020671
b =	6.10499144				
k =	171.70465088				
FREUNDLICH	5	2.3308990	0.8501906	0.9981	0.05784982
K =	214.23922729				
N =	0.85019058				
MODIFIED FREUNDLICH	5	1.1575382	0.8768305	0.9988	0.04698000
A =	287.45388794				
B =	0.87683052				
KD =	20.89964867				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

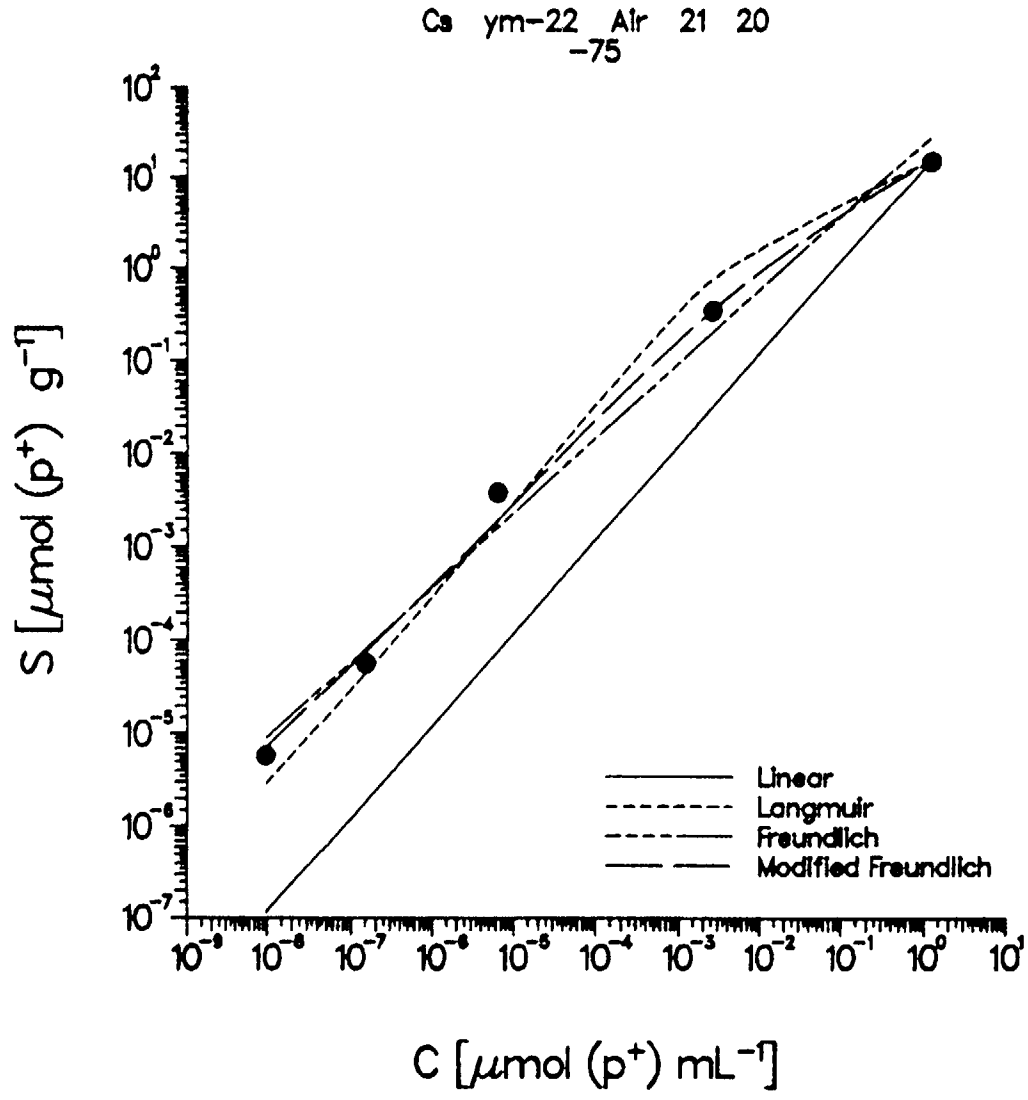

Ba ym-22 Air 21 20
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

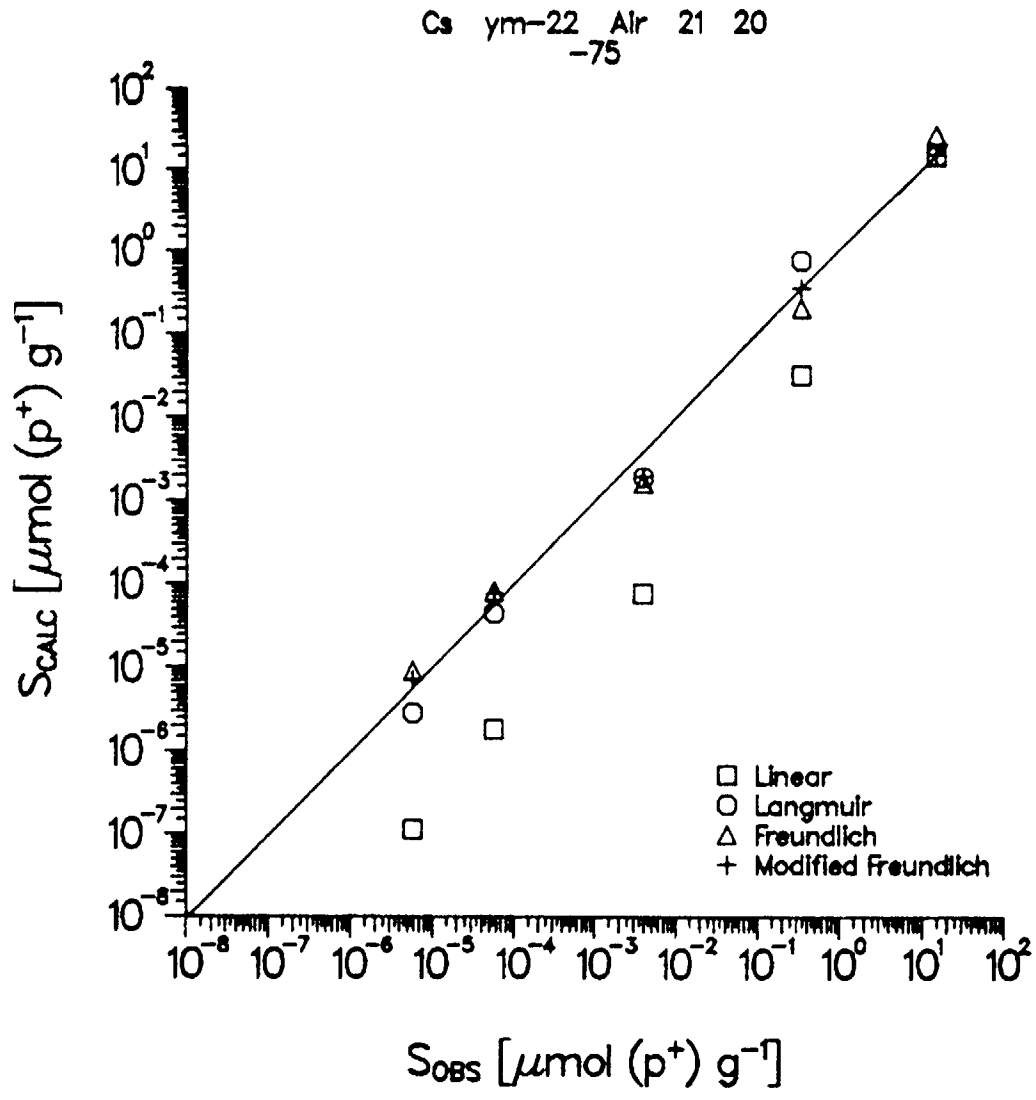

Ba ym-22 Air 21 20
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	12.0005379	0.9996	0.18185401
Kd =	12.00053787				
LANGMUIR	5	0.0033563	0.0639887	0.9954	0.00281587
b =	15.62775517				
k =	19.06508446				
FREUNDLICH	5	1.3633571	0.7989938	0.9883	0.33001456
K =	23.08644485				
N =	0.79899383				
MODIFIED FREUNDLICH	5	0.4750488	0.8635553	0.9963	0.20003089
A =	59.71435928				
B =	0.86355525				
KD =	3.54901743				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

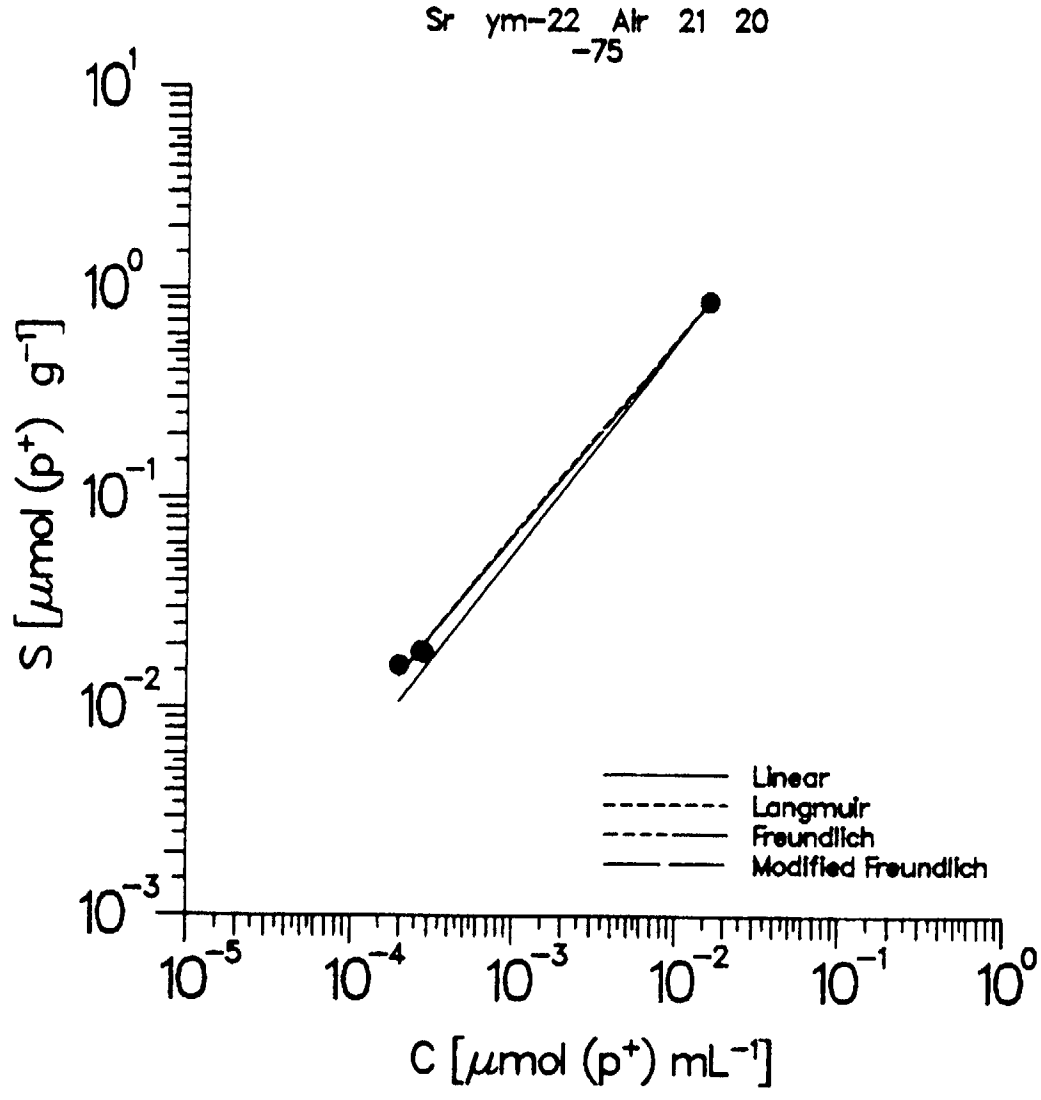

Cs ym-22 Air 21 20
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

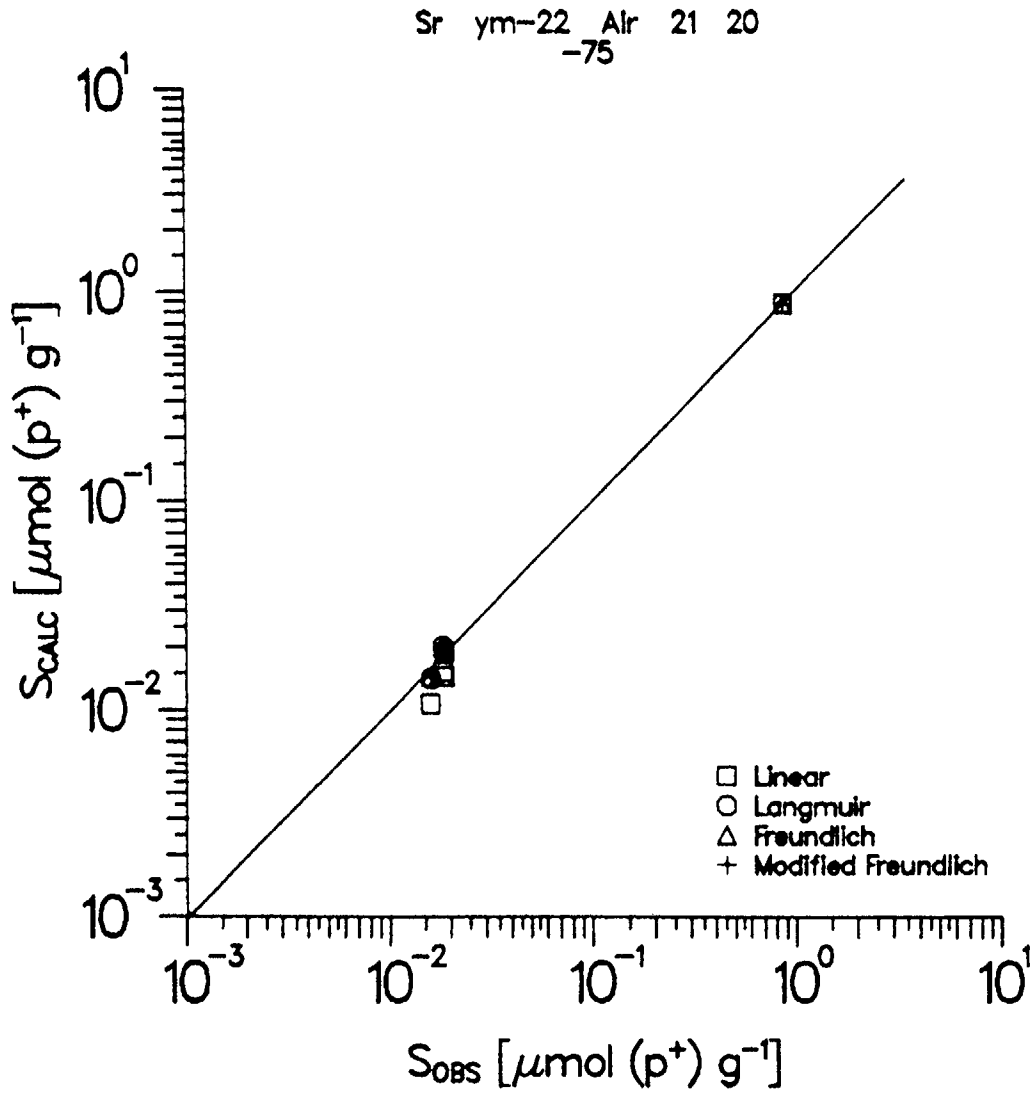

Cs ym-22 Air 21 20
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	4	0.0000000	54.0857773	0.9999	0.00529847
Kd =	54.08577728				
LANGMUIR	4	0.0139199	0.2828040	0.7761	0.00148362
b =	3.53601766				
k =	20.31651306				
FREUNDLICH	4	1.6035200	0.9297567	0.9984	0.04173877
K =	40.13470078				
N =	0.92975670				
MODIFIED FREUNDLICH	4	0.3405390	0.9401864	0.9984	0.04254356
A =	43.80956650				
B =	0.94018638				
KD =	2.30252147				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

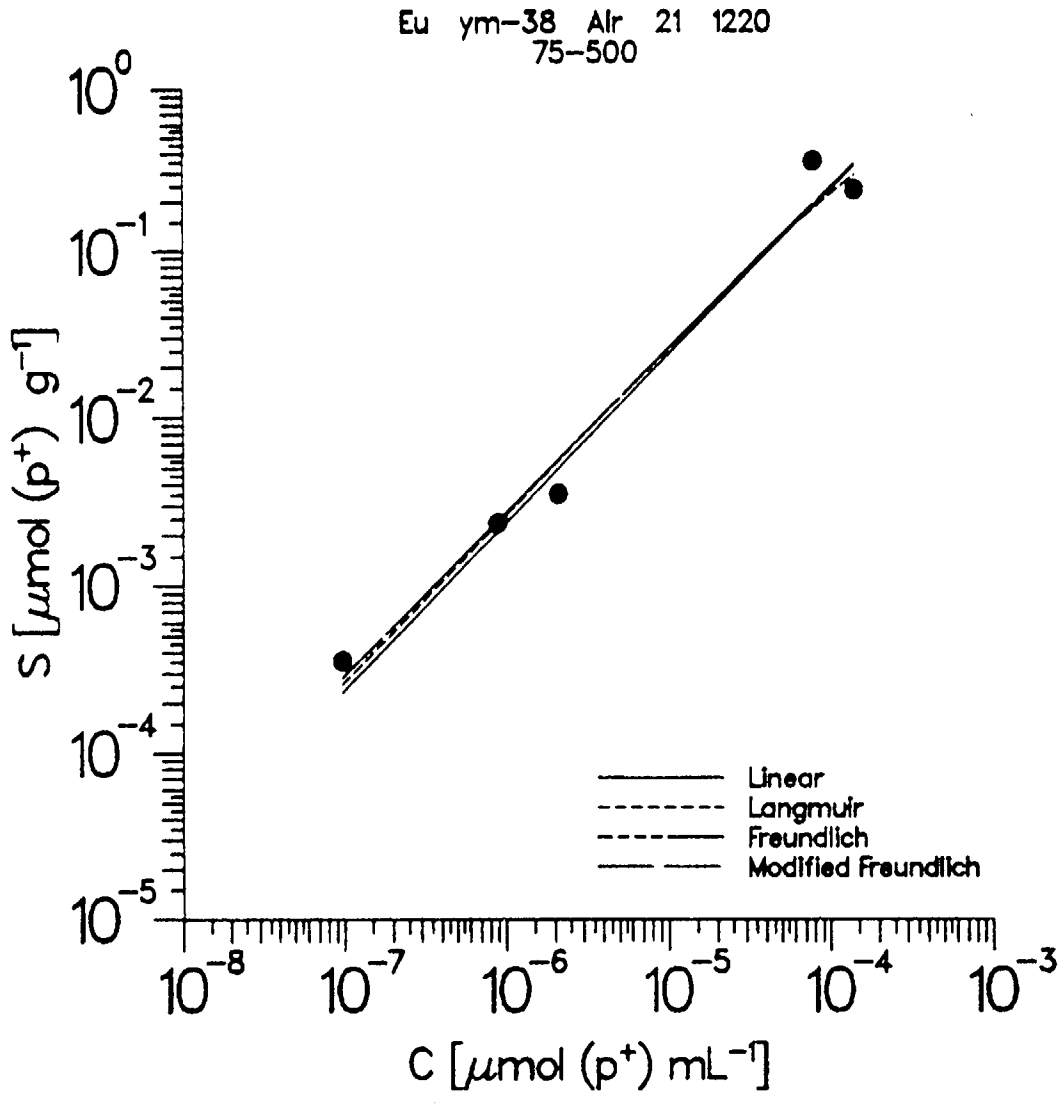

Sr ym-22 Alr 21 20
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

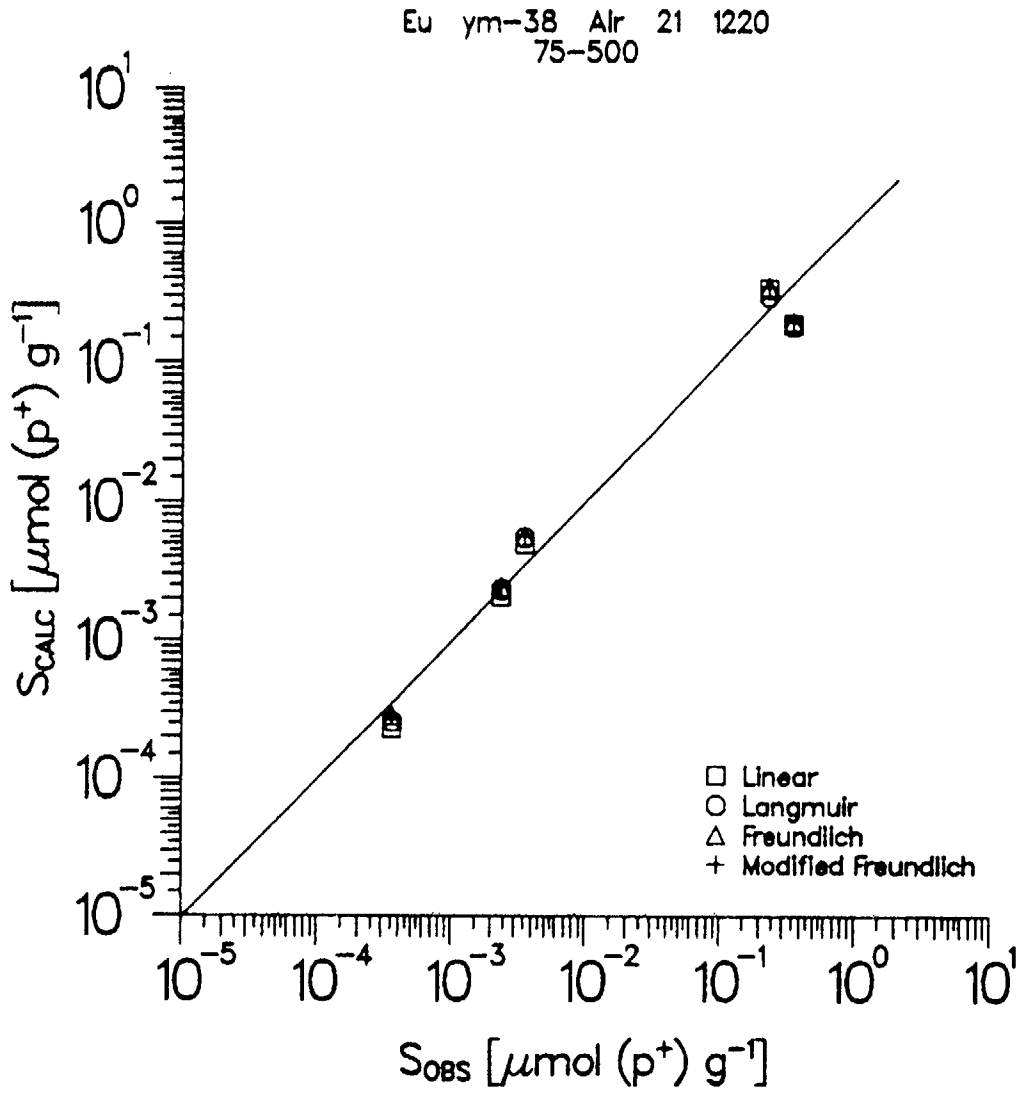

Sr ym-22 Air 21 20
-75
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	2379.0139160	0.7882	0.11408564
Kd =	2379.01391602				
LANGMUIR	5	0.0003761	0.7063261	0.0650	0.00019503
b =	1.41577661				
k =	1878.22998047				
FREUNDLICH	5	3.2917325	0.9751889	0.9786	0.22248343
K =	1957.63879395				
N =	0.97518891				
MODIFIED FREUNDLICH	5	0.2056379	0.9752305	0.9786	0.22250593
A =	1958.83459473				
B =	0.97523052				
KD =	1.62502801				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

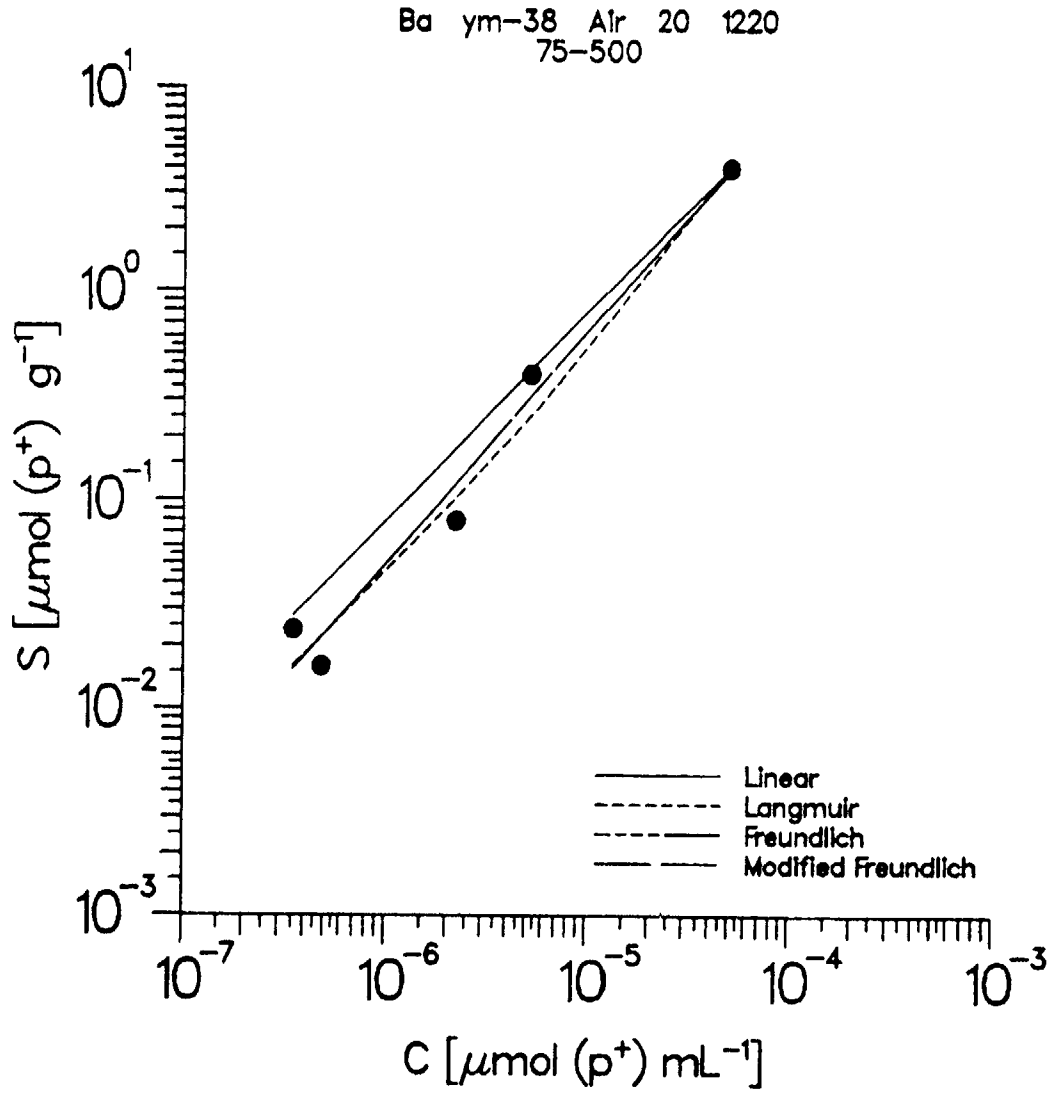

Eu ym-38 Air 21 1220
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

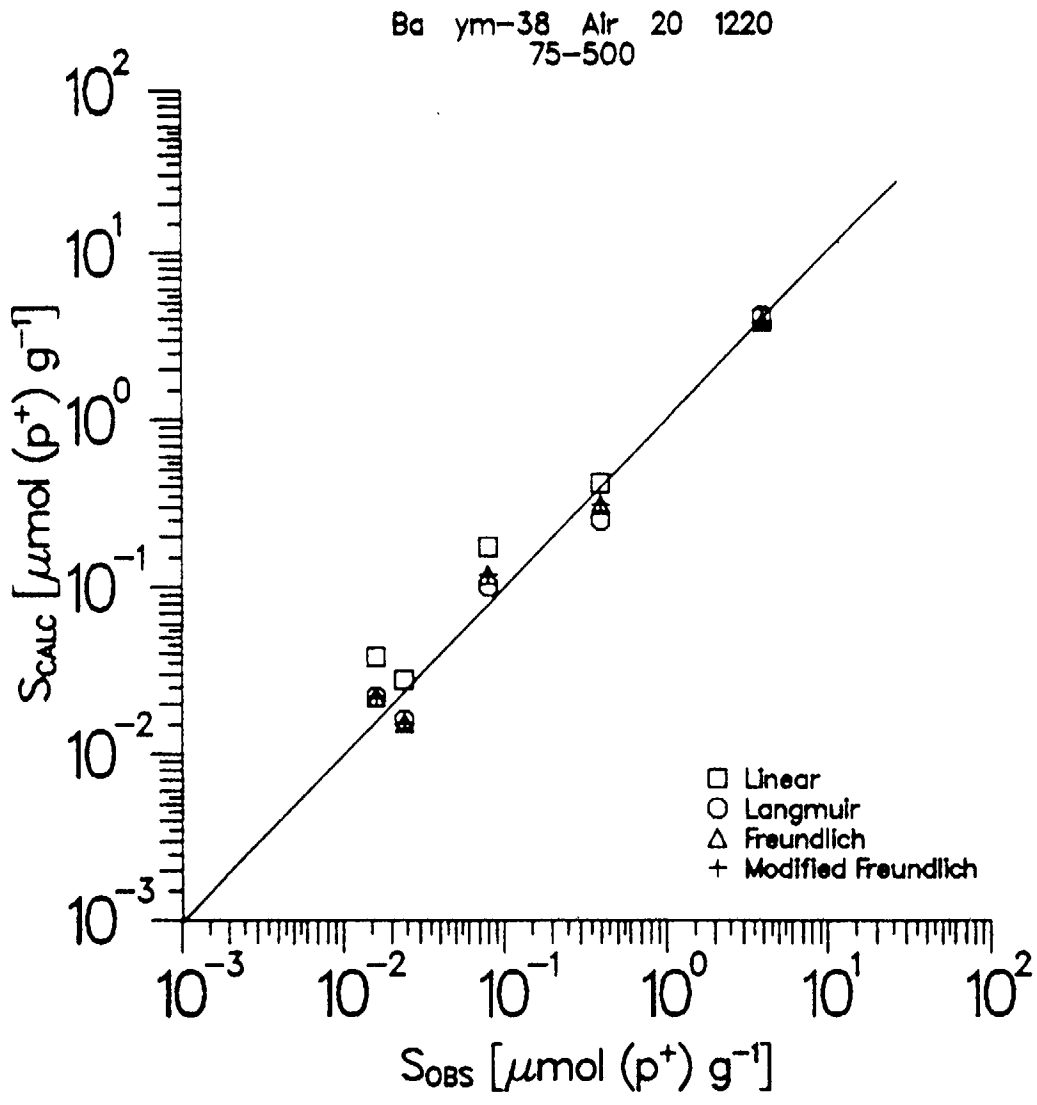

Eu ym-38 Air 21 1220
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	78921.1015625	0.9994	0.05786219
Kd = 78921.10156250					
LANGMUIR	5	0.0000221	-0.1961672	0.2496	0.00000856
b = -5.09769106					
k = -8891.04296875					
FREUNDLICH	5	5.3600082	1.1114445	0.9750	0.17941441
K = 229091.10937500					
N = 1.11144447					
MODIFIED FREUNDLICH	5	2.2774434	1.1120648	0.9750	0.17947264
A = 231101.76562500					
B = 1.11206484					
KD = 111.67121887					

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

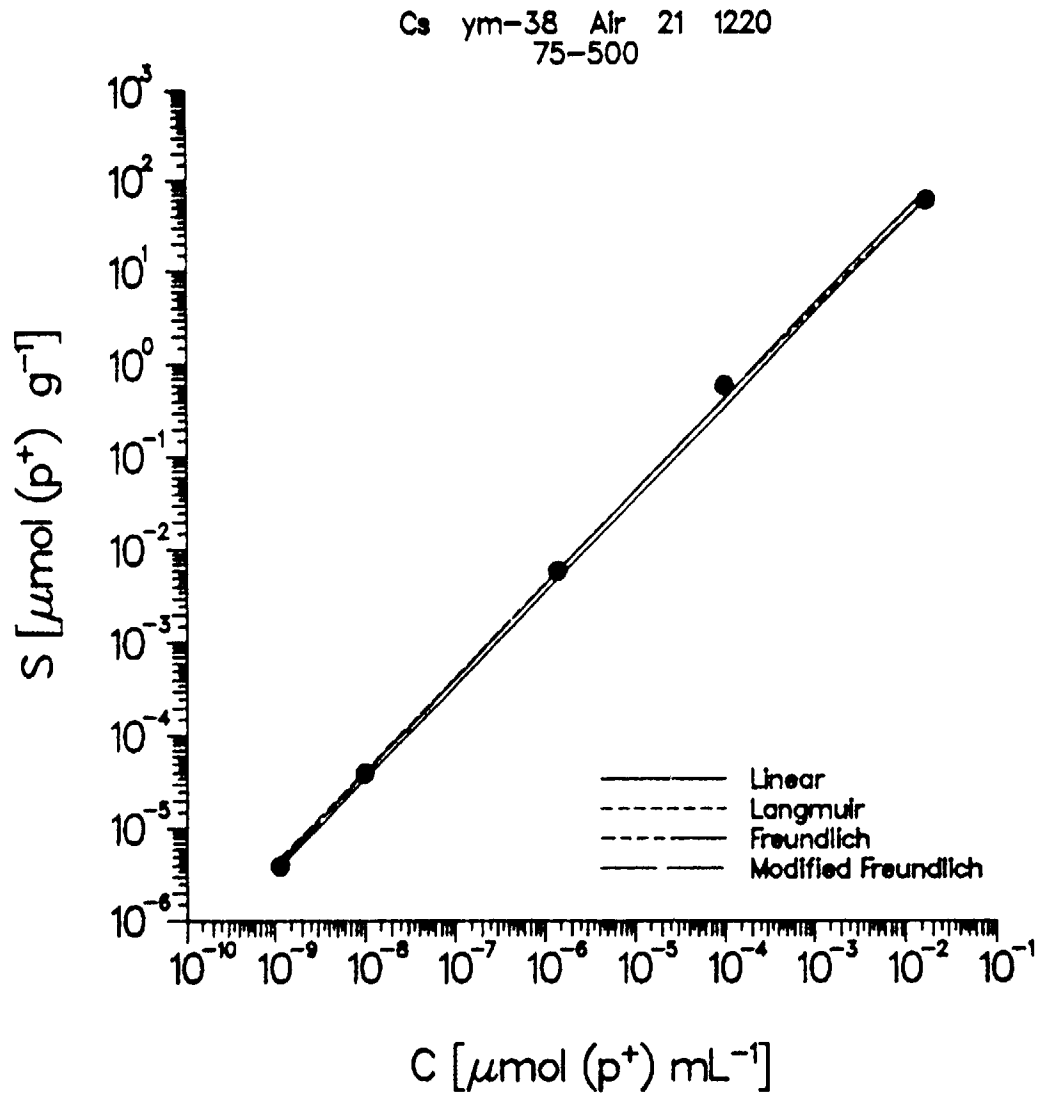

Ba ym-38 Air 20 1220
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

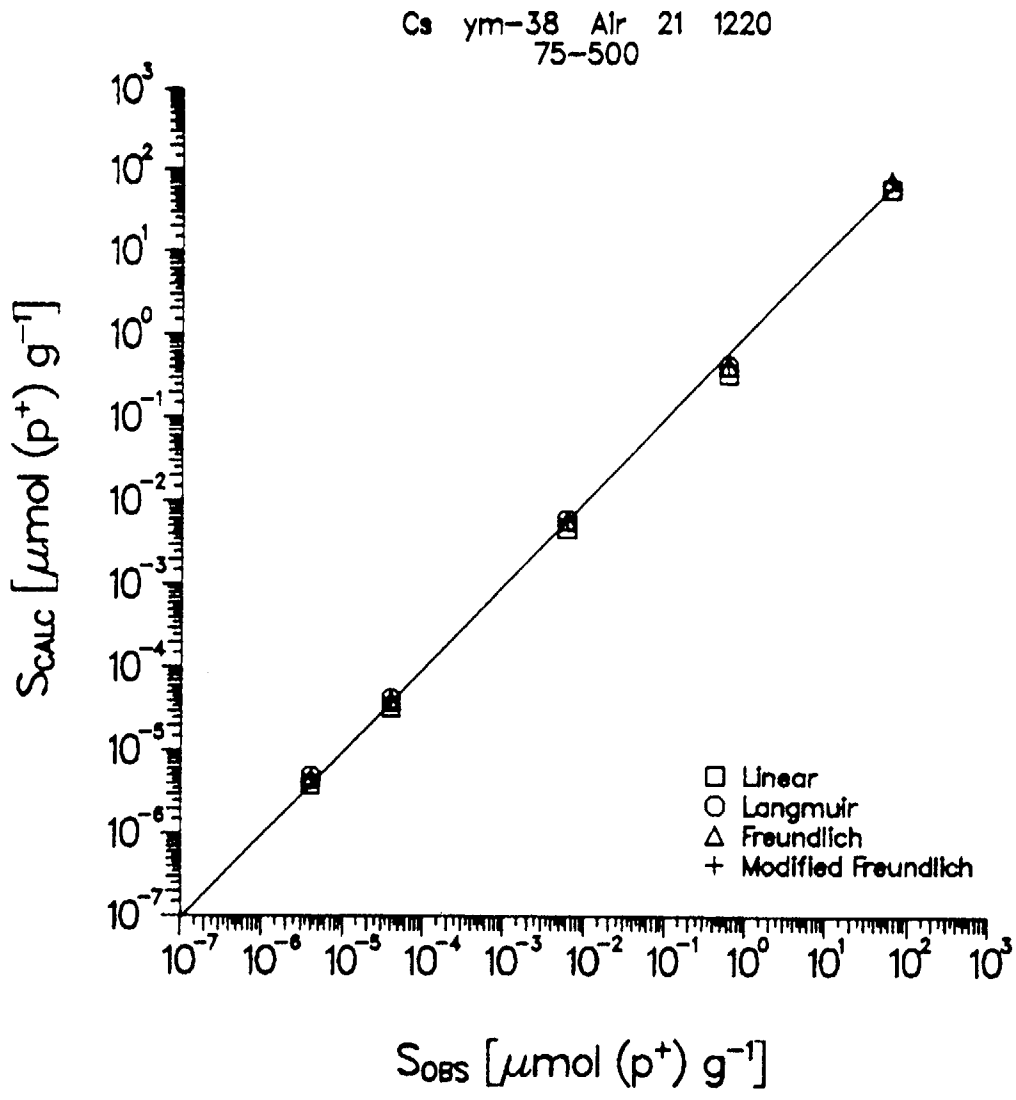

Ba ym-38 Air 20 1220
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	3405.7980957	1.0000	0.14959799
Kd =	3405.79809570				
LANGMUIR	5	0.0002353	0.0033123	0.2611	0.00005028
b =	301.90576172				
k =	14.07886696				
FREUNDLICH	5	3.6511989	1.0062014	0.9989	0.11190912
K =	4479.18359375				
N =	1.00620139				
MODIFIED FREUNDLICH	5	0.5836210	1.0087211	0.9991	0.10500961
A =	4677.14550781				
B =	1.00872111				
KD =	3.78944159				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

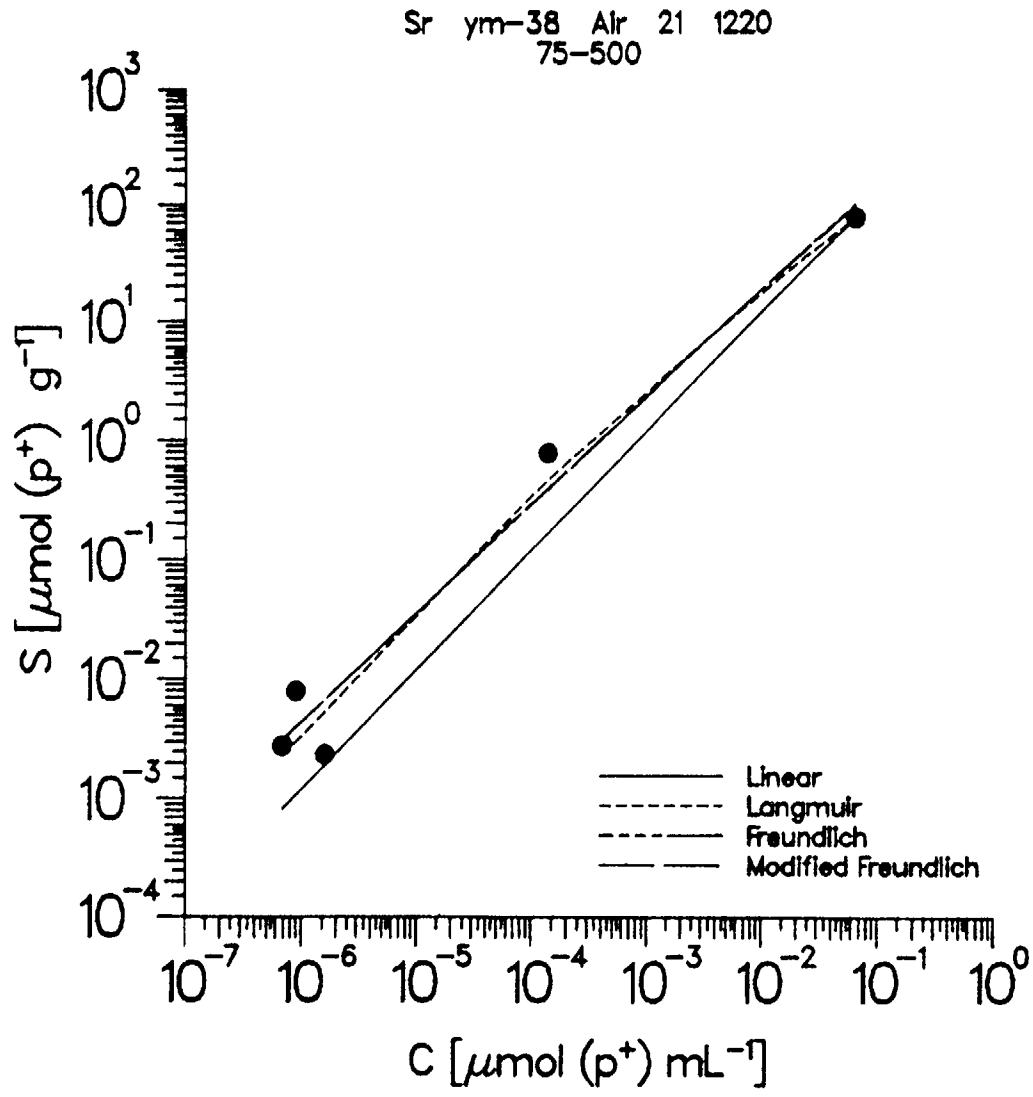

Cs ym-38 Air 21 1220
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

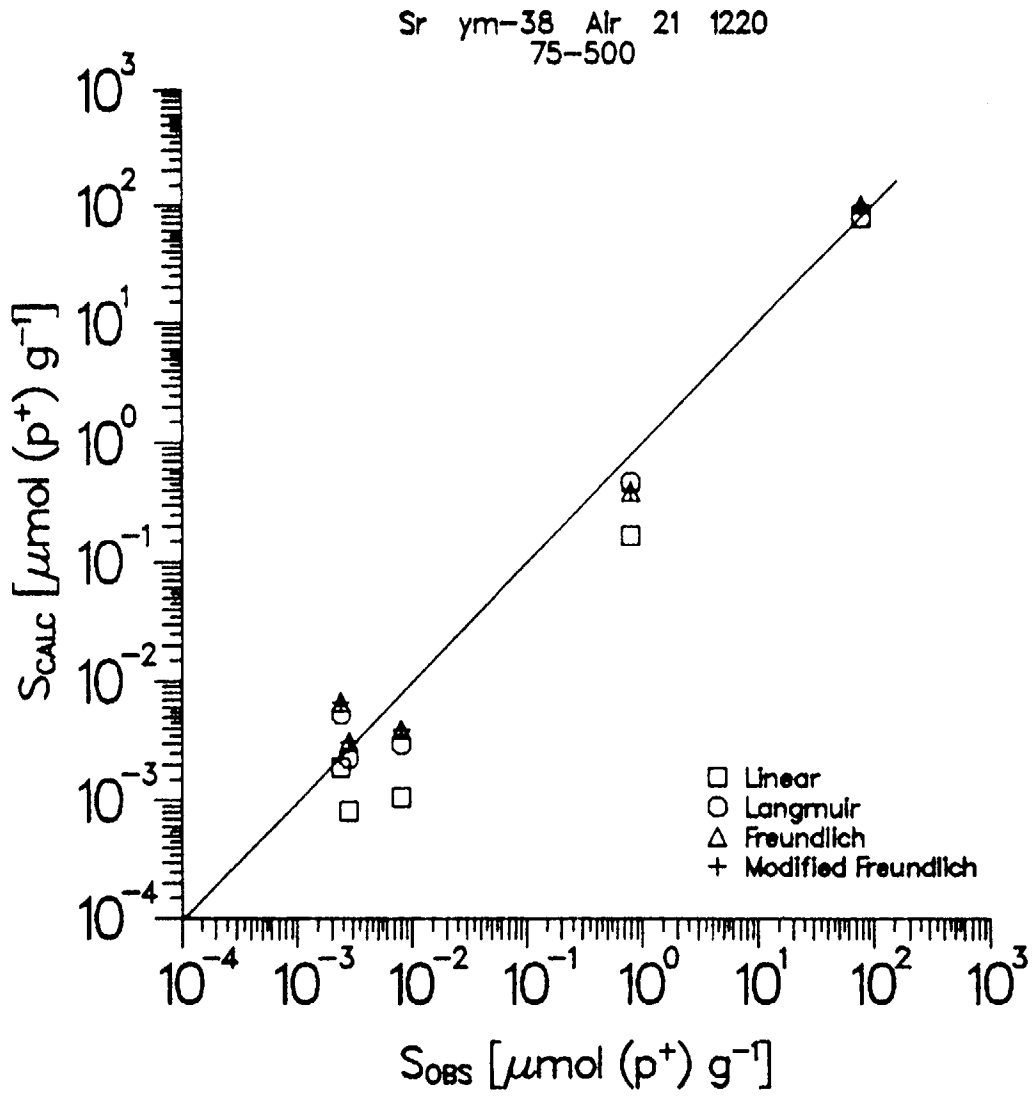

Cs ym-38 Air 21 1220
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	1199.7155762	0.9999	0.36309218
Kd =	1199.71557617				
LANGMUIR	5	0.0002991	0.0081434	0.5468	0.00025100
b =	122.79814148				
k =	27.22876549				
FREUNDLICH	5	3.0871513	0.9071071	0.9736	0.36863047
K =	1222.22534180				
N =	0.90710711				
MODIFIED FREUNDLICH	5	0.0317945	0.9125617	0.9743	0.36566234
A =	1312.66650391				
B =	0.91256166				
KD =	1.08353019				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

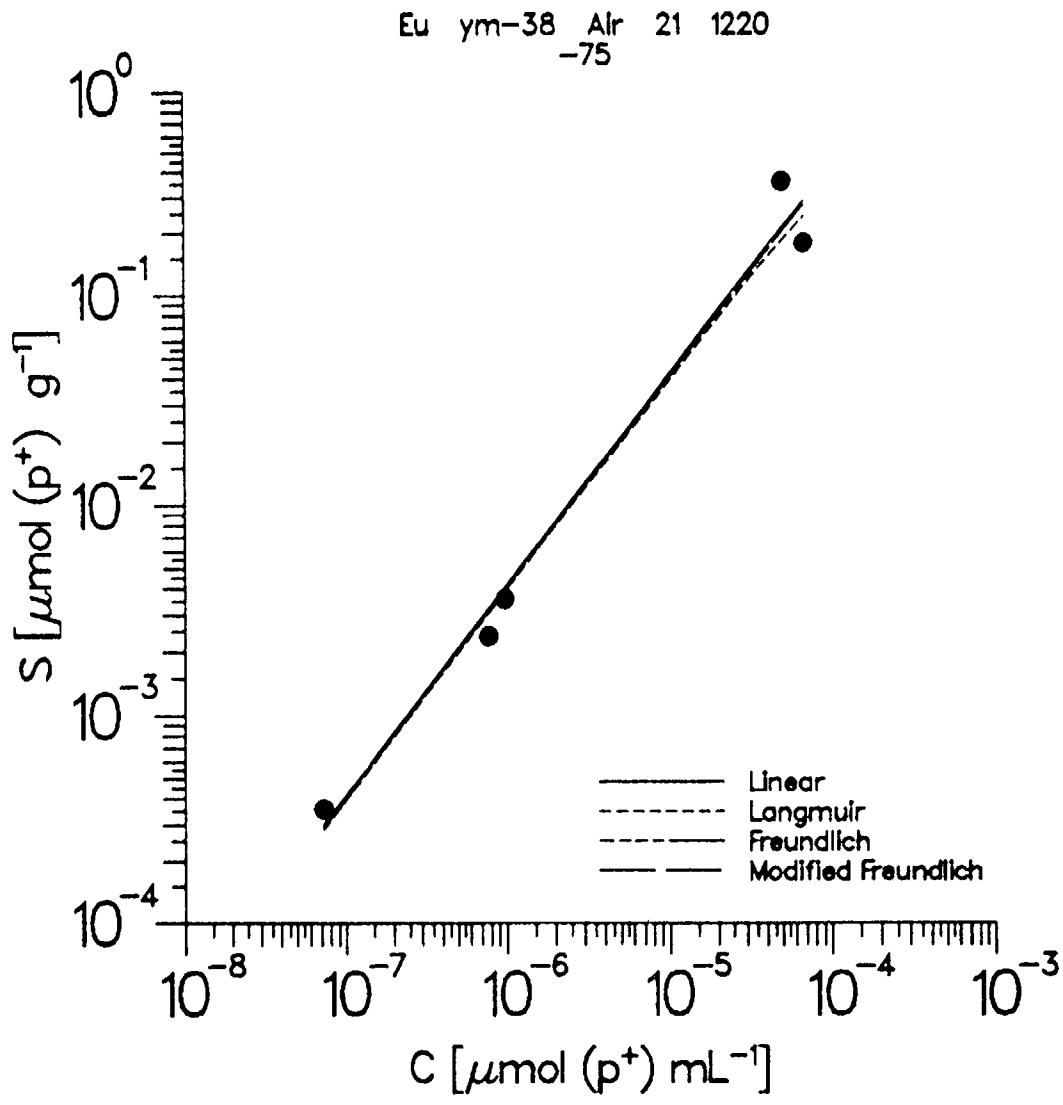

Sr ym-38 Air 21 1220
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

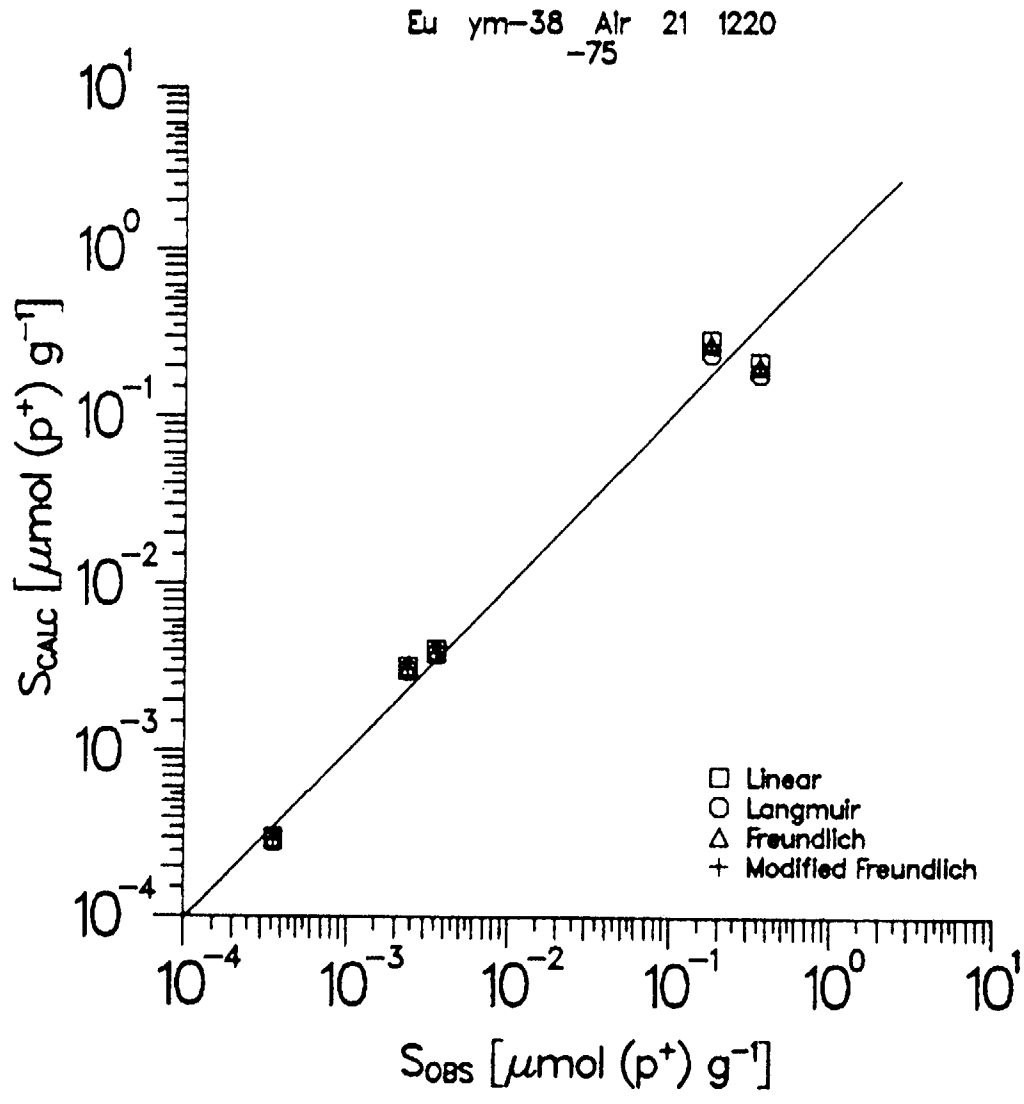

Sr ym-38 Air 21 1220
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	4184.2578125	0.7921	0.10560074
Kd =	4184.25781250				
LANGMUIR	5	0.0002519	0.4829596	0.0273	0.00010977
b =	2.07056642				
k =	1917.30212402				
FREUNDLICH	5	3.5856454	0.9965077	0.9820	0.19962683
K =	3851.63769531				
N =	0.99650770				
MODIFIED FREUNDLICH	5	0.4995337	0.9965454	0.9820	0.19965670
A =	3853.83813477				
B =	0.99654543				
KD =	3.17150402				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

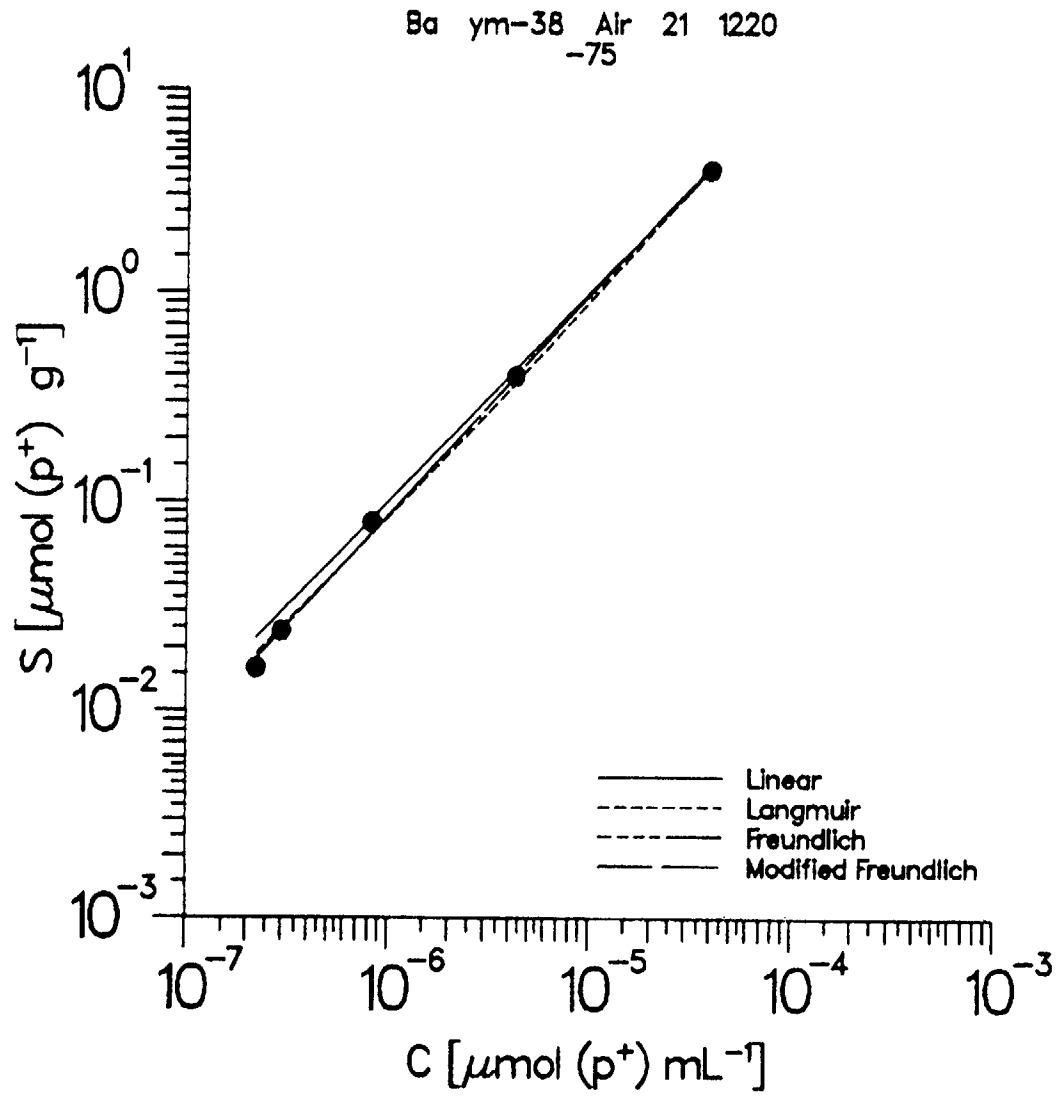

Eu ym-38 Air 21 1220
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

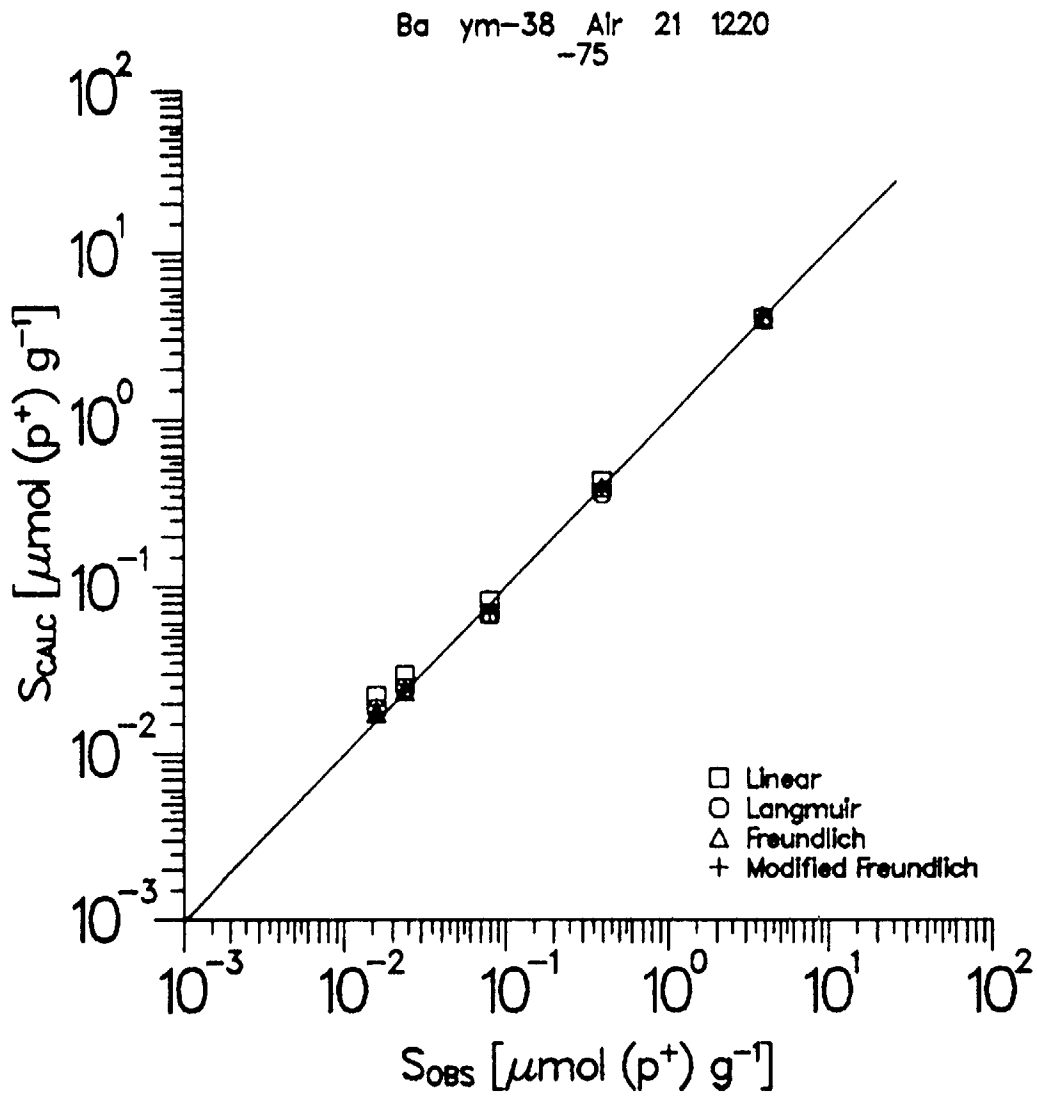

Eu ym-38 Air 21 1220
-75
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	99917.1875000	0.9999	0.01795388
Kd = 99917.18750000					
LANGMUIR	5	0.0000119	-0.0510031	0.2966	0.00000157
b = -19.60666275					
k = -4278.86962891					
FREUNDLICH	5	5.2373405	1.0504571	0.9986	0.04213389
K = 172719.14062500					
N = 1.05045712					
MODIFIED FREUNDLICH	5	2.1547260	1.0510467	0.9986	0.04188322
A = 174215.12500000					
B = 1.05104673					
KD = 112.22155762					

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

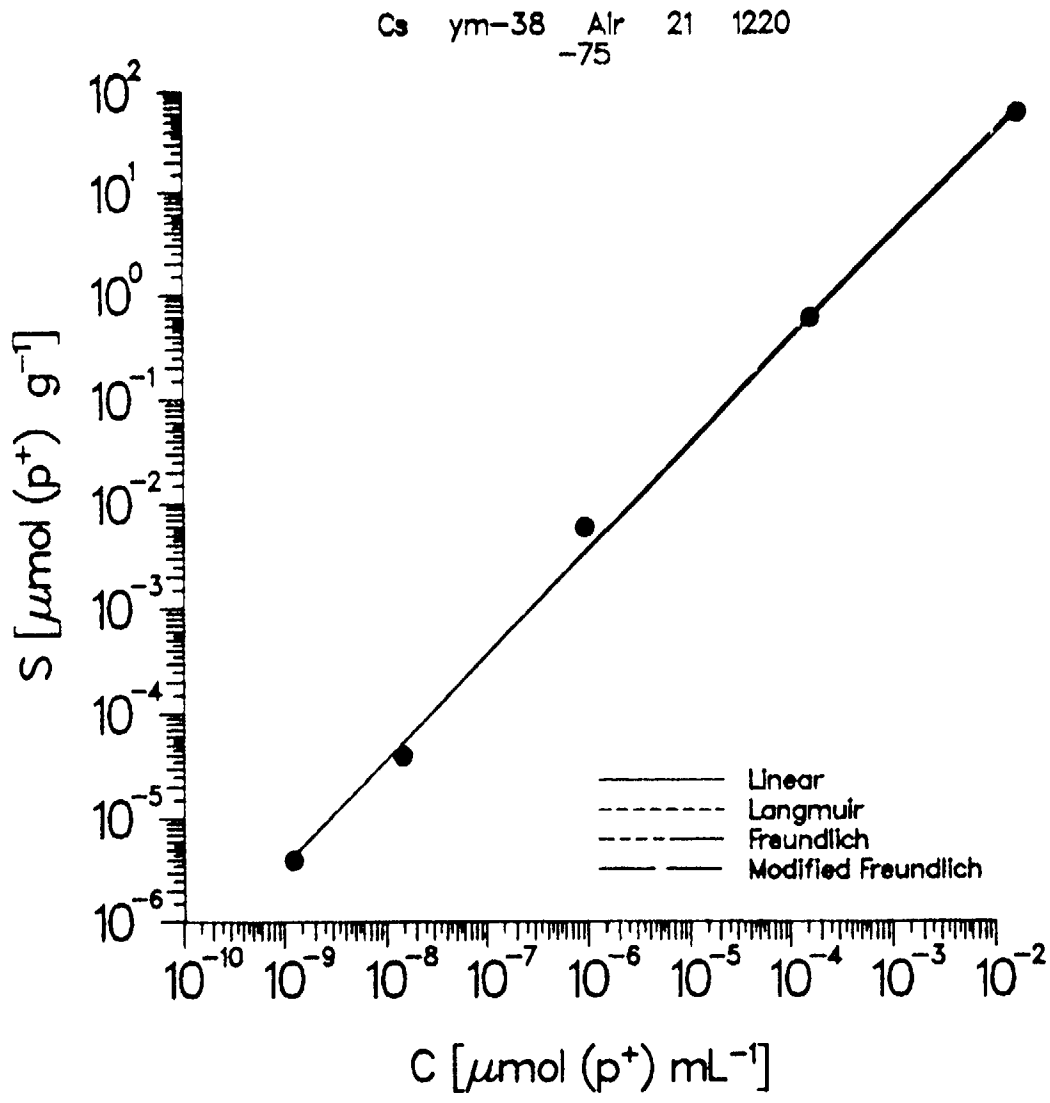

Ba ym-38 Air 21 1220
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

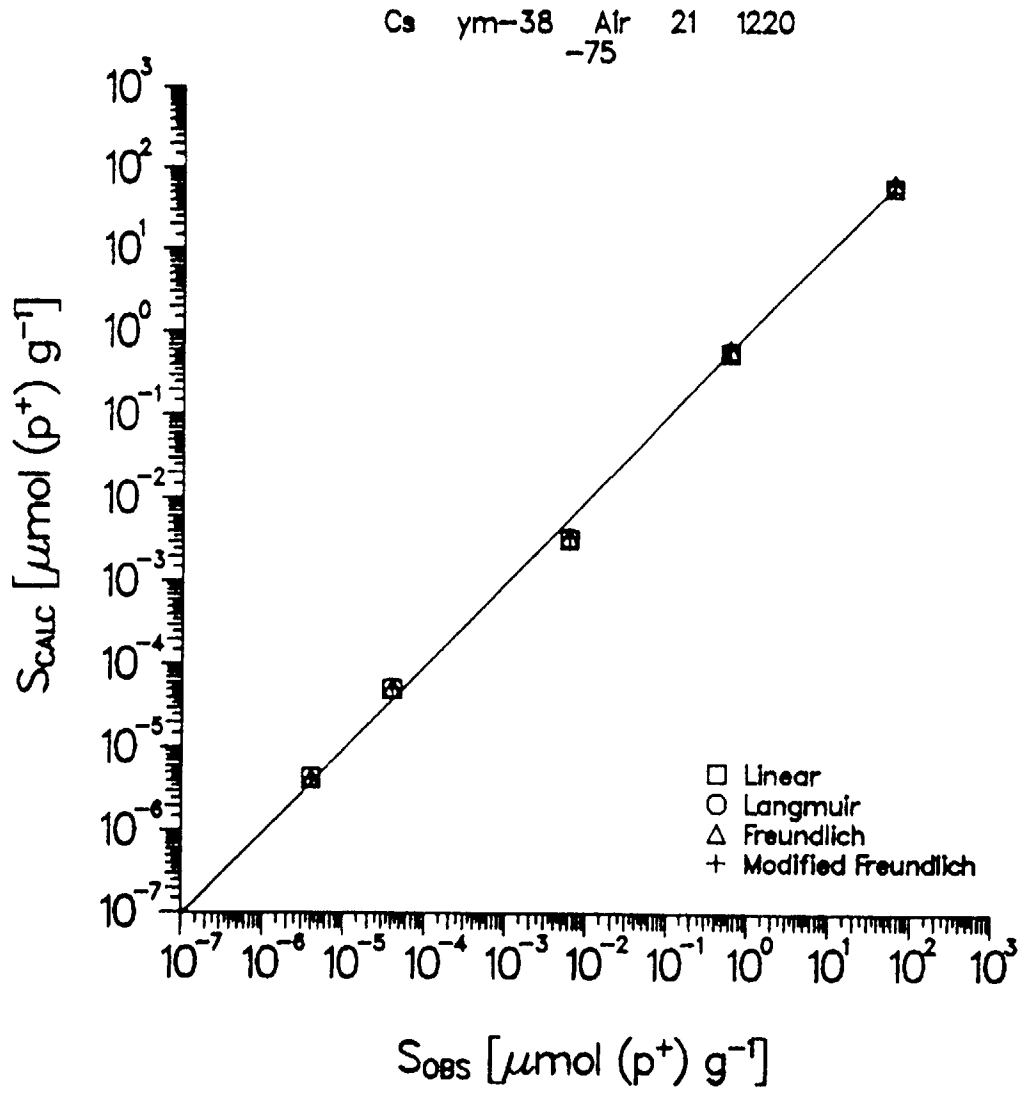

Ba ym-38 Air 21 1220
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	3511.7822266	1.0000	0.01804220
Kd =	3511.78222656				
LANGMUIR	5	0.0002776	0.0004188	0.0017	0.00008934
b =	2388.02954102				
k =	1.50872052				
FREUNDLICH	5	3.6249123	1.0096211	0.9979	0.15633136
K =	4216.11328125				
N =	1.00962114				
MODIFIED FREUNDLICH	5	0.5571618	1.0121293	0.9980	0.15352440
A =	4400.69873047				
B =	1.01212931				
KD =	3.55209684				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

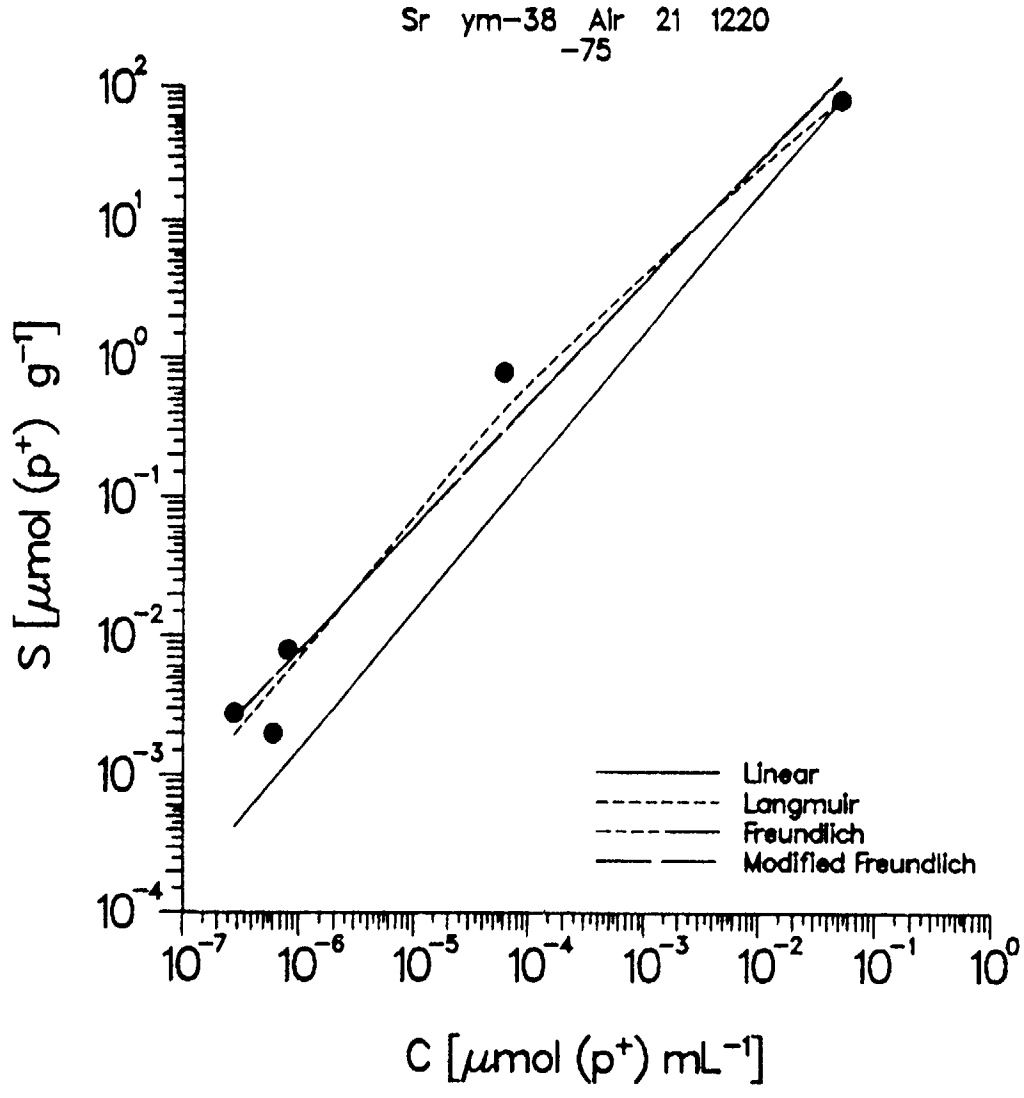

Cs ym-38 Air 21 1220
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

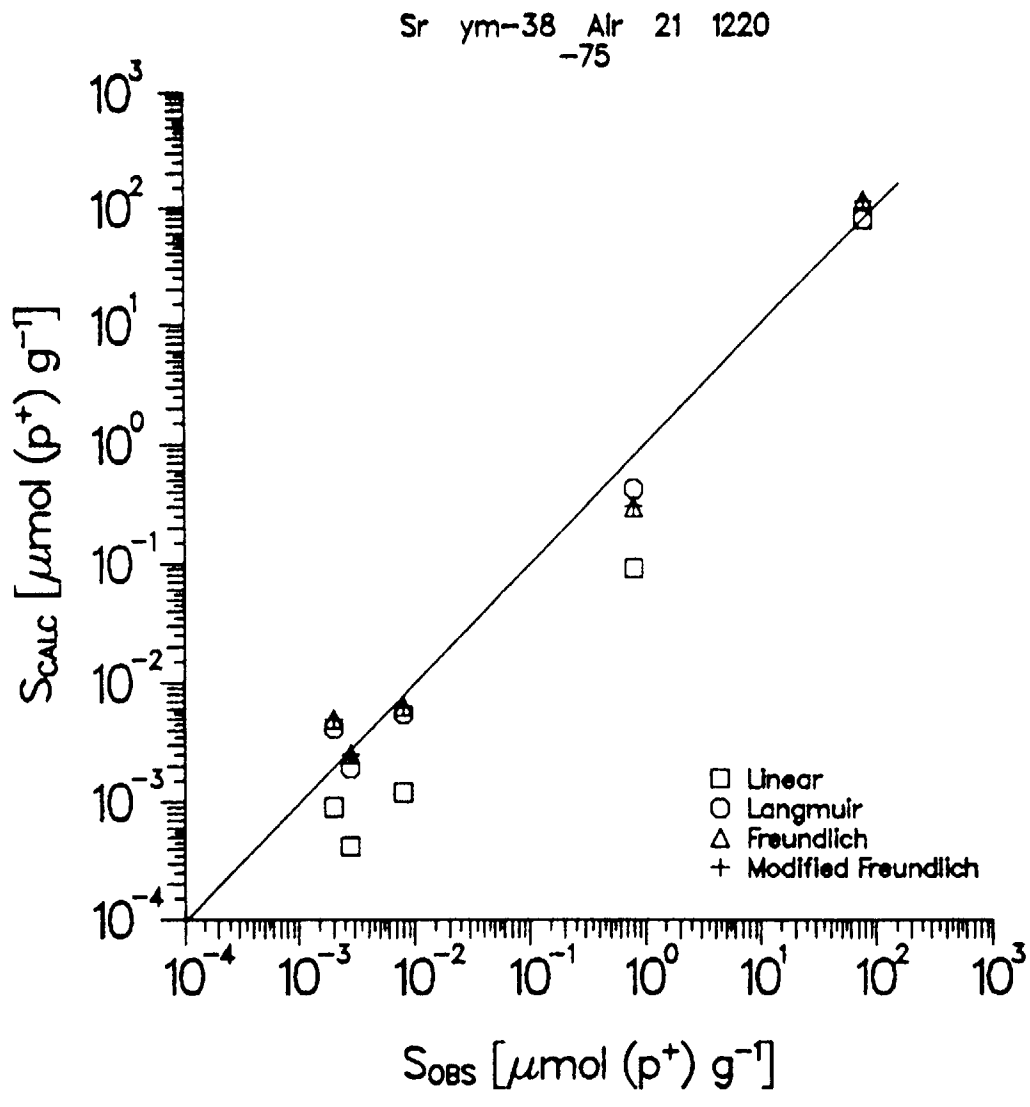

Cs ym-38 Air 21 1220
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1220 micromol (p+)/g
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	1500.0157471	0.9999	0.40804890
Kd =	1500.01574707				
LANGMUIR	5	0.0001447	0.0099218	0.8664	0.00010581
b =	100.78855133				
k =	68.56639862				
FREUNDLICH	5	3.2027719	0.8852442	0.9756	0.35726085
K =	1595.04113770				
N =	0.88524419				
MODIFIED FREUNDLICH	5	0.1483974	0.8906047	0.9764	0.35271487
A =	1716.94848633				
B =	0.89060467				
KD =	1.46766007				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

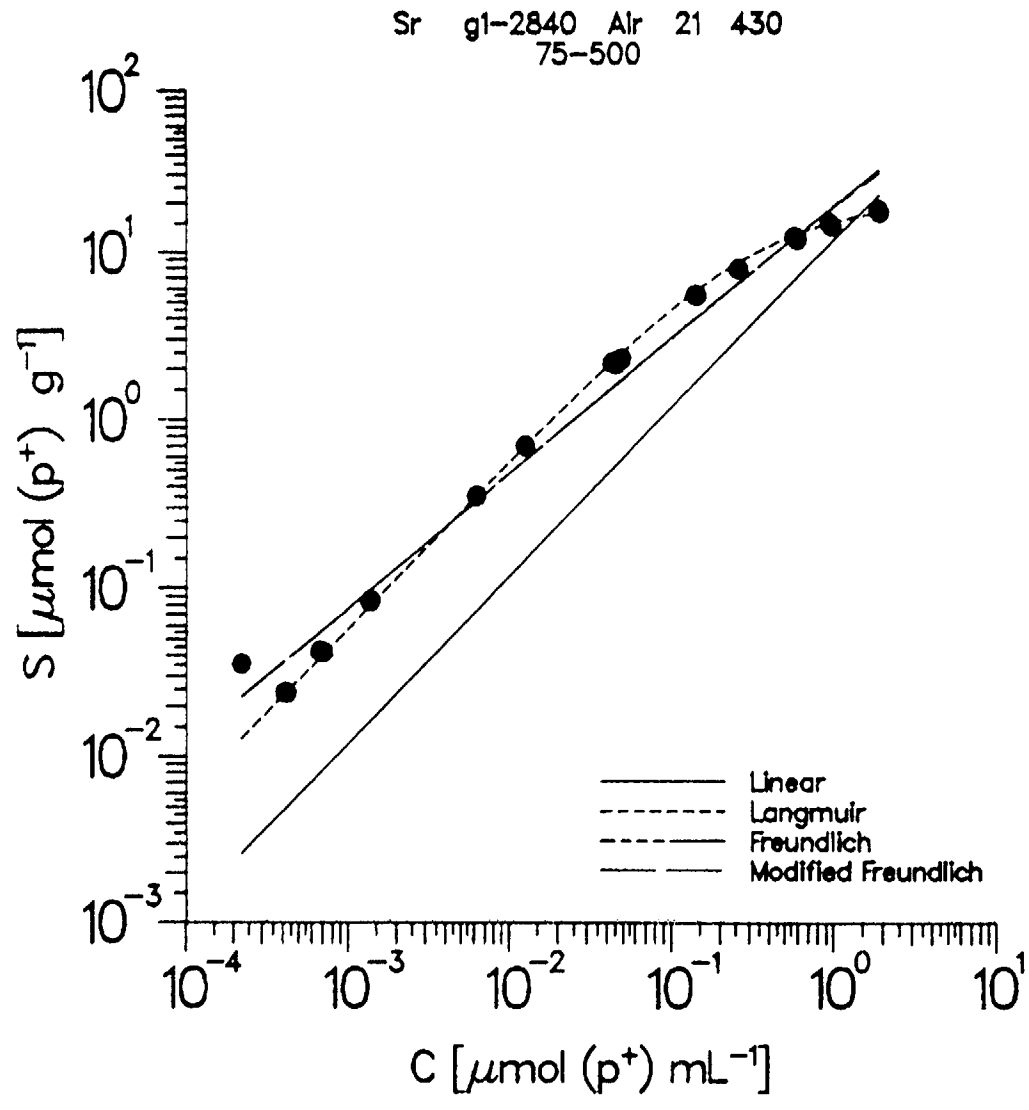

Sr ym-38 Air 21 1220
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

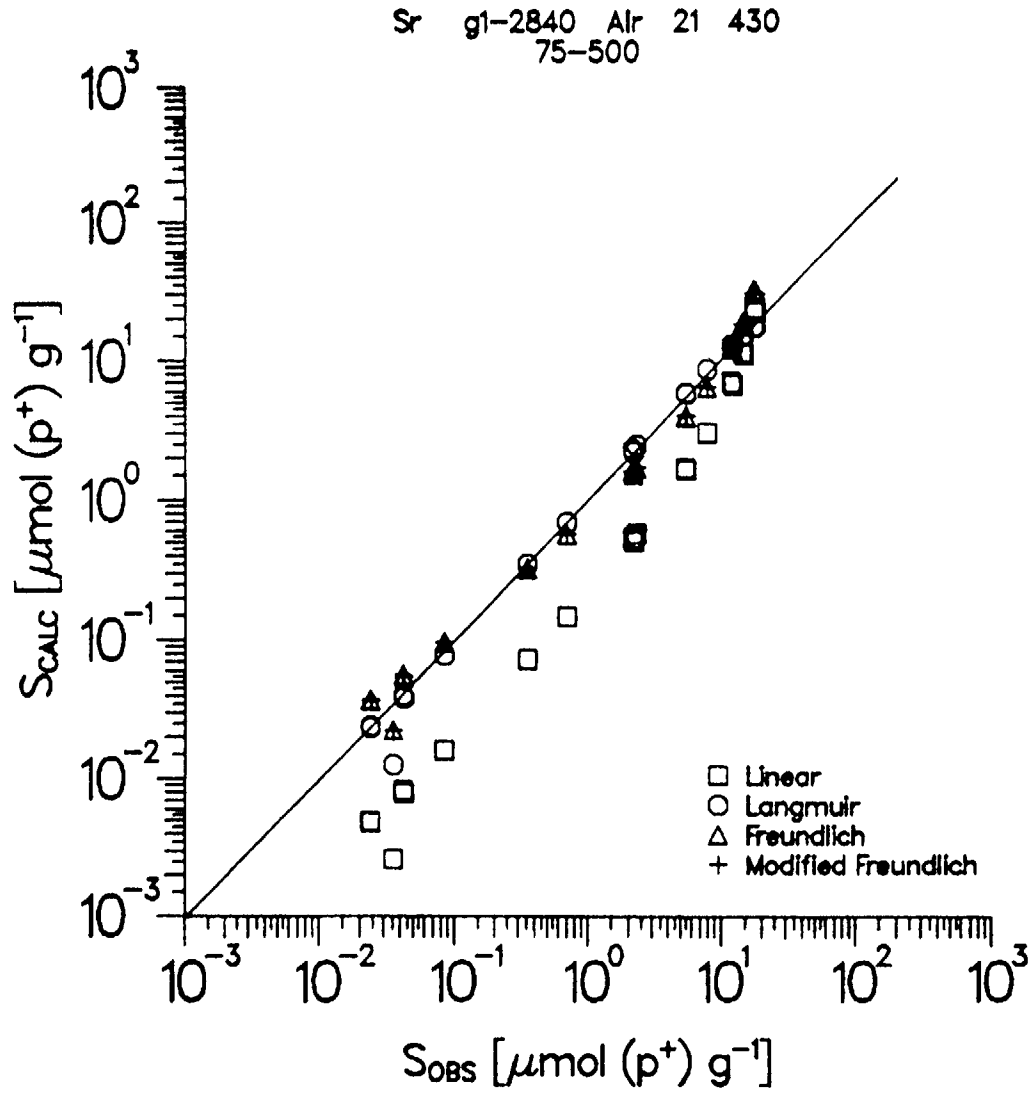

Sr ym-38 Air 21 1220
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = gl-2840
TIME = 21 days
ATMOS = Air
CEC = 430 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	25	0.0000000	11.7581921	0.8664	3.04291487
Kd =	11.75819206				
LANGMUIR	25	0.0174508	0.0477379	0.9879	0.00300400
b =	20.94772720				
k =	2.73556852				
FREUNDLICH	25	1.2794104	0.8004495	0.9825	0.13864766
K =	19.02875519				
N =	0.80044949				
MODIFIED FREUNDLICH	25	-1.3419210	0.8048776	0.9833	0.13619611
A =	19.56804657				
B =	0.80487758				
KD =	0.02151611				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

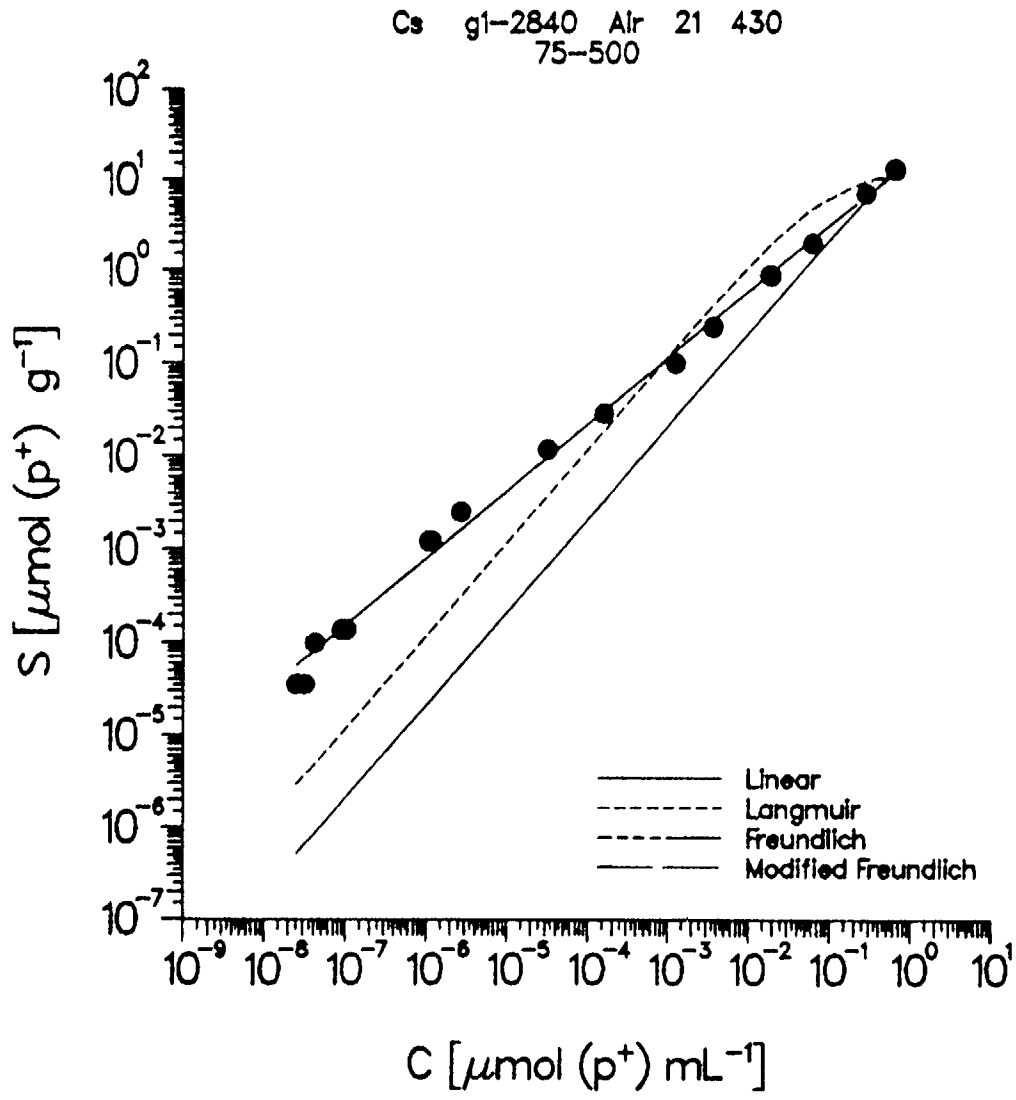

Sr g1-2840 Air 21 430
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

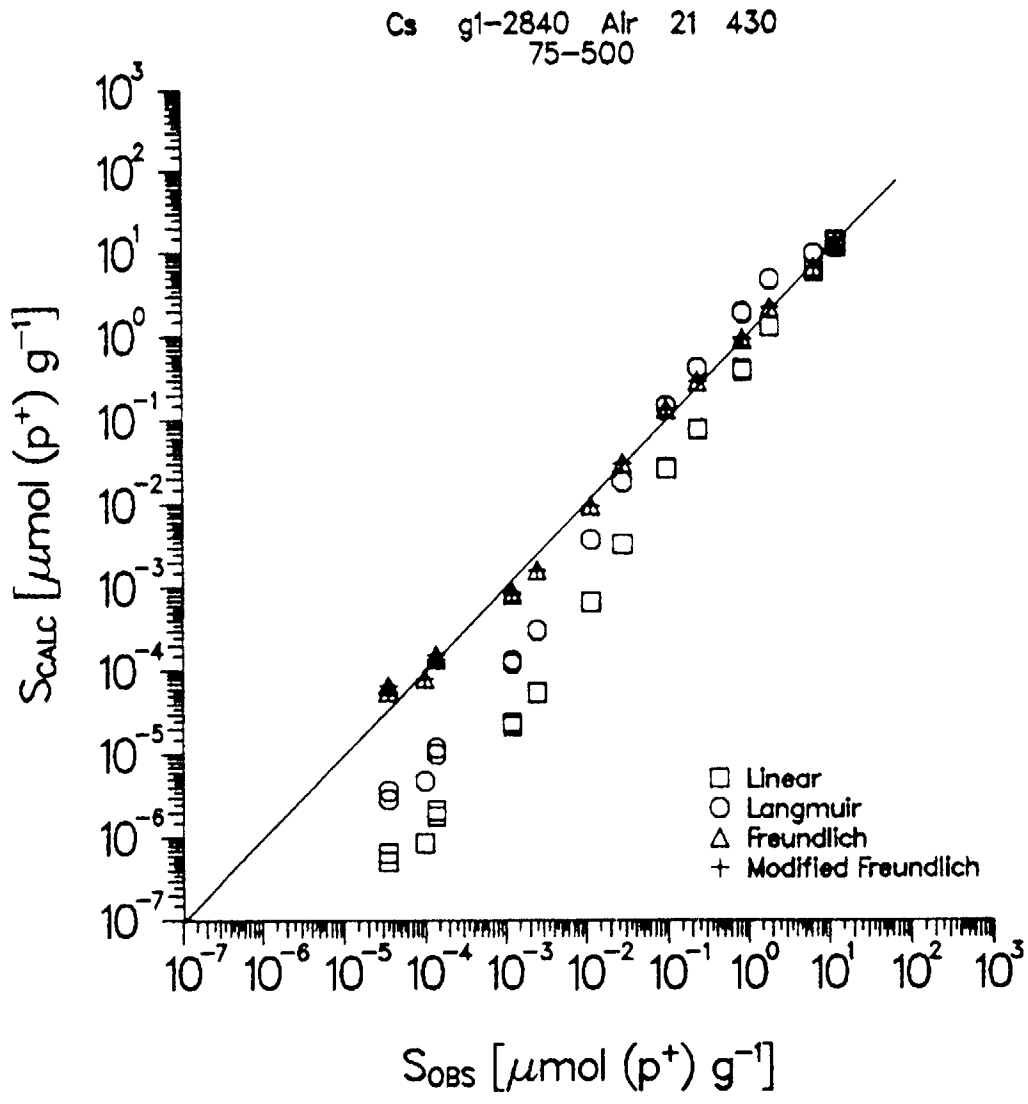

Sr g1-2840 Air 21 430
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = gl-2840
TIME = 21 days
ATMOS = Air
CEC = 430 micromol (p+)/g
SIZE = 75-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	25	0.0000000	20.7846336	0.9886	0.46947831
Kd =	20.78463364				
LANGMUIR	25	0.0085994	0.0745548	0.6991	0.00939863
b =	13.41295528				
k =	8.66975880				
FREUNDLICH	25	1.2029345	0.7163849	0.9959	0.11907169
K =	15.95638466				
N =	0.71638495				
MODIFIED FREUNDLICH	25	-1.4248178	0.7174003	0.9958	0.11960261
A =	16.16778946				
B =	0.71740025				
KD =	0.01032560				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.


Cs g1-2840 Air 21 430
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich


Cs g1-2840 Air 21 430
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

Appendix D

Isotherms Modeling: Case 2

In Appendix D, modeling efforts for case 2 are presented. Results from this case are summarized in Tables X and XI in the main body of this report. The information for each data set is sequentially organized as follows:

1. A table with estimated constants and statistical parameters for each isotherm.
2. Curves of adsorbed concentration S [μmol(p^+)/g] versus concentration in solution [μmolg(p^+)/mL] in a logarithmic scale. Both raw data and predictions by isotherms are included.
3. A graph with the calculated S-values versus observed S-values for all tested isotherms.

Tables and figures for the same data set are identified by the conditions defined in the table heading, which are also included in each figure in the same order but without units.

Units for constants are as follows: K_d in mL/g; b in μmol(p+)/g and k in mL/μmol(p+); K, N, A, β, and K_d have units corresponding to S in μmol(p+)/g and C in μmol(p+)/mL.

The following table of contents serves as a guide to locate the sample, e.g., YM-22, and respective experimental conditions, e.g., CEC = 14 micromol(p+)/g for particle sizes less than 75 microns, that identify the set used for isotherm modeling.

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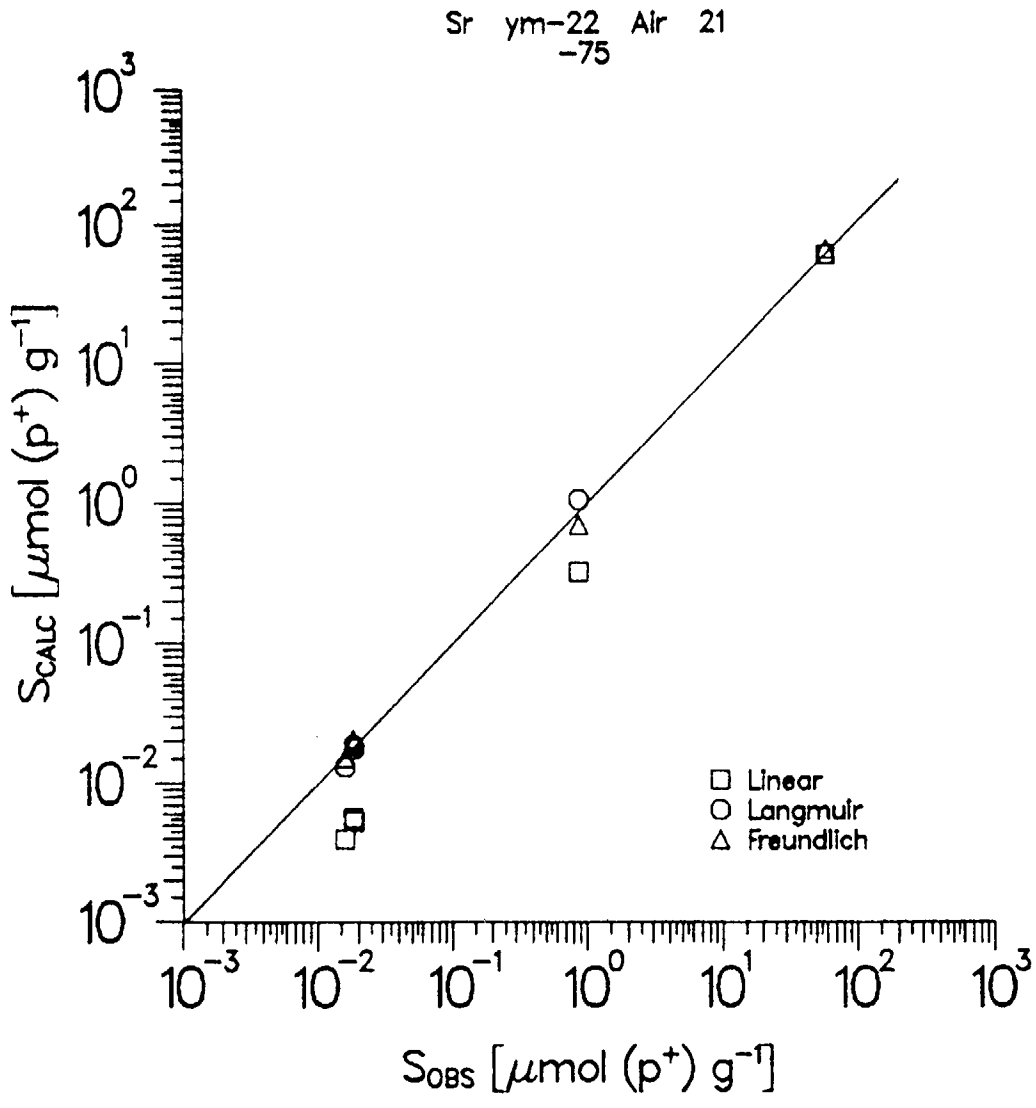
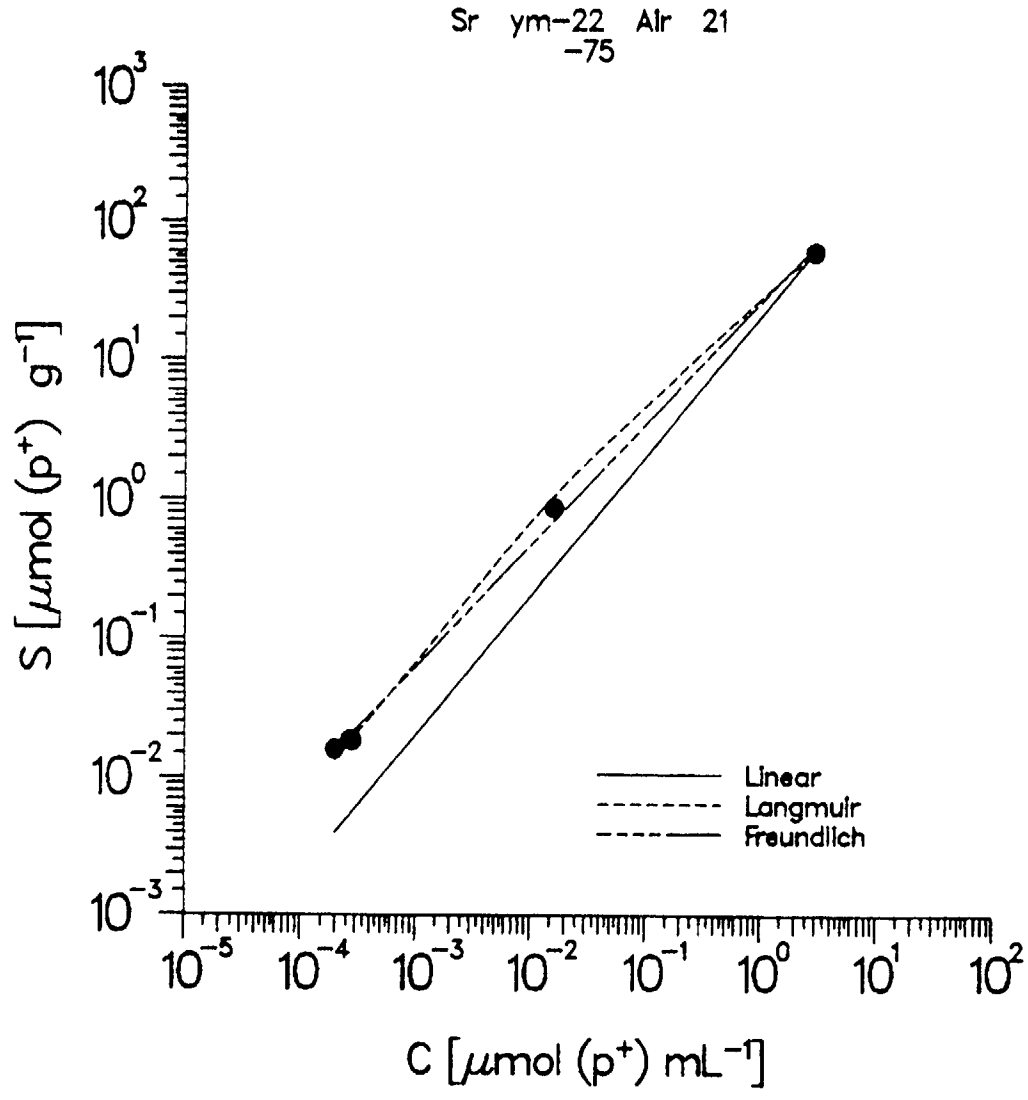
Printouts for Sr Isotherms (YM-22, 20 micromol(p+)/g, <75 μm). 236
Printouts for Sr Isotherms (YM-22, 20 micromol(p+)/g, 75-500 μm) 239

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = air
SIZE = - 75 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	20.0009956	0.9999	0.31881636
Kd =	20.00099564				
LANGMUIR	5	0.0150644	0.0116510	0.9814	0.00247881
b =	85.82984161				
k =	0.77341026				
FREUNDLICH	5	1.4042658	0.8698474	0.9985	0.06964244
K =	25.36680412				
N =	0.86984736				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K and N in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

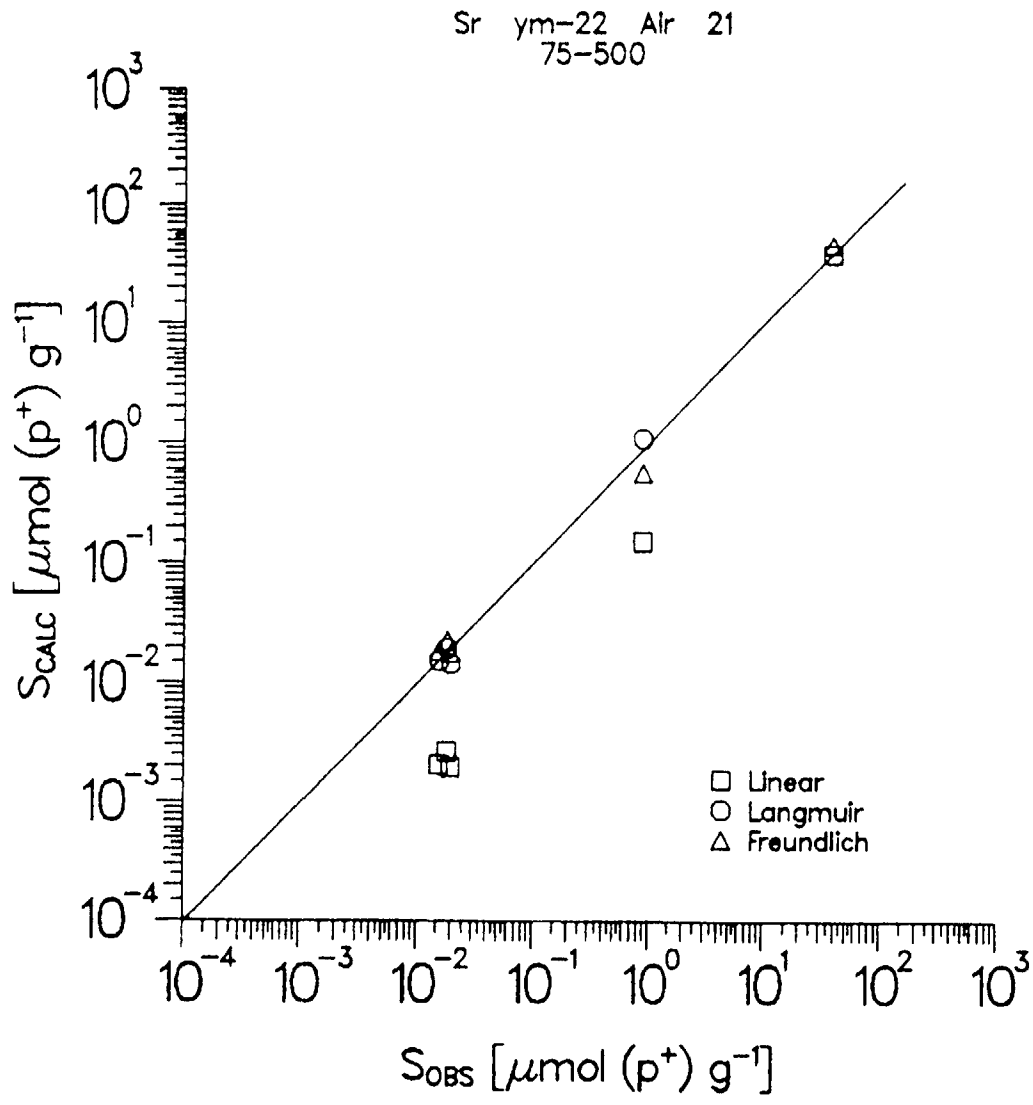

Sr ym-22 Air 21
-75
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
Linear
Langmuir
Freundlich

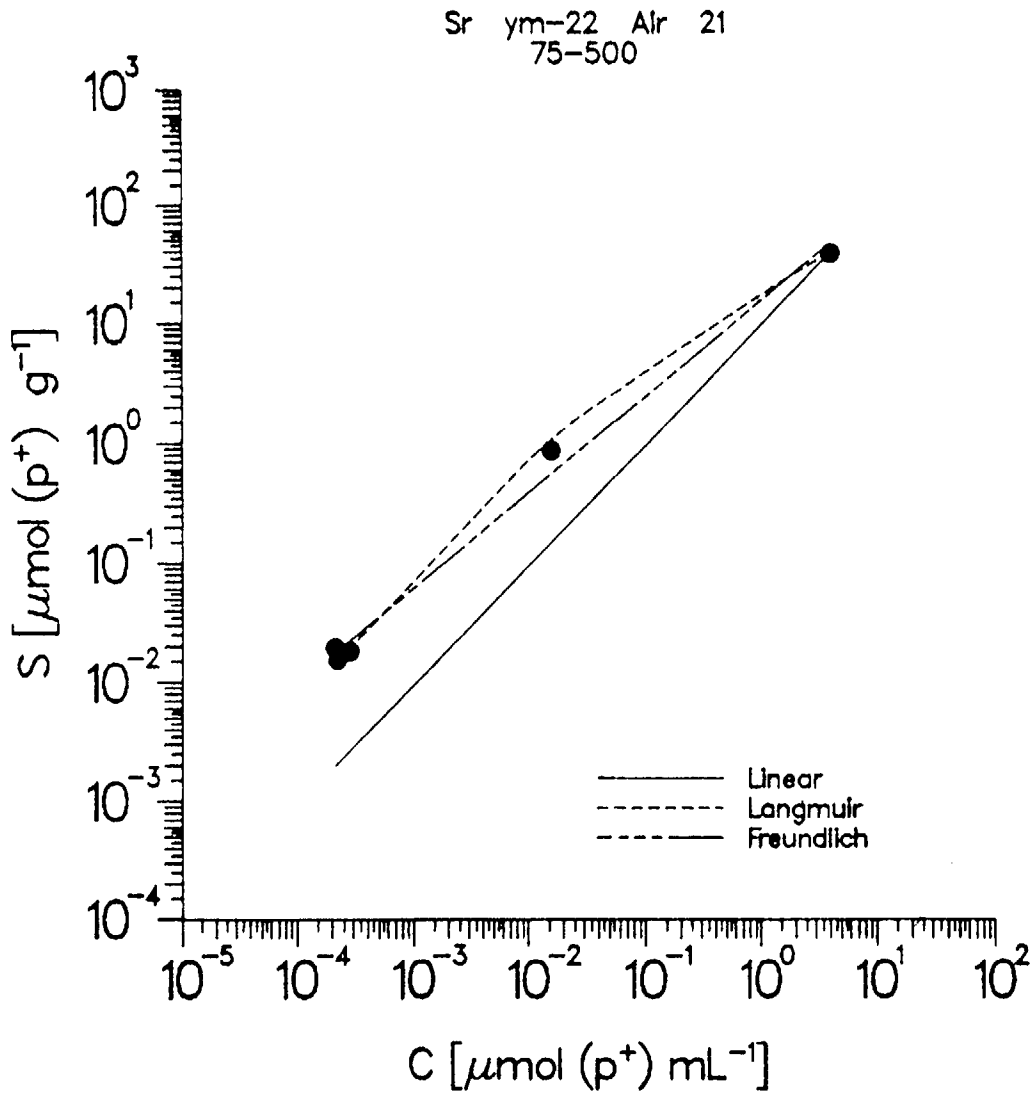

Sr ym-22 Alr 21
-75
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
SIZE = 75-500 microns

ISOTHERM	N	ALPHA	BETA	R**2	SSE
LINEAR	5	0.0000000	9.4124680	0.9996	0.42134419
Kd =	9.41246796				
LANGMUIR	5	0.0144442	0.0225046	0.9959	0.00302514
b =	44.43531036				
k =	1.5580374002				
FREUNDLICH	5	1.1803710	0.7967290	0.9933	0.14156452
K =	15.14854908				
N =	0.79672903				

N = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K and N in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.


Sr ym-22 Air 21
75-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3}
Linear
Langmuir
Freundlich


Sr ym-22 Alr 21
75-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich

Appendix E

Isotherms Modeling: Case 3

In Appendix E, modeling efforts for case 3 are presented. Results from this case are summarized in Tables XIII and XIV in the main body of this report. The information for each data set is sequentially organized as follows:

1. A table with estimated constants and statistical parameters for each isotherm.
2. Curves of adsorbed concentration S (μmol(p+)/g) versus concentration in solution (μmol(p+)/mL) in a logarithmic scale. Both raw data and predictions by isotherms are included.
3. A graph with the calculated S-values versus observed S-values for all tested isotherms.

Tables and figures for the same data set are identified by the conditions defined in the table heading, which are also included in each figure in the same order but without units.

Units for constants are as follows: K_d in mL/g; b in μmol(p+)/g and k in mL/μmol(p+); K, N, A, β, and K_d have units corresponding to S in μmol(p+)/g and C in μmol(p+)/mL.

The following table of contents serves as a guide to locate the sample, e.g., YM-22, and respective experimental conditions, e.g., CEC = 20 micromol(p+)/g and particle sizes less than 75, 75-500, and 106-500 microns, that identify the set used for isotherm modeling.

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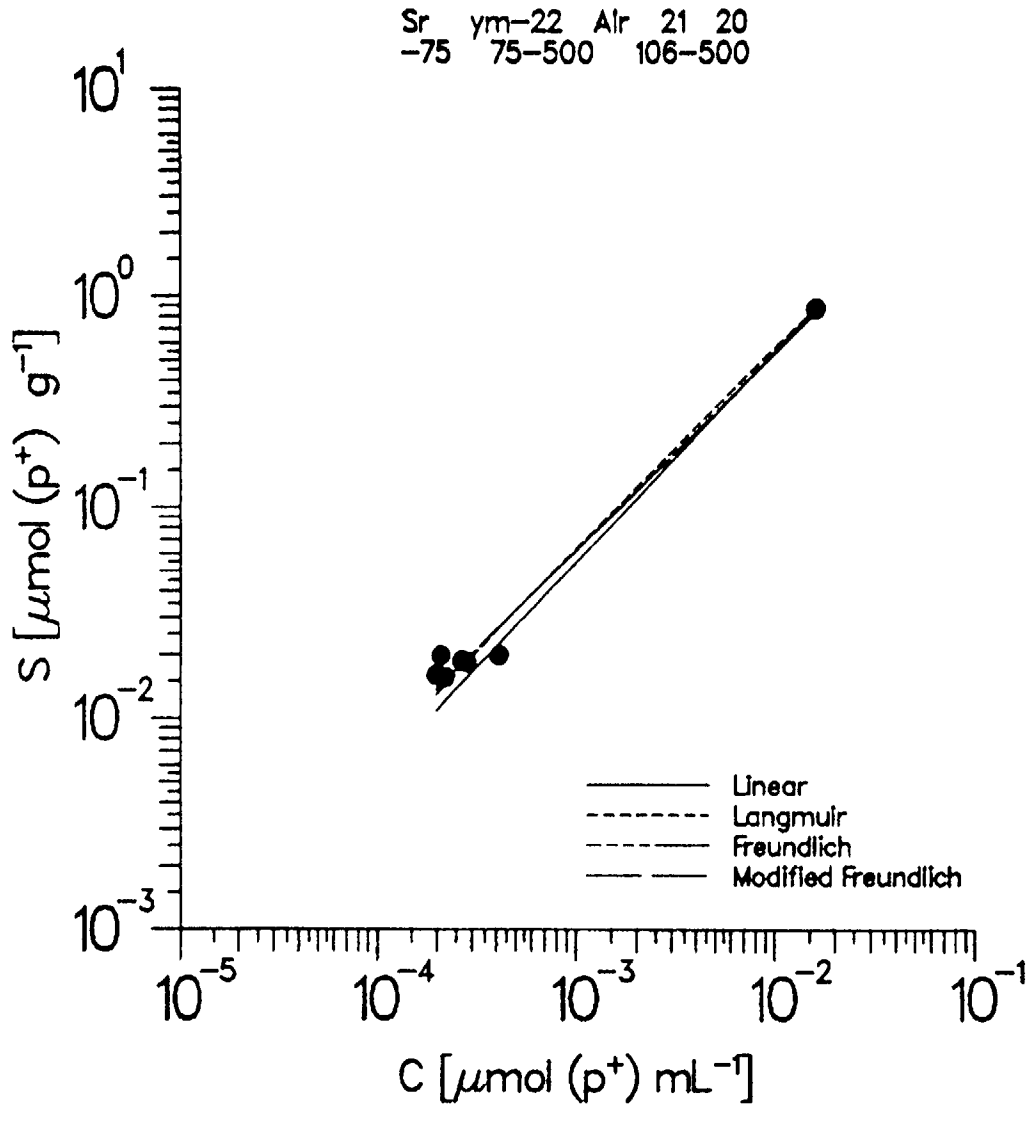
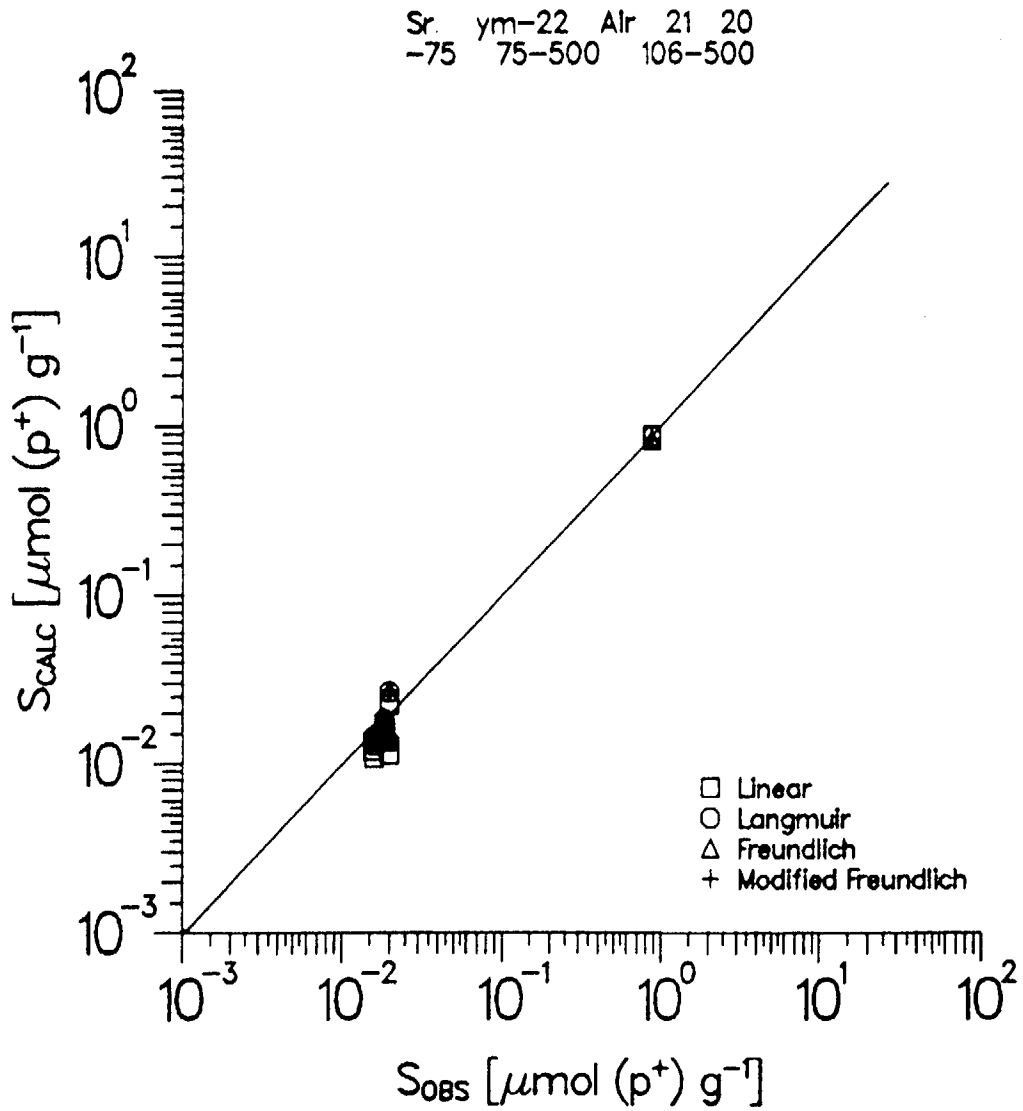
Printouts for Sr Isotherms (YM-22, 20 micromol(p+)/g, <75, 75-500, 106-500 μm) 244
Printouts for Cs Isotherms (YM-22, 20 micromol(p+)/g, <75, 75-500, 106-500 μm) 247
Printouts for Ba Isotherms (YM-22, 20 micromol(p+)/g, <75, 75-500, 106-500 μm) 250
Printouts for Eu Isotherms (YM-22, 20 micromol(p+)/g, <75, 75-500, 106-500 μm) 253
Printouts for Sr Isotherms (YM-38, 1,520 micromol(p+)/g, <38, <75, 38-106, 75-500, 106-500 μm) 256
Printouts for Cs Isotherms (YM-38, 1,520 micromol(p+)/g, <38, <75, 38-106, 75-500, 106-500 μm) 259
Printouts for Ba Isotherms (YM-38, 1,520 micromol(p+)/g, <38, <75, 38-106, 75-500, 106-500 μm) 262
Printouts for Eu Isotherms (YM-38, 1,520 micromol(p+)/g, <38, <75, 38-106, 75-500, 106-500 μm) 265
Printouts for Ba Isotherms (g1-2363, 48 micromol(p+)/g, <38, <500, 38-106, 106-500 μm) 268

ELEMENT = Sr
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	10	0.0000000	54.5393600	0.9998	0.00582366
Kd =	54.53936005				
LANGMUIR	10	0.0153770	0.1880609	0.1317	0.00341514
b =	5.31742668				
k =	12.23002911				
FREUNDLICH	10	1.6015043	0.9366708	0.9861	0.08878801
K =	39.94885254				
N =	0.93667084				
MODIFIED FREUNDLICH	10	0.3386314	0.9472536	0.9861	0.08996011
A =	43.61756516				
B =	0.94725364				
KD =	2.27765322				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

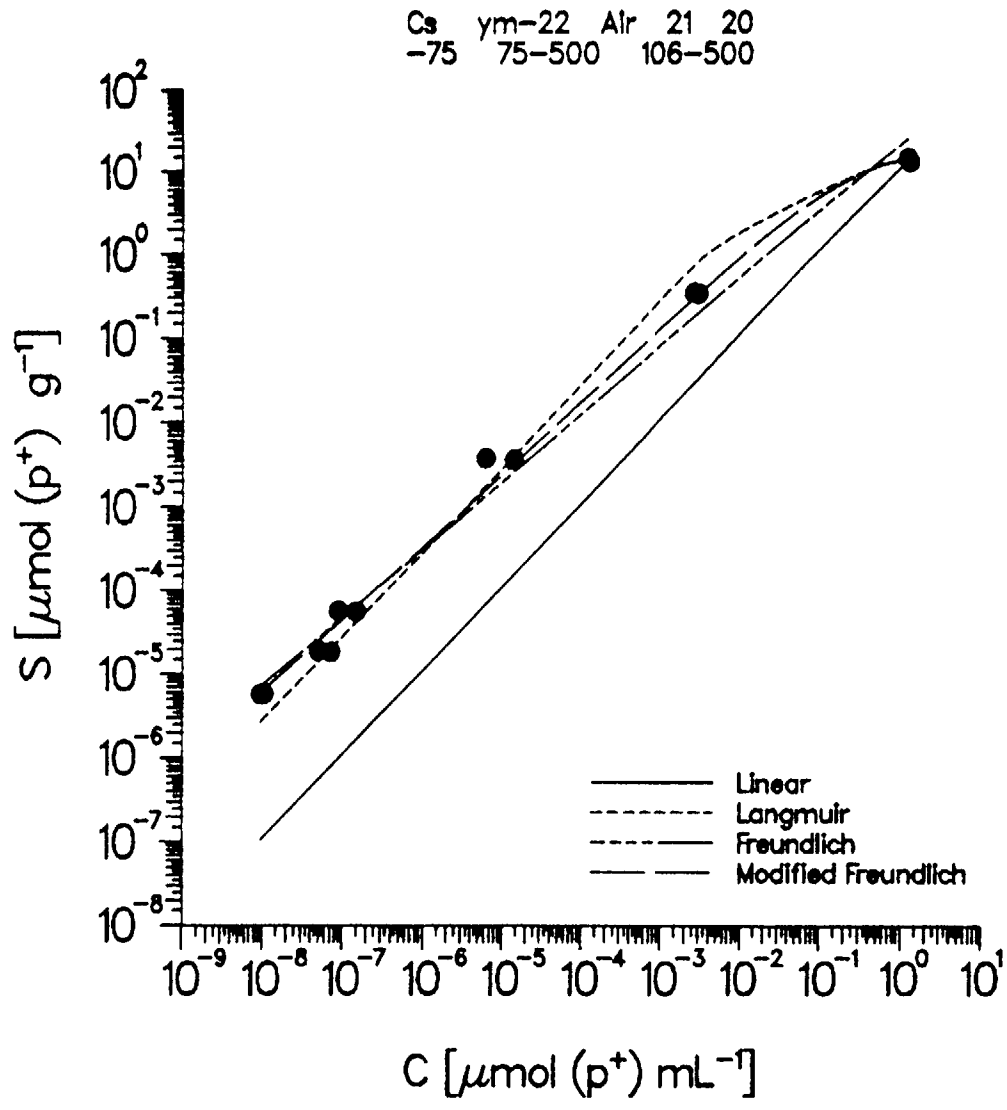

Sr ym-22 Alr 21 20
-75 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

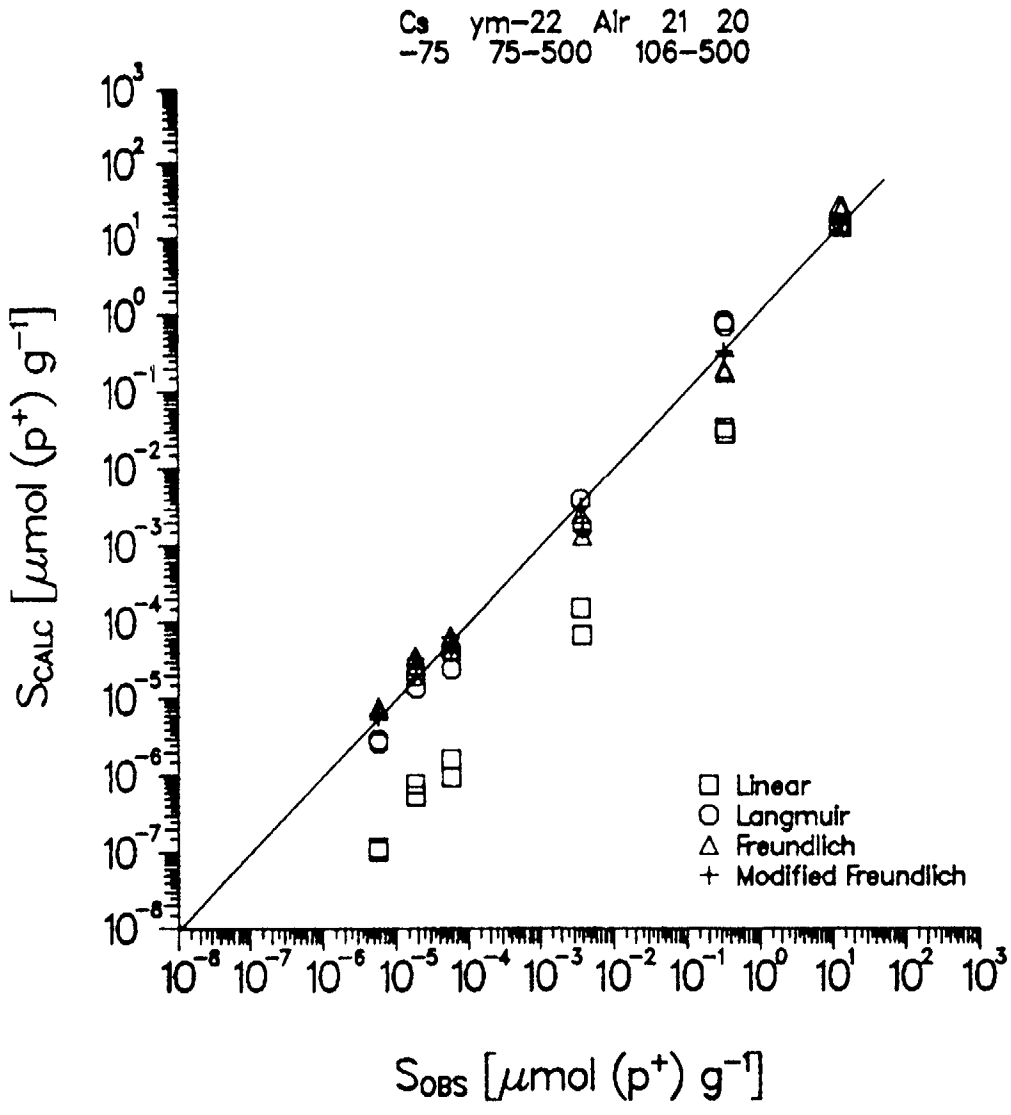

Sr. ym-22 Air 21 20
-75 75-500 106-500
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	12	0.0000000	10.9385805	0.9913	0.59263873
Kd =	10.93858051				
LANGMUIR	12	0.0035609	0.0684417	0.9906	0.00351194
b =	14.61098099				
k =	19.22049904				
FREUNDLICH	12	1.3249748	0.8066162	0.9899	0.25780362
K =	21.13366318				
N =	0.80661625				
MODIFIED FREUNDLICH	12	0.3855188	0.8614295	0.9959	0.17385446
A =	48.59021378				
B =	0.86142951				
KD =	2.80242372				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

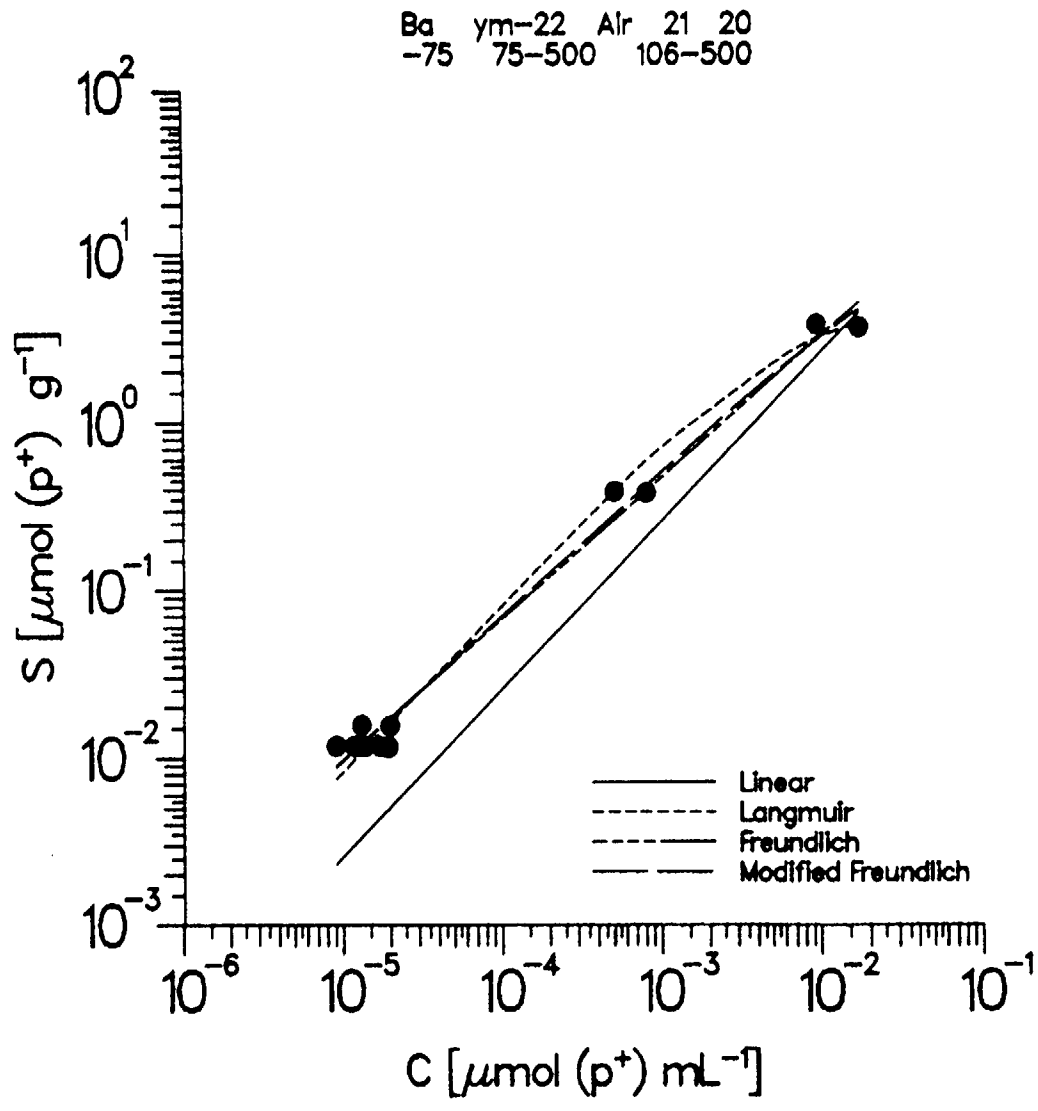

Cs ym-22 Air 21 20
-75 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

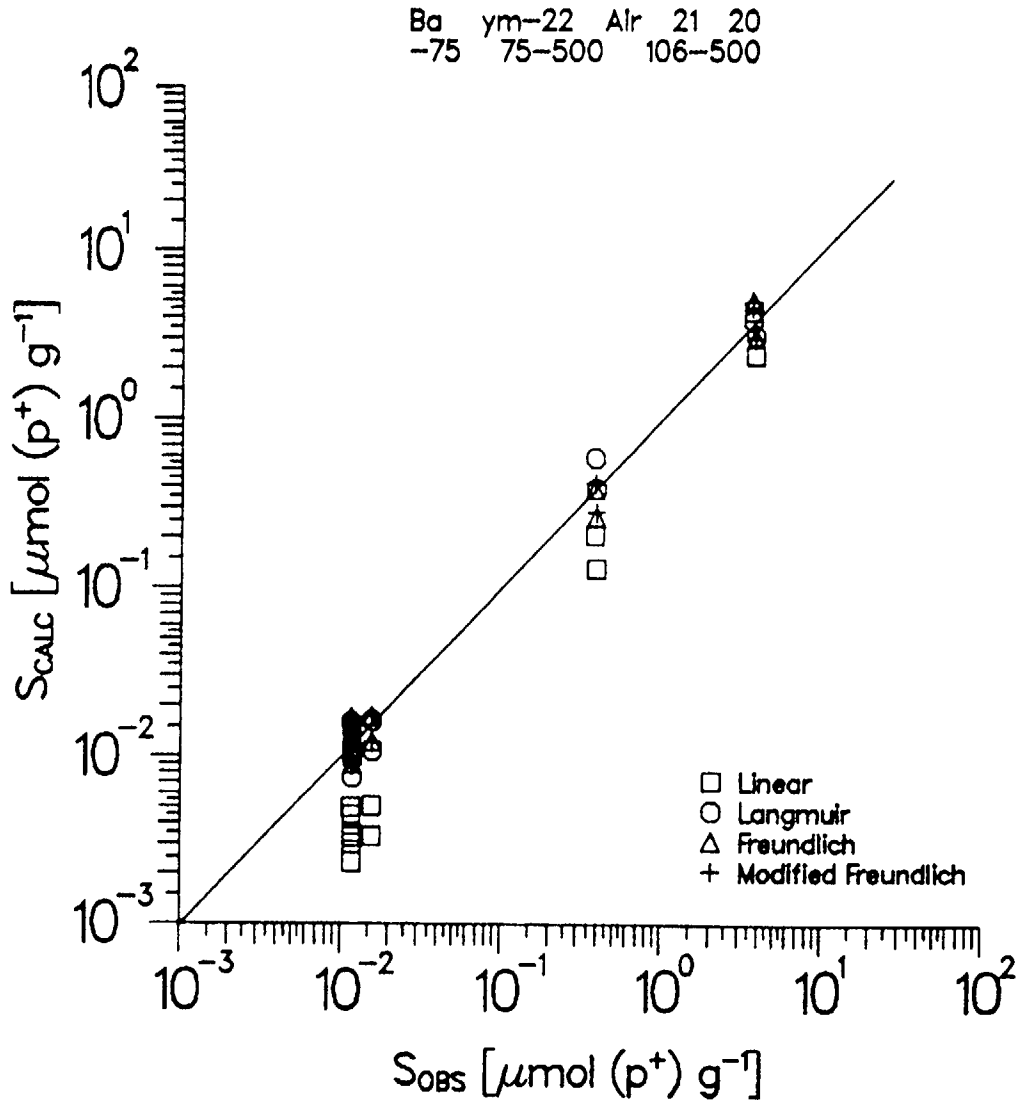

Cs ym-22 Air 21 20
-75 75-500 106-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	12	0.0000000	254.3512726	0.9066	0.51274031
Kd =	254.35127258				
LANGMUIR	12	0.0012210	0.1893229	0.8803	0.00039931
b =	5.28198004				
k =	155.06182861				
FREUNDLICH	12	2.1852295	0.8399234	0.9886	0.11406526
K =	153.18969727				
N =	0.83992344				
MODIFIED FREUNDLICH	12	1.0037611	0.8651865	0.9895	0.11285319
A =	201.73956299				
B =	0.86518645				
KD =	14.45996952				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

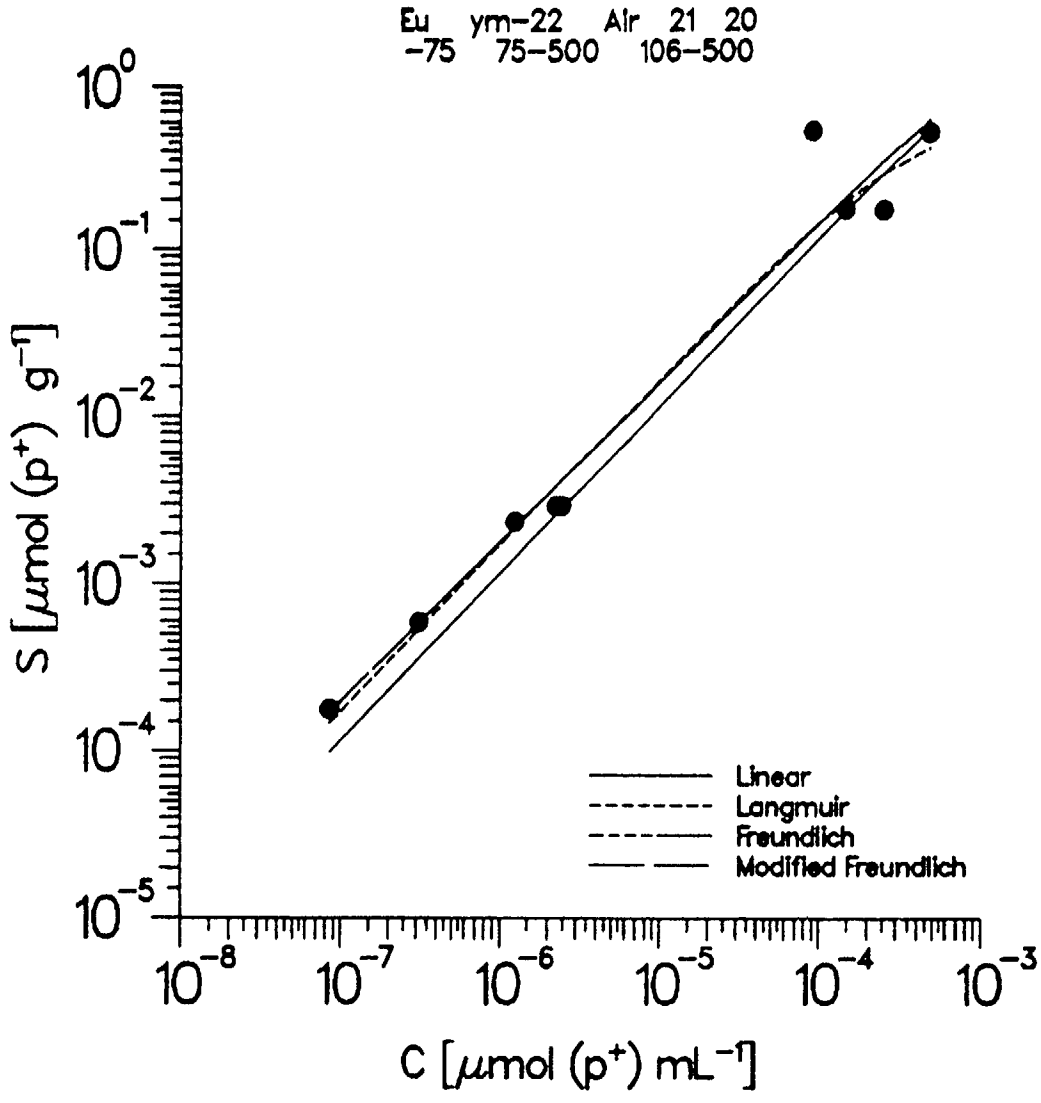

Ba ym-22 Air 21 20
-75 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

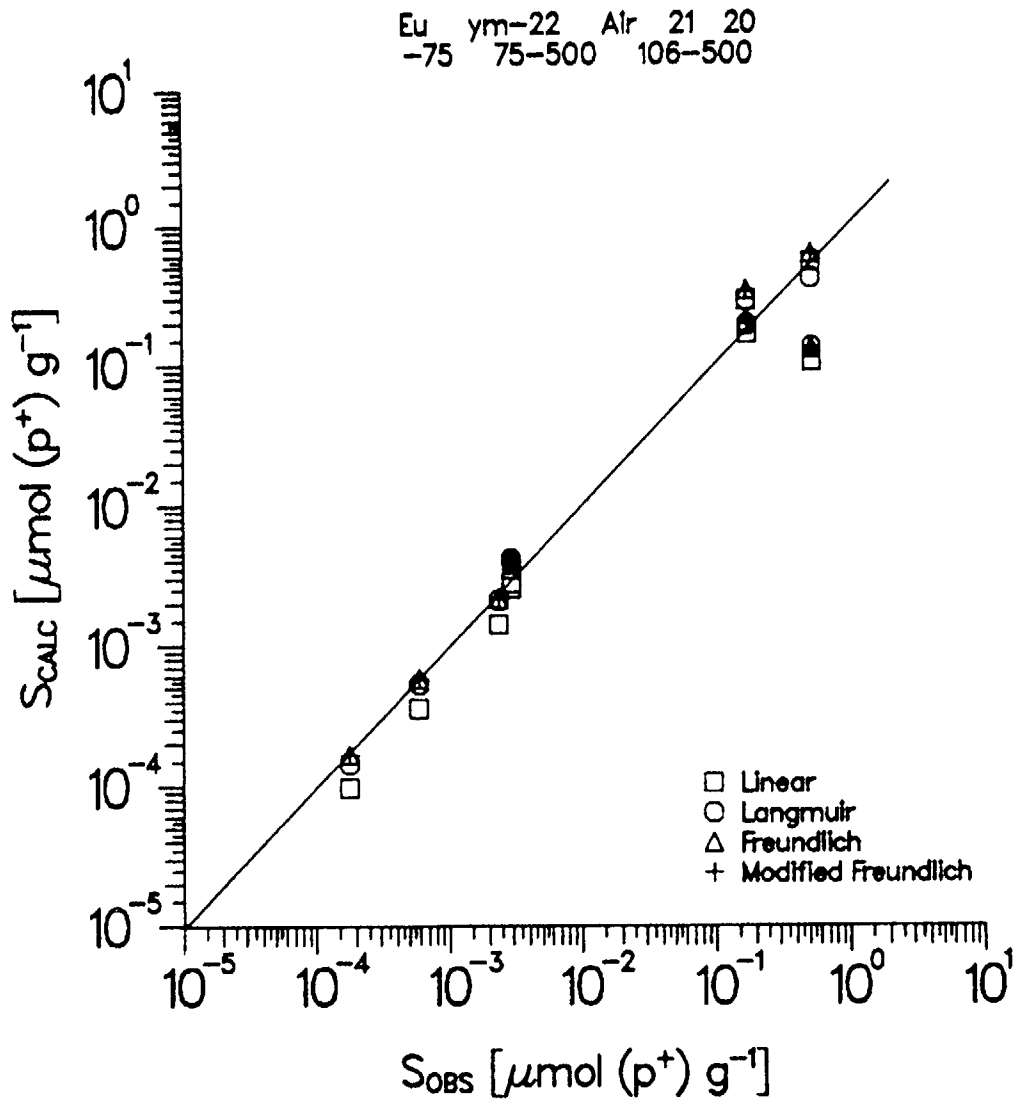

Ba ym-22 Air 21 20
-75 75-500 106-500
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-22
TIME = 21 days
ATMOS = Air
CEC = 20 micromol (p+)/g
SIZE = - 75 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	11	0.0000000	1148.7070313	0.6831	0.14920272
Kd =	1148.70703125				
LANGMUIR	11	0.0005836	1.1533434	0.2902	0.00029408
b =	0.86704445				
k =	1976.29272461				
FREUNDLICH	11	2.9629719	0.9523998	0.9691	0.23760702
K =	918.27325439				
N =	0.95239985				
MODIFIED FREUNDLICH	11	1.6794996	0.9551916	0.9687	0.23989715
A =	956.15789795				
B =	0.95519161				
KD =	57.31728745				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

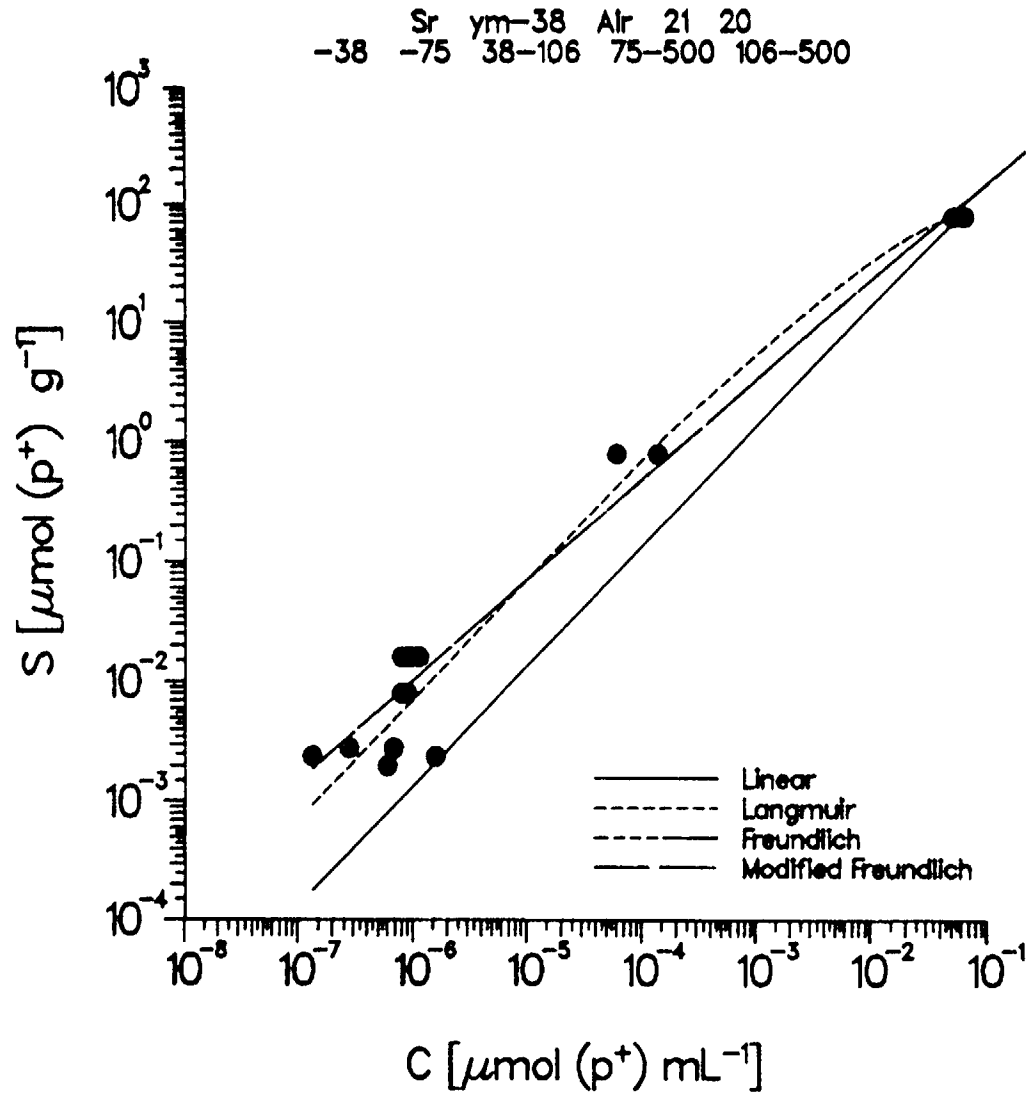

Eu ym-22 Air 21 20
-75 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

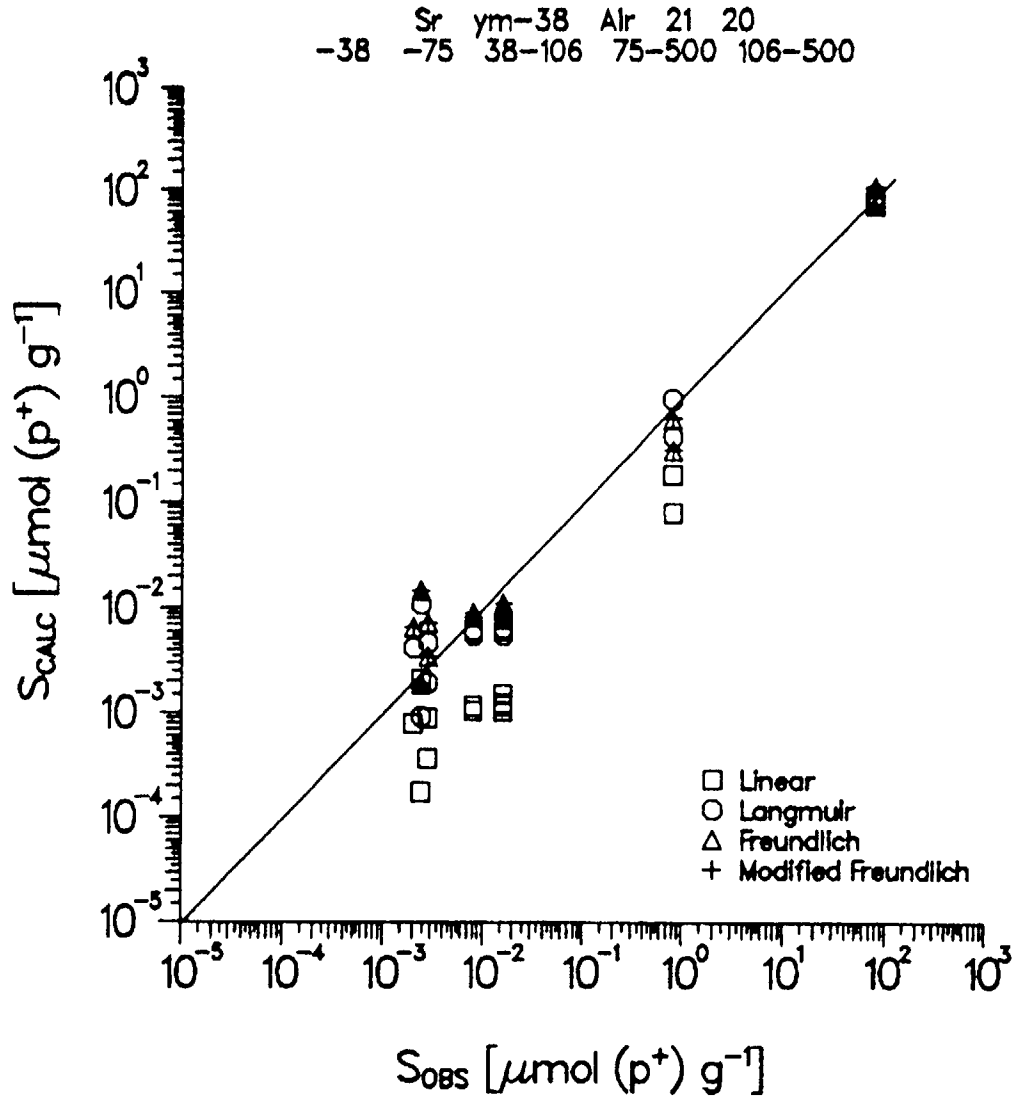

Eu ym-22 Air 21 20
-75 75-500 106-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Sr
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 38 microns
= - 75 microns
= 38-106 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	17	0.0000000	1317.2322998	0.9877	3.19127631
Kd =	1317.23229980				
LANGMUIR	17	0.0001441	0.0102849	0.6385	0.00015791
b =	97.23000336				
k =	71.37462616				
FREUNDLICH	17	3.0131795	0.8349179	0.9515	0.33346391
K =	1030.81213379				
N =	0.83491790				
MODIFIED FREUNDLICH	17	-0.1443238	0.8389689	0.9521	0.33269158
A =	1090.23413086				
B =	0.83896887				
KD =	0.67293757				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

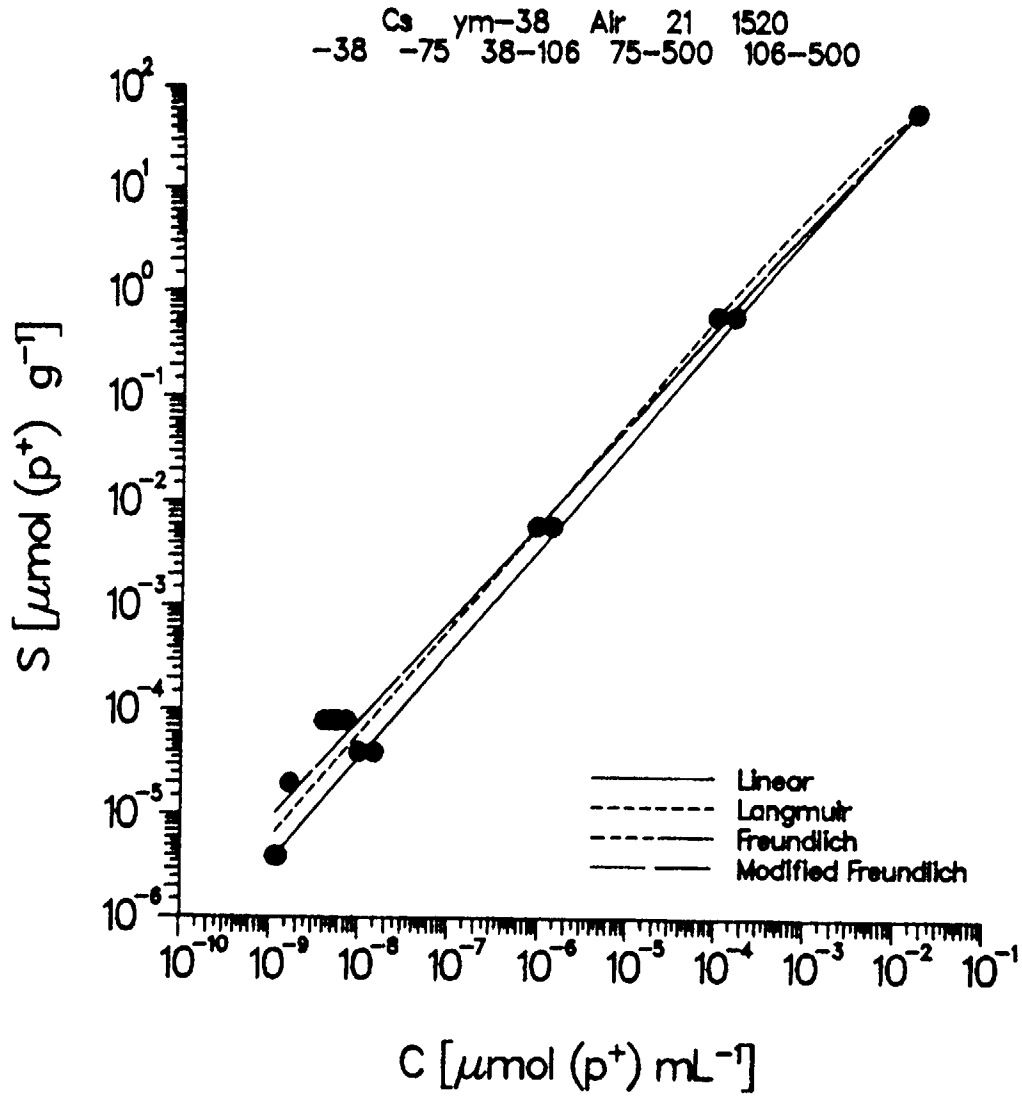

Sr ym-38 Air 21 20
-38 -75 38-106 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

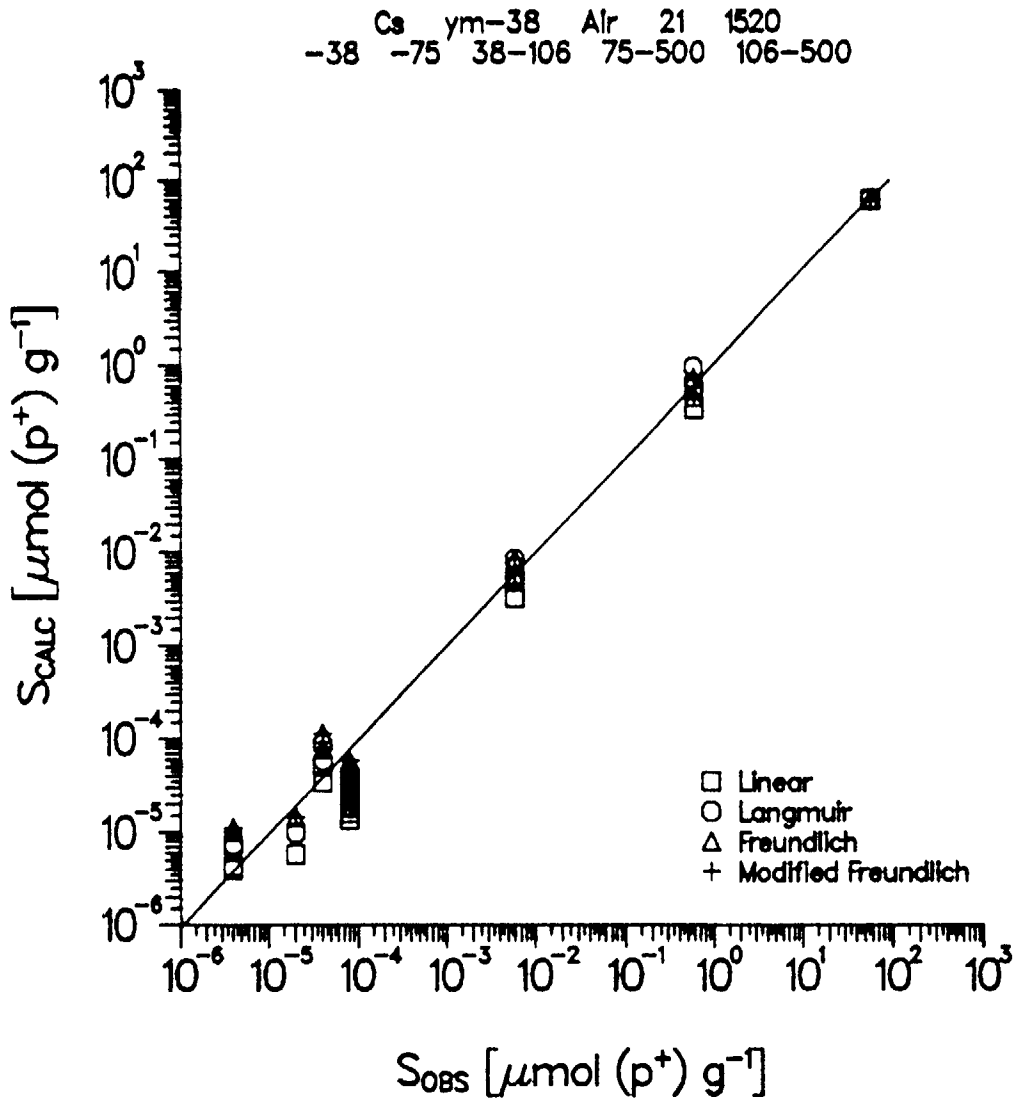

Sr ym-38 Alr 21 20
-38 -75 38-106 75-500 106-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Cs
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 38 microns
= - 75 microns
= 38-106 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	17	0.0000000	3457.2561035	0.9998	0.34041947
Kd =	3457.25610352				
LANGMUIR	17	0.0001694	0.0069739	0.1337	0.00010496
b =	143.39193726				
k =	41.17168045				
FREUNDLICH	17	3.4329979	0.9419580	0.9868	0.27824274
K =	2710.17871094				
N =	0.94195795				
MODIFIED FREUNDLICH	17	0.2654014	0.9437543	0.9868	0.27832225
A =	2800.56054688				
B =	0.94375432				
KD =	1.91081536				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

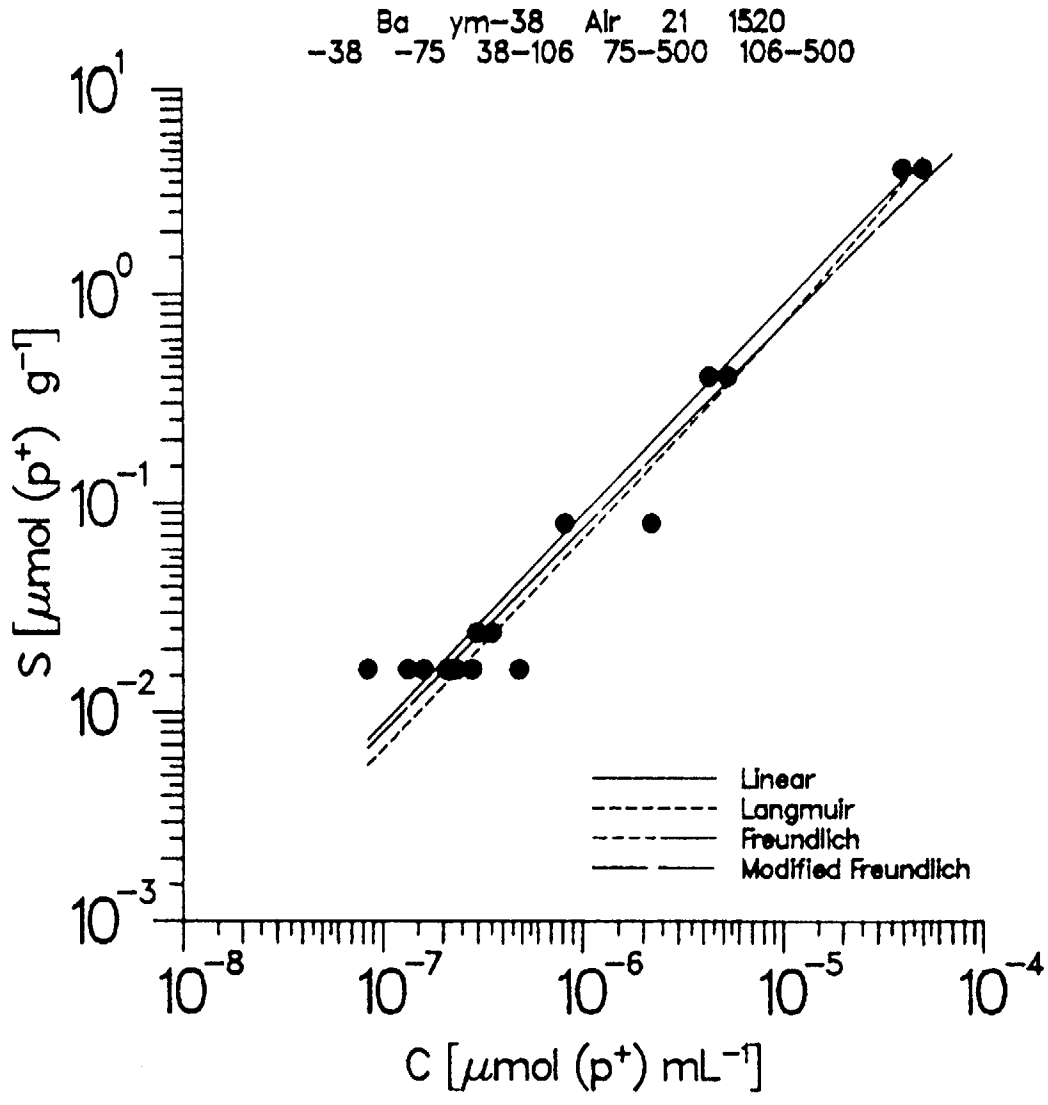

Cs ym-38 Air 21 1520
-38 -75 38-106 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

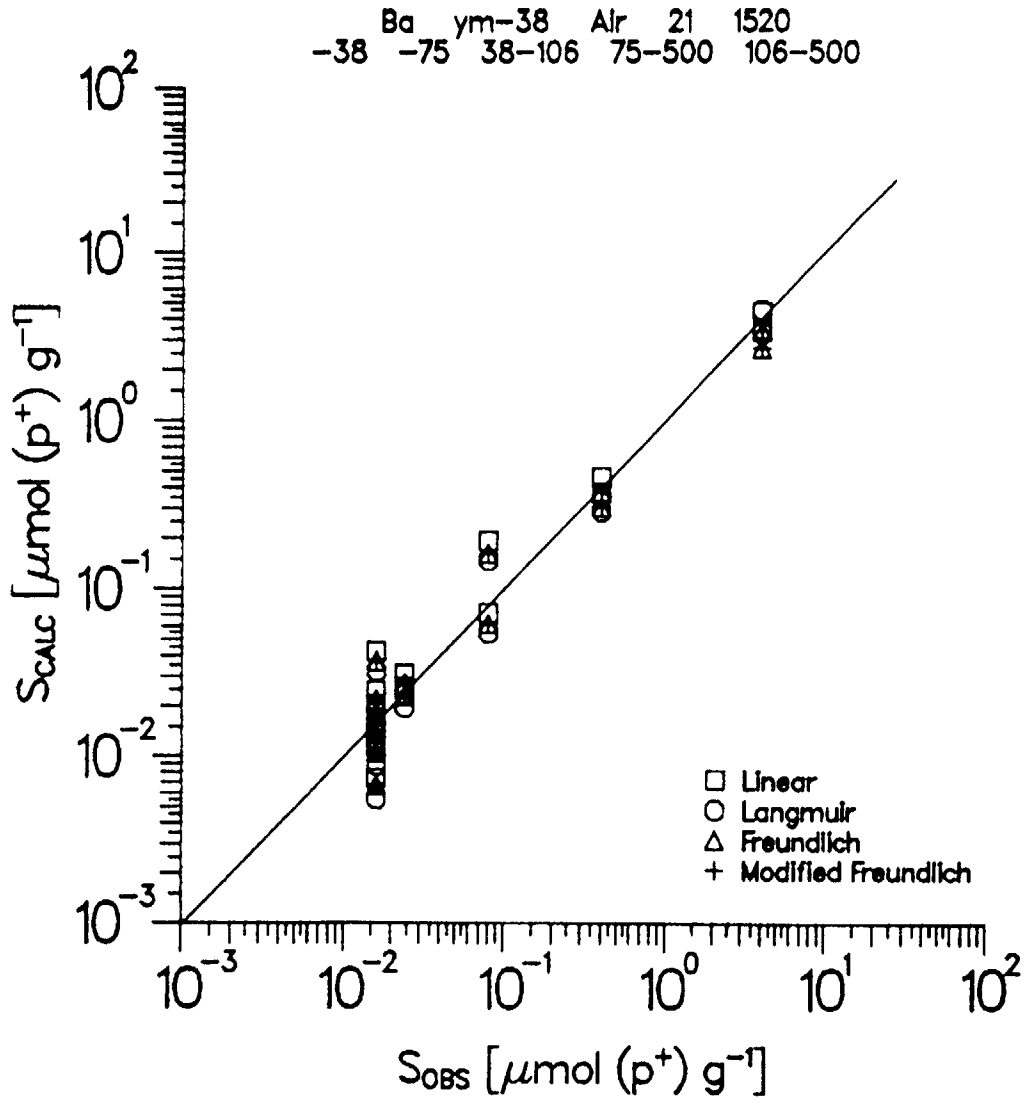

Cs ym-38 Air 21 1520
-38 -75 38-106 75-500 106-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 38 microns
= - 75 microns
= 38-106 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	18	0.0000000	86987.0078125	0.9860	0.16796449
Kd = 86987.00781250					
LANGMUIR	18	0.0000152	-0.0784722	0.0242	0.00000746
b = -12.74335957					
k = -5168.04736328					
FREUNDLICH	18	4.7089090	0.9729112	0.9448	0.19998336
K = 51157.46875000					
N = 0.97291118					
MODIFIED FREUNDLICH	18	1.5295391	0.9732894	0.9448	0.20006576
A = 51449.68359375					
B = 0.97328943					
KD = 37.28337860					

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

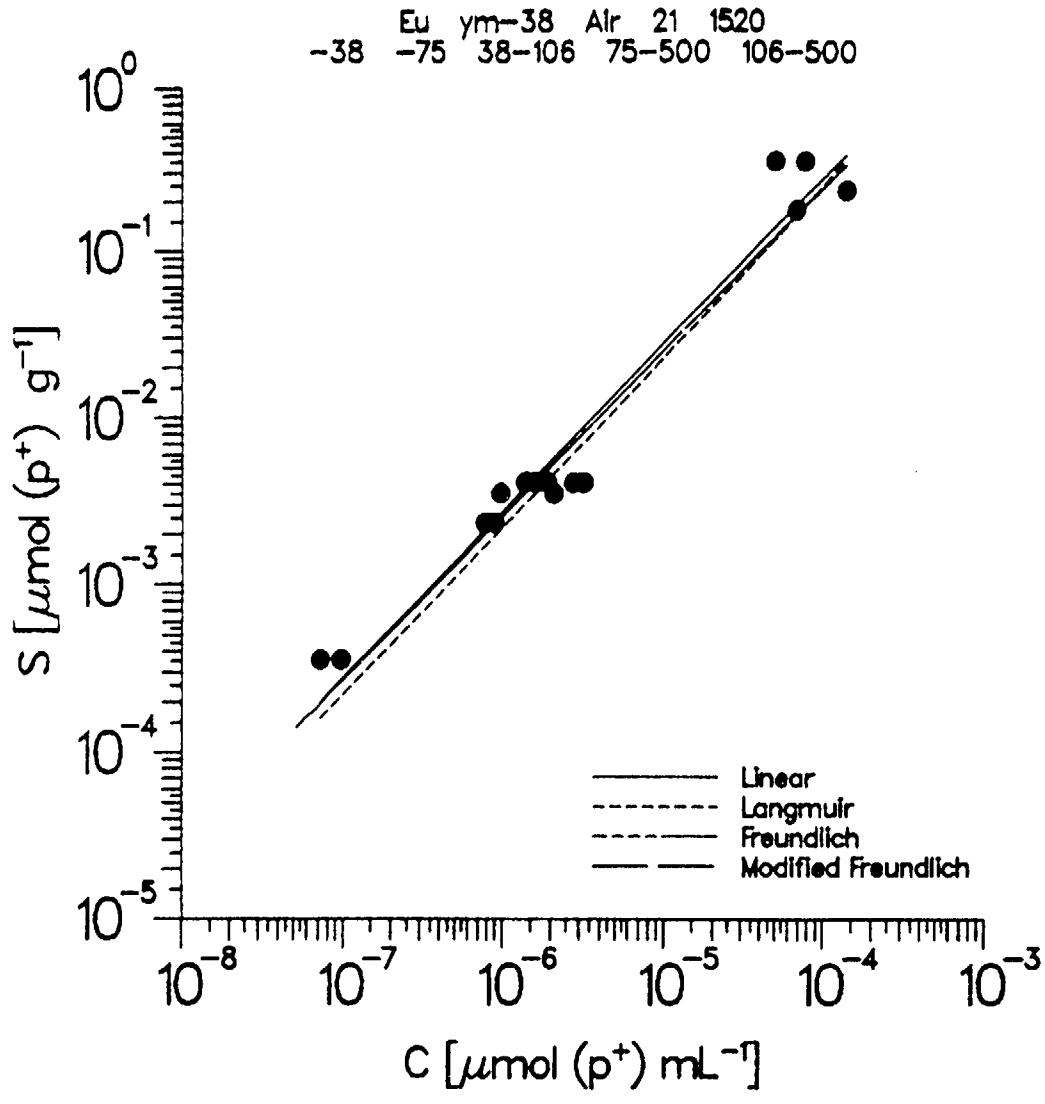

Ba ym-38 Air 21 1520
-38 -75 38-106 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

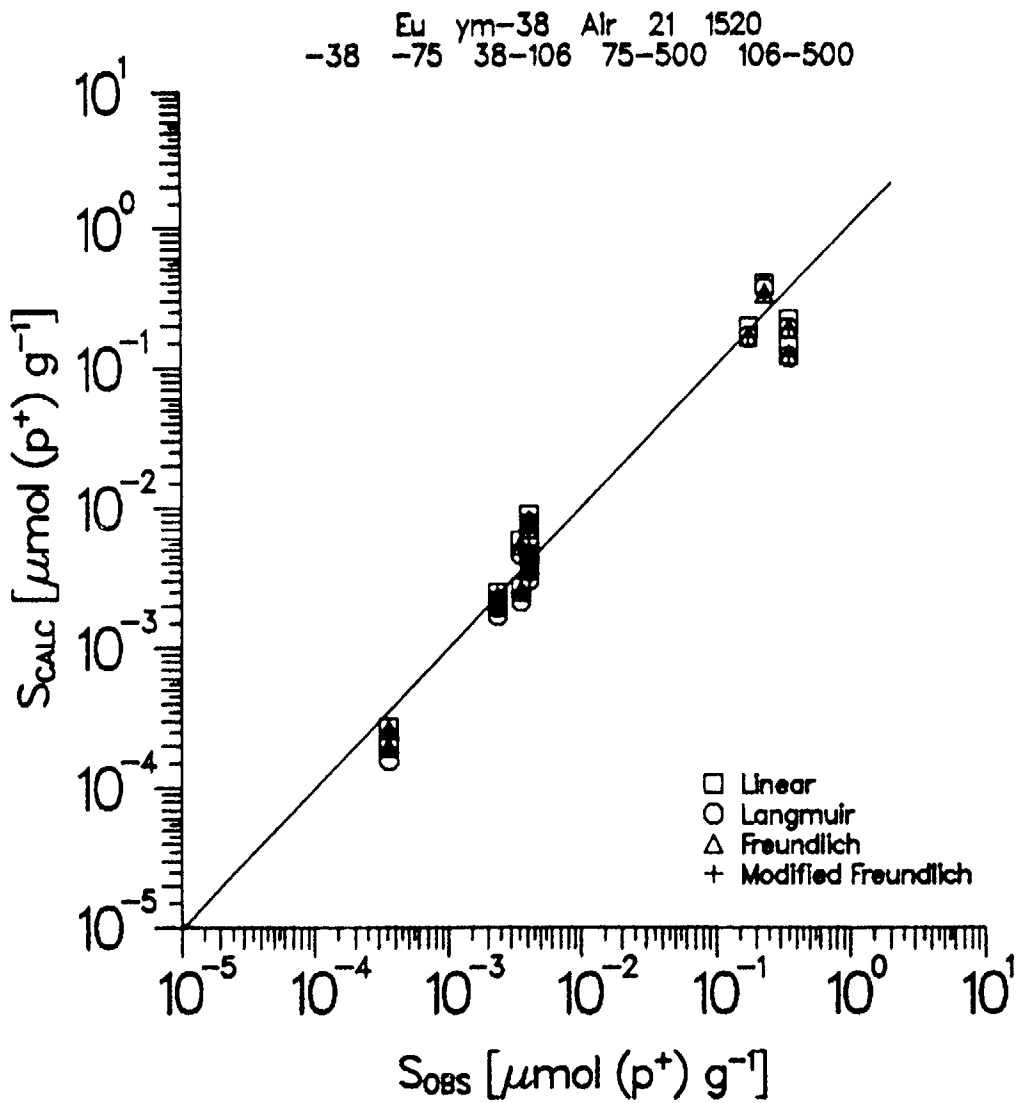

Ba ym-38 Air 21 1520
-38 -75 38-106 75-500 106-500
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Eu
SAMPLE = ym-38
TIME = 21 days
ATMOS = Air
CEC = 1520 micromol (p+)/g
SIZE = - 38 microns
= - 75 microns
= 38-106 microns
= 75-500 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	17	0.0000000	2776.1760254	0.7364	0.07791777
Kd =	2776.17602539				
LANGMUIR	17	0.0004510	-0.4749461	0.0081	0.00021657
b =	-2.10550237				
k =	-1053.04907227				
FREUNDLICH	17	3.3141580	0.9833670	0.9456	0.22879520
K =	2061.37963867				
N =	0.98336697				
MODIFIED FREUNDLICH	17	0.1325002	0.9833972	0.9456	0.22880284
A =	2062.26171875				
B =	0.98339725				
KD =	1.36375761				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.

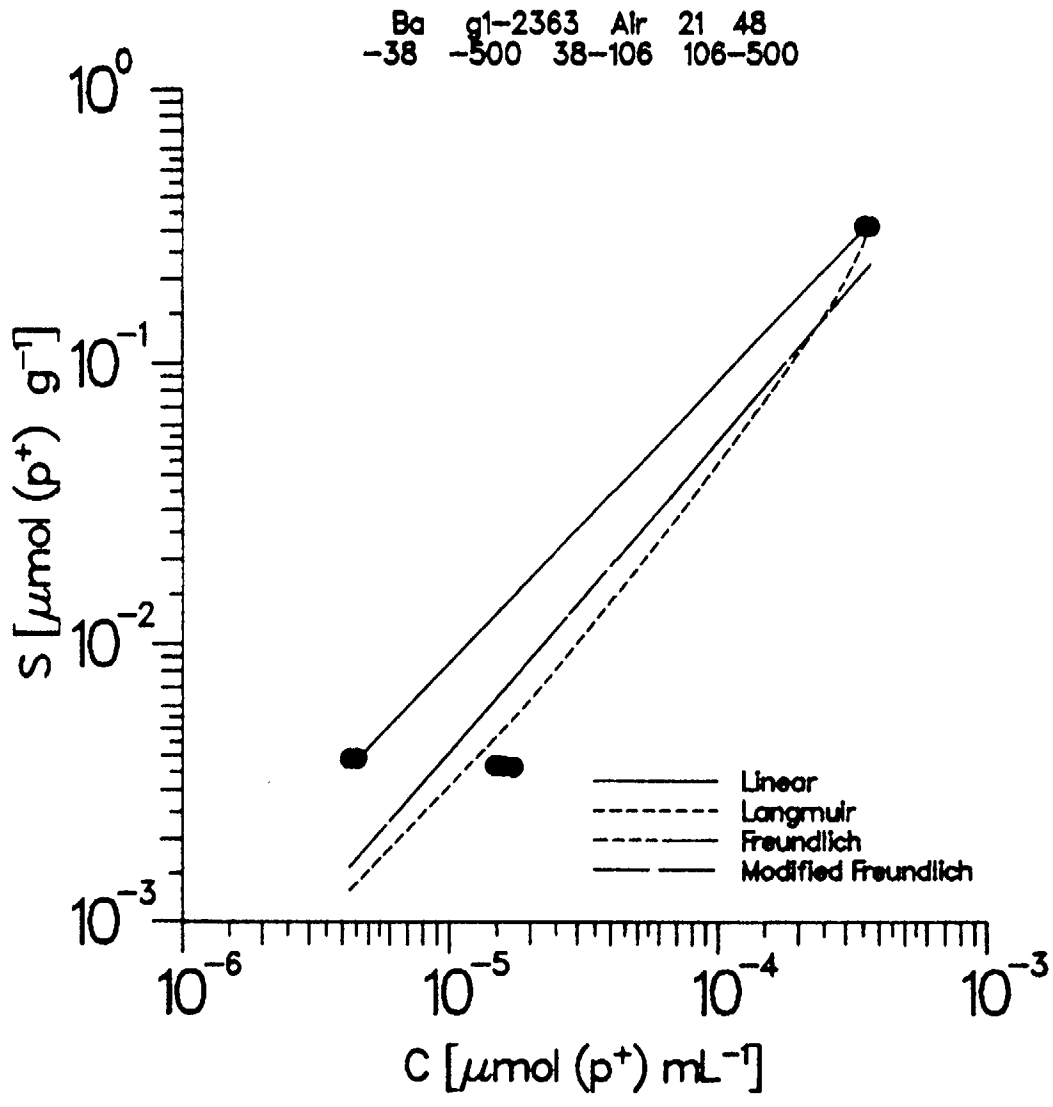

Eu ym-38 Air 21 1520
-38 -75 38-106 75-500 106-500
S [μmol (p+) g-1]
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich

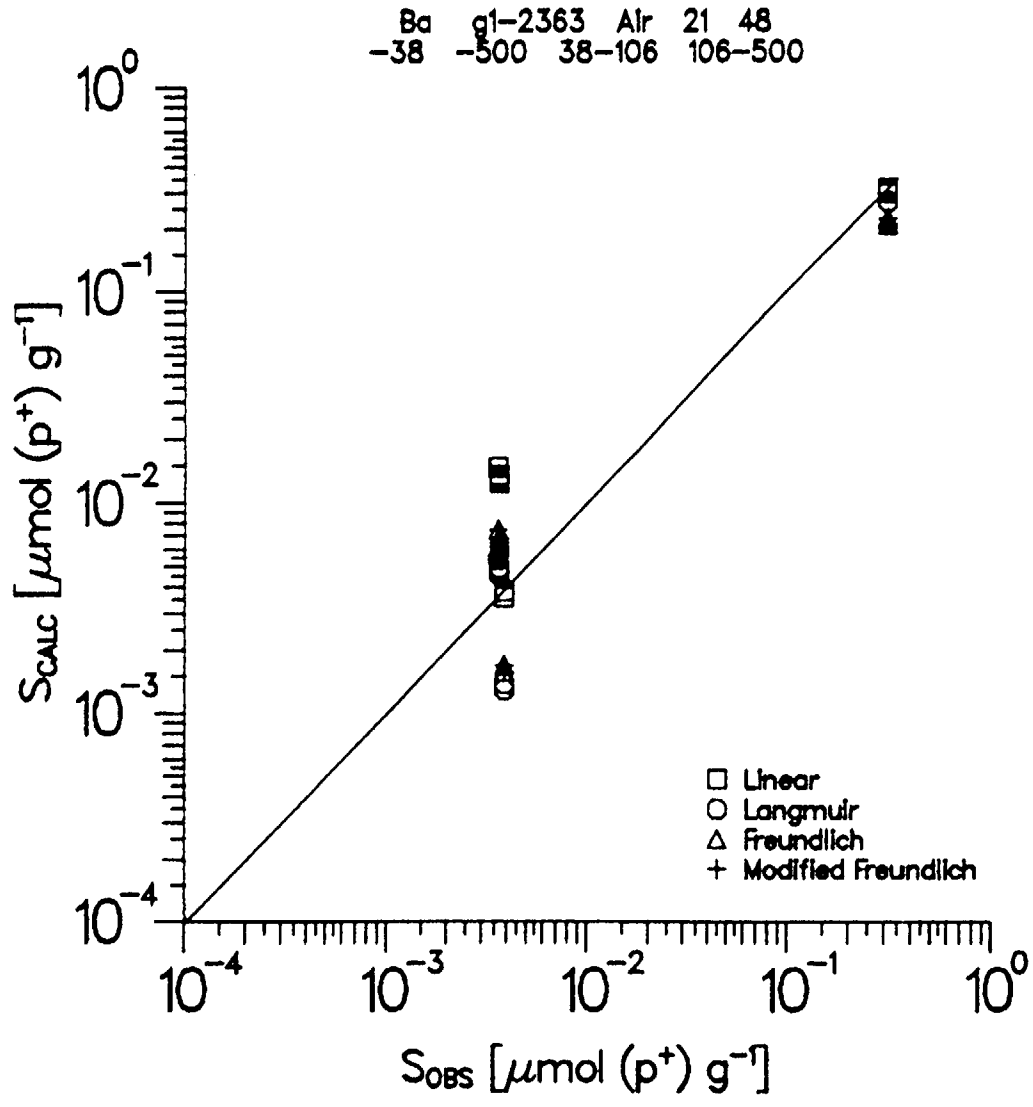

Eu ym-38 Air 21 1520
-38 -75 38-106 75-500 106-500
S_{CALC} [μmol (p^+) g^{-1}]
S_{OBS} [μmol (p^+) g^{-1}]
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Linear
Langmuir
Freundlich
Modified Freundlich

ELEMENT = Ba
SAMPLE = gl-2363
TIME = 21 days
ATMOS = Air
CEC = 48 micromol (p+)/g
SIZE = - 38 microns
= -500 microns
= 38-106 microns
= 106-500 microns

ISOTHERM	n	ALPHA	BETA	R**2	SSE
LINEAR	8	0.0000000	850.8080444	0.9972	0.00962229
Kd =	850.80804443				
LANGMUIR	8	0.0032997	-5.6113749	0.2896	0.00155677
b =	-0.17820944				
k =	-1700.54919434				
FREUNDLICH	8	3.1418917	1.1064124	0.8880	0.32131281
K =	1386.41015625				
N =	1.10641241				
MODIFIED FREUNDLICH	8	1.4688416	1.1080341	0.8880	0.32176229
A =	1412.80688477				
B =	1.10803413				
KD =	21.16549301				

n = the number of experimental points
ALPHA and BETA are respectively the intercept and slope from the linear regression analysis
R = correlation coefficient
SSE = standard error
Kd in mL/g
b in micromol(p+)/g and k in mL/micromol(p+)
K,N,A,B and KD in units corresponding to solute adsorbed S in micromol(p+)/g and solute in solution C in micromol(p+)/mL.


Ba g1-2363 Air 21 48
-38 -500 38-106 106-500
10^0
10^{-1}
10^{-2}
10^{-3}
S [μmol (p+) g-1]
10^{-6}
10^{-5}
10^{-4}
10^{-3}
C [μmol (p+) mL-1]
Linear
Langmuir
Freundlich
Modified Freundlich


Ba g1-2363 Air 21 48
-38 -500 38-106 106-500
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
S_{CALC} [μmol (p^+) g^{-1}]
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^0
S_{OBS} [μmol (p^+) g^{-1}]
Linear
Langmuir
Freundlich
Modified Freundlich