SUMMARY REPORT ON THE EVALUATION OF A 1977-1985 EDITED SORPTION DATA BASE FOR ISOTHERM MODELING

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W. L. Polzer
H. R. Fuentes[1]
C. Yong[2]
Environmental Science Group

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Contributors:
R. J. Beckman, A-1
M. G. Rao[3], HSE-12
P. Chan[2], HSE-12

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A. Meijer, Principal Investigator
Los Alamos National Laboratory

[1]Los Alamos Collaborator, University of Texas at El Paso
[2]GRA, University of Texas at El Paso
[3]Los Alamos Collaborator, Howard University

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by

W. L. Polzer, H. R. Fuentes, and C. Yong

ABSTRACT

Sorption data bases collected by Los Alamos National Laboratory (LANL) from 1977 to 1985 for the Yucca Mountain Project (YMP) have been inventoried and fitted with isotherm expressions. Effects of variables (e.g., particle size) on the isotherm were also evaluated. The sorption data are from laboratory batch measurements which were not designed specifically for isotherm modeling. However a limited number of data sets permitted such modeling. The analysis of those isotherm data can aid in the design of future sorption experiments and can provide expressions to be used in radionuclide transport modeling.

Over 1200 experimental observations were inventoried for their adequacy to be modeled by isotherms and to evaluate the effects of variables on isotherms. About 15% of the observations provided suitable data sets for modeling. The data sets were obtained under conditions that include ambient temperature and two atmospheres, air and CO_2.

The Linear, Langmuir, Freundlich, and Modified Freundlich isotherms were used in modeling the data; the first three because of their simplicity and widespread use in transport codes, the fourth because of its derivation from more fundamental concepts. In general the data were more uniformly distributed for regression by the Freundlich and Modified Freundlich expressions than for regression by the Linear and Langmuir expressions; sorption experiments should be designed with specific models in mind. The parameters from the Freundlich and Modified Freundlich expressions should better predict sorption in transport. In general replication and particle size had no effect on the regression of data for the four isotherms. An effect of particle size on the regression for the sorption of barium on YM-22 tuff was observed. Hysteresis was observed to have an effect on the isotherms, but major mineralogy did not. These observations are limited to the evaluated data sets. Examples on how to estimate free energies of adsorption for the exchange of monovalent radionuclides (cesium) for a monovalent ion (sodium) on tuff material are also included.

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Figure C.88. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-49 Tc 42 air 106-500 amb 1170.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 desorption; the variable being tested is hysteresis . . . 252

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SUMMARY REPORT ON THE EVALUATION OF A 1977-1985 EDITED SORPTION DATA BASE FOR ISOTHERM MODELING

by

W. L. Polzer, H. R. Fuentes, and C. Yong

ABSTRACT

Sorption data bases collected by Los Alamos National Laboratory (LANL) from 1977 to 1985 for the Yucca Mountain Project (YMP) have been inventoried and fitted with isotherm expressions. Effects of variables (e.g., particle size) on the isotherm were also evaluated. The sorption data are from laboratory batch measurements which were not designed specifically for isotherm modeling. However a limited number of data sets permitted such modeling. The analysis of those isotherm data can aid in the design of future sorption experiments and can provide expressions to be used in radionuclide transport modeling.

Over 1200 experimental observations were inventoried for their adequacy to be modeled by isotherms and to evaluate the effects of variables on isotherms. About 15% of the observations provided suitable data sets for modeling. The data sets were obtained under conditions that include ambient temperature and two atmospheres, air and CO_2.

The Linear, Langmuir, Freundlich, and Modified Freundlich isotherms were used in modeling the data; the first three because of their simplicity and widespread use in transport codes, the fourth because of its derivation from more fundamental concepts. In general the data were more uniformly distributed for regression by the Freundlich and Modified Freundlich expressions than for regression by the Linear and Langmuir expressions; sorption experiments should be designed with specific models in mind. The parameters from the Freundlich and Modified Freundlich expressions should better predict sorption in transport. In general replication and particle size had no effect on the regression of data for the four isotherms. An effect of particle size on the regression for the sorption of barium on YM-22 tuff was observed. Hysteresis was observed to have an effect on the isotherms, but major mineralogy did not. These observations are limited to the evaluated data sets. Examples on how to estimate free energies of adsorption for the exchange of monovalent radionuclides (cesium) for a monovalent ion (sodium) on tuff material are also included.

1.0 INTRODUCTION

Los Alamos National Laboratory (Los Alamos) has conducted sorption studies from 1977 to 1985 in support of site selection activities for the Yucca Mountain Project (previously referred to as the Nevada Nuclear Waste Storage Investigations Project). The studies evaluate the extent of sorption for a group of radioactive elements on samples from the unsaturated zone of Yucca Mountain using laboratory batch experiments. The experiments were designed to scope the effects of a number of variables on sorption behavior of selected elements on Yucca Mountain tuffs.

The elements studied were americium, barium, cesium, cerium, europium, neptunium, plutonium, radium, selenium, strontium, technetium, thorium, tin, and uranium. Among the variables investigated were mineralogy, temperature, particle size, solution concentration, water composition, time, atmosphere and pH. However, no effort was made to carry out experiments in which the effects of these variables were systematically investigated.

For all batch experiments tuff samples were pretreated with Well J-13 groundwater for at least two weeks and then 1 g of crushed tuff was contacted with 20 mL of the same water traced with the radioactive form of the target element. Radioactivities in solution were measured before and after various contact periods during which the tubes were continuously shaken. These activities were used to calculate a simple distribution coefficient,

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

Note that $R_d = K_d$ when equilibrium conditions exist. Detailed information on the scope of these studies, the experimental procedures, and measurements for

all the elements as a function of the previously listed variables has been provided by Thomas (1987).

The need to validate the experimental sorption data motivated the evaluation of this data in terms of isotherms and potential sorption models. This report presents the results of this evaluation. This report is the conclusion of the work previously documented in Fuentes et al. (1987a) and Fuentes et al. (1987b). It is important to mention that the data bases were not originally collected with the purpose of developing isotherms.

This report focuses on an evaluation of data that were selected from a statistically refined data base (Beckman et al., 1988). Results from an inventory of the refined data base, the criteria to select the data sets, the results of fitting by isotherms equations, the effects of variables on fitting parameters, and estimates of free energies of adsorption are included in this report. Analyses of these results illustrate a variety of problems that may be encountered with the available data sets, and there is no attempt to exhaustively analyze all and each data set. Considerations that may aid in the experimental and statistical design of future sorption studies are outlined. However, the evaluation does provide information that puts in perspective the value of the present data base and serves as background to better design future isotherm experiments.

2.0 INVENTORY OF DATA BASE

A refined data base (Beckman et al., 1988) was inventoried to select data sets appropriate for isotherm fitting and to evaluate the effects of variables on isotherms parameters. First, the data base was organized systematically by elements and experimental conditions, such as adsorption and desorption at a

specific temperature and atmosphere. The inventory is a tabulation of all the data sets at ambient temperature and two atmospheres, air and CO_2. This inventory is a more effective organization than the original data base reported by Thomas (1987) because it provides complete information on the data available for each element. The tables in the inventory present the total number of observations, the cation exchange capacity, the particle size range, the contact time, the initial concentration in solution, and the pH for each combination of tuff from a given lithologic unit and radionuclides listed in Section 1.0. Although the entire data base from Beckman et al. (1988) was inventoried, this inventory does not include experiments conducted at temperatures other than ambient and experiments performed under controlled atmosphere (ca) conditions. The air atmosphere refers to the ambient atmosphere; the CO_2-atmosphere is 5% enriched with CO_2; and the controlled atmosphere or nitrogen atmosphere (ca) has less than 0.2 ppm (parts per million) O_2 and less than 20 ppm CO_2. Those experiments were excluded because these data sets could not be fit by isotherm equations. The inventory is documented as TWS-EES15-7-89-12 in the resident file of the Environmental Science Group, EES-15, at Los Alamos.

A data set is defined as a group of observations that was obtained for the sorption of a radionuclide onto a given tuff sample for a specific range of experimental conditions. Different conditions, such as different temperatures or particle sizes, were not combined for modeling except when the purpose was to test a significant difference caused by one variable on a specific isotherm.

The selection of the best data sets was based on the following criteria:

1. Availability of at least two sets with the same experimental

conditions except one (e.g., temperature) so that the effect of one variable on isotherms can be evaluated.

2. Each data set should be capable of being fit by isotherms. A set is capable of being modeled when at least three observations at three different concentrations of the radionuclide in solution are available; the three concentrations should not form two clusters of points as this would lead to an indetermination.

A major assumption of the modeling discussed here is that equilibrium applies. An additional criterion was introduced; only those sets were considered that showed a large difference (equal or greater than one order of magnitude) between the initial solution concentration and the changes in concentration at different contact times. This criterion increased the possibility of having an equilibrium or at least a pseudo equilibrium. The selected sets are tabulated in Appendix A and include cases for both adsorption and desorption. The sets correspond to cases that permit the evaluation of the effects of the following variables on isotherms; replication, particle size, mineralogy, and hysteretic behavior between adsorption and desorption. Although the number of sets is limited, their analysis yields considerations of prime concern in experimental design and modeling of isotherm data. The computer codes SOS, MINMATCH, and GETDATA were used to inventory the data bases and to select the best sets. These codes are also documented as TWS-EES15-7-89-13 in the resident file of the Environmental Science Group, Group EES-15, at Los Alamos. In the rest of this report, the word "model" and its derivatives are generally used to refer to all the mathematical aspects of evaluating the applicability of isotherms and their comparison. The word "fit" and its derivatives specifically refer to statistical regression techniques, such as the least squares.

3.0 METHODS OF ANALYSIS

Concentrations of Radionuclides Adsorbed and in Solution

Once the selected sets were defined (Appendix A), the Rd (simple distribution coefficient), the initial radionuclide concentration (radioactive tracer) in solution, and its final concentration in solution were used to calculate the concentrations adsorbed (S) and in solution (C) at equilibrium, or at pseudo-equilibrium. The adsorbed and solution concentrations were computed using the following equations:

$$C = \frac{C_o EV(1000)}{Z(R_d W + V)} \tag{2}$$

$$S = \frac{CEV(1000)}{WZ} \left[1 - \frac{V}{R_d W + V}\right] \tag{3}$$

where

C = amount of radioactive tracer in solution (μmol (p+) mL^{-1}),

S = amount of radioactive tracer on solid fraction (μmol (p+) g^{-1}),

C_o = initial concentration of radioactive tracer in solution (μmole mL^{-1}),

E = formula weight of radioactive tracer (g mol^{-1}),

V = volume of solution in reactive mixture (mL),

W = weight of solids in reactive mixture (g), and

Z = (p+) equivalent of the solute (valence).

Rd = distribution coefficient (mL g^{-1}).

Isotherm Parameters

The values for S and C are given in Appendix A. The S (adsorbed

concentration) and C (solution concentration) values became the dependent and independent variables, respectively, for the evaluation of isotherms. Each set was fitted to four isotherms; the Linear, the Langmuir, the Freundlich, and the Modified Freundlich. These isotherms are relatively simple and consequently have been widely used in transport equations and in their computer codes (Travis and Etnier 1981) with the exception of the Modified Freundlich. Whereas the Linear and Freundlich isotherms are the most popular to represent sorption on manmade and natural porous media, they are a very simplistic representation of the sorption process. On the other hand, the Langmuir and Modified Freundlich isotherms have some theoretical foundations so that, when applicable, they can provide an improved understanding of sorption processes.

The simplest and most widely used equilibrium sorption isotherm is the linear relationship

$$S = K_d C \tag{4}$$

where

S = concentration of radioactive tracer (solute) in the solid (μmol (p+) g^{-1}),

C = concentration of radioactive tracer (solute) in solution (μmol (p+) mL^{-1}), and

K_d = distribution coefficient (mL g^{-1}).

This expression is widely used in transport models to describe the sorption of reactive solutes by solids. One limitation is that it does not include a

maximum quantity of adsorption. The distribution coefficient, K_d, is a measure of the retention of solute by the solid and is assumed to be independent of concentration. This independence does not always occur, and thus conclusions based on assumptions of linear behavior may not be valid.

Langmuir (1918) developed a quantitative model that has also been widely applied to describe experimental data. The Langmuir equation was derived for the sorption of gases on a solid surface, but it has been extended to include the sorption of solutes to solids. The basic expression takes the form

$$S = \frac{k\ b\ C}{1 + kC} \tag{5}$$

where

k, b = empirical constants.

Linearization of Equation (5) provides the following transformation for estimating parameter constants from experimental data,

$$C/S = (1/b)C + 1/kb. \tag{6}$$

In this expression, k is a measure of the strength of the sorption bond and b is the maximum amount of solute that can be sorbed by the solid. This isotherm is based on the theoretical assumption that the sorption sites are homogeneously distributed over the surface relative to energy potentials.

The Freundlich isotherm has the form

$$S = KC^N \tag{7}$$

where

K,N = empirical constants.

Constants can be estimated by logarithmic transformation of Equation (7) to

$$\text{Log } S = N \log C + \log K. \tag{8}$$

This expression is also very popular in the literature because of the flexibility of the exponential function to fit experimental data.

The Linear and Langmuir isotherms assume that the energy of adsorption is uniformly distributed on the adsorbent surface. However, this assumption fails in many cases because adsorption sites on pure minerals or multi-mineral aggregates may have different energies (heterogeneity). These differences among site energies require the identification of energy distributions that characterize the heterogeneity of a particular adsorbent-solute interaction. Equations such as the Freundlich isotherm are more appropriate than the Linear and Langmuir isotherms for modeling adsorption in these cases.

Sips (1948) introduced and discussed an isotherm that implied a Gaussian-like statistical function to represent the distribution of site-solute interactions. This isotherm, which is based on the assumption of localized adsorption without interaction among sites, was presented as an expansion of the conventional Freundlich isotherm. Sposito (1980) following Sips (1948) and using a Langmuir isotherm to define site-solute interactions, derived a Gaussian-like statistical function that defines variation of the relative affinity of a solute for a site on a solid phase. The isotherm, referred to as Modified Freundlich, can be expressed as

$$\frac{S}{S_{max}} = \frac{K_D{}^{\beta}C^{\beta}}{1 + K_D{}^{\beta}C^{\beta}} \tag{9}$$

where

S_{max} = maximum available exchange capacity of solid phase and

K_D, β = parameters that define the solute-solid phase interaction.

If this isotherm applies, then a more comprehensive representation of the heterogeneity of the adsorption is gained from the meaning of K_D and β. These two parameters can be found by regression analysis of a given set of data on the following transformation of Equation (9),

$$\log \frac{S}{S_{max} - S} = \beta \log C + \log (K_D{}^{\beta}). \tag{10}$$

The parameter β has been described (Sposito, 1980) as a measure of how sharply peaked the statistical function for the distribution of surface binding energies at equilibrium is about an average value; the parameter has also been described by Crickmore and Wojciechowski (1977) as the spread of the statistical function for the distribution of adsorption-desorption rate constants. The parameter K_D has been implicitly related (Sposito, 1980) to an average "distribution coefficient," or an average adsorption energy or affinity. Crickmore and Wojciechowski (1977), on the other hand, define K_D as the ratio of the reaction rate constants that represent simultaneous β-order adsorption-desorption rates. Both parameters, β and K_D, are temperature and

pH dependent. It is important to note that Equation (9) can be viewed as a general formulation, and the other three isotherms (Equations 4, 5 and 7) are special cases of the general isotherm. When the denominator of equation (9) is approximately one ($1 << K_D^{\beta}C^{\beta}$) or when the denominator of equation (10) is approximately S_{max} ($S_{max} - S \cong S_{max}$), then the equation degenerates into the Freundlich isotherm; this condition occurs when the reactive solute is in trace concentrations. If $\beta = 1$, i.e. sorption energies are homogeneous, then the equation degenerates into the Langmuir isotherm. If $\beta = 1$ and the reactive tracer is in trace quantities, then the equation degenerates into the Linear isotherm.

Although this report focuses on these four isotherms, other expressions, such as those summarized by Travis and Etnier (1981), can also be evaluated. A major drawback of other expressions and models, such as electrochemical or surface complexation models (Sposito 1984; Cederberg et al., 1985), is the need to couple them to transport codes.

Each data set was fitted to the four isotherms using SAS routines (SAS 1985) that performed the linear regression analyses and provided the statistics to define the accuracy and precision of the isotherms. The computer programs mentioned in Section 2.0 were used to retrieve, organize, feed, analyze the sets, and file the resultant calculations for later tabulation and graphing. The calculated statistics and the estimates for isotherm parameters are presented in tables in Appendix B.

Statistical Parameters

The parameters that were used to compare isotherms were the index of determination (R^2), the coefficient of variation (CV), and the sum of squared

errors (SSE). The index of determination gives the fraction of the total variation of the dependent variable that is due to its relationship with the variation of the independent variable (Freund and Williams 1972). For example, if R^2 is 0.9 for the regression of the sorption data using the Freundlich model, then 0.9 of the total variation in log S is accounted for by its relationship with log C. However, it should be noted that the R^2 does not establish a cause-and-effect relationship, but only that a relationship exists. A cause-and-effect relationship is established by logical argument, not high values of R^2. It is also possible to find a numerically high degree of correlation in a sample drawn from a population in which there is no correlation whatever (Freund and Williams 1972). Therefore, it is appropriate to use additional statistics to evaluate how well the sorption data are represented by the isotherm models.

The coefficient of variation is another criterion for comparison and is defined as the standard deviation divided by the mean. Thus, the deviations are normalized with respect to the mean, which defines a relative standard deviation.

The sum of squared errors from the regression line is another criterion for comparing results. However, a comparison of models when the variables are different (e.g., the dependent variable in the linear model is S, but the dependent variable in the Freundlich model is log S) is not appropriate unless the dependent variable is the same. Consequently, the equations of the four models were expressed as a function of S after each regression, and then the sums of squared deviations were determined and compared.

Equivalent Isotherm Parameters

The four models are also compared on the basis of equivalent isotherm parameters. This comparison provides an insight on the affects of using different isotherms to represent the same data in transport codes when all considered isotherms fit the same data with relatively good correlation. In addition, this comparison should permit the evaluation of the concept that the Freundlich, Langmuir, and Linear models are special cases of the general Modified Freundlich. The transformation from isotherm parameters of each isotherm to the equivalent parameter is given in Table I. The parameters of the four isotherm models are compared on the basis of the equivalent K_d of the Linear model and on the basis of the equivalent K_D and β of the Modified Freundlich model. These comparisons have been made because the Linear isotherm is the simplest and perhaps the most commonly used sorption expression in transport models. The Modified Freundlich isotherm, on the other hand, describes the extent of sorption heterogeneity and, therefore, it can be used to predict the variability of retardation (or "dispersion" caused by sorption) of radionuclides under flow conditions when local equilibrium exists. For example, the K_D can be described as an average K_D that can give an indication of the average breakthrough of a radionuclide under flow conditions; the β can be described as the spread or dispersion of individual K_D's about the mean K_D that can give an indication of the "dispersion" of a radionuclide due to sorption.

A small K_D predicts a relatively fast average breakthrough; a large K_D predicts a relatively slow average breakthrough. The β should vary between zero and one. A value of one indicates homogeneity of sorptive energies and thus no dispersion due to sorption; a value less than one indicates

TABLE I
Equations Used to Transform Parameters of Four Isotherms Into the Equivalent Parameters of the Linear and Modified Freundlich Isotherms

Isotherm	Transformation Equation
Linear	$K_d = K_d$ $K_D = K_d/S_{max}$ $\beta = 1$
Langmuir	$K_d = kb$ $K_D = k$ $\beta = 1$
Freundlich	$K_d = (K/S_{max})^{1/N} S_{max}$ $K_D = (K/S_{max})^{1/N}$ $\beta = N$
Modified Freundlich	$K_d = K_D\ S_{max}$ $K_D = K_D$ $\beta = \beta$

heterogeneity of sorptive energies and thus dispersion due to sorption (dispersion should increase as β approaches zero).

Effects of Variables on Isotherms

The effects of replication, particle size, mineralogy, and hysteresis were tested using F-test calculations. For example, if two sets of data were obtained in which the conditions were the same, except for particle size, then a regression line is determined for each data set. A third regression line is also obtained using the combined data from the two sets. The F value is then calculated from the following ratio;

$$F = \frac{(SS - SS_1 - SS_2)/(m - 1)2}{(SS_1 + SS_2)/(n - 2m)} \tag{11}$$

where

SS = the sum of squares from the combined data set,

SS_1 = The sum of squares from the regression on data set 1,

SS_2 = The sum of squares from the regression on data set 2,

m = The number of data sets (2),

n_1 = number of data points in data set 1, and

n_2 = number of data points in data set 2.

n = number of data points for both data sets.

If the two lines are the same, the calculated F-value is smaller than the critical value for an F-distribution with (m-1)2 and n-2m degrees of freedom (i.e., 2 and n-4 for two data sets).

These tests were performed with programs that use SAS routines (SAS 1985). The effects of the variables on the isotherms were generally

classified as significant or insignificant at the 95% level of confidence. This level was selected as a reasonable value, but this selection does not exclude levels lower or higher. Test results are summarized in Appendix C in tabulated and graphical form.

Thermodynamic Parameters

As a manner of illustrating the application of isotherm parameters to derive thermodynamic properties of sorption processes, the parameters of the Modified Freundlich have been used to estimate the thermodynamic equilibrium constant and free energy of adsorption of appropriate data sets. These estimates are based on assumptions and information (Fuentes et al., 1988) that apply when data modeled by the Modified Freundlich isotherm also represents ion exchange. The free energy values define the energy associated with the sorption process in a general thermodynamic concept and provide an indication of the strength of the bonding.

The thermodynamic equilibrium constant can be determined from the following equation according to Gaines and Thomas (1953) for ion exchange,

$$\ln Keq_B^A = (z_B - z_A) + \int_0^1 \ln K_{rB}^A \, d\bar{X}_B \tag{12}$$

$$K_{rB}^A = \frac{\bar{X}_A{}^{z_B}}{\bar{X}_B{}^{z_A}} \circ \frac{C_B{}^{z_A}}{C_A{}^{z_B}} \circ \frac{\gamma_B{}^{z_A}}{\gamma_A{}^{z_B}} \tag{13}$$

where

$\bar{X}_A$, $\bar{X}_B$ = equivalent fractions of A and B sorbed, respectively;

C_A, C_B = concentrations of A and B, respectively, μmoles/mL^{-1};

γ_A, γ_β = activity coefficient of A and B, respectively;

z_A, z_B = valences of A and B, respectively;

K_{rB}^{A} = rational selectivity coefficient; and

A,B = radionuclide being adsorbed and chemical species being desorbed, respectively.

The Modified Freundlich equation can be written with the same parameters as follows;

$$\frac{\bar{X}_A}{\bar{X}_B} = K_D^{\beta} z_A^{\beta} C_A^{\beta} \tag{14}$$

where

K_D = Modified Freundlich parameter, mL^{-1} μmoles, and

β = Modified Freundlich parameter, dimensionless.

This analysis assumes that sorption occurs by ion exchange and that the experimental data are also well represented by the Modified Freundlich isotherm. Adsorbed equivalent fractions are estimated from equation (14), which assumes that B is an average cation occupying all the sites measured by the cation exchange capacity, but excluding those used by cation A. After substituting equation (14) into equation (13), and equation (13) into equation (12) and integrating, equation (12) can then be rewritten as

$$\begin{aligned} \ln Keq_B^A = & -z_A \left[\left(\frac{C_{Bo}}{\frac{w}{v}\bar{C}_{Bo}}\right) \ln C_{Bo} + 1\right] \\ & + z_A \left[1 + \frac{C_{Bo}}{\frac{w}{v}\bar{C}_{Bo}}\right] \ln \left[\frac{w}{v}\bar{C}_{Bo} + C_{Bo}\right] \\ & + z_B \ln K_D + z_B \ln z_A + z_A \ln \gamma_B - z_B \ln \gamma_A \end{aligned} \tag{15}$$

where

w = weight of solid, g,

v = volume of liquid, mL,

C_{Bo} = initial concentration of B, μmoles/mL$^{-1}H_2O$, and

$\bar{C}_{Bo}$ = initial concentration of B sorbed, μmoles/g^{-1}solid.

For these sorption studies

w/v = 1g/20mL;

$\bar{C}_{Bo}$ = cation exchange capacity of the tuff;

C_{Bo} = the concentration of an average cation in J-13 water that exchanges with A (the primary cations in J-13 water are sodium and calcium);

γ_A, γ_B = activity coefficients calculated from the Debye Huckel equation (Garrels and Christ 1965) using the chemical composition of J-13 water; and

z_B = estimated valence of the average cation.

An average cation has a valence that is an average of the valences of those cations (B) that exchange with the cation of concern (A). For these analyses, a range of composite valences of the composite cation was assumed and the equilibrium constant calculated for each (Appendix B).

The Gibbs' free energy of sorption is related to the thermodynamic equilibrium constant by

$$\Delta G = -RT \ln Keq_B^A \tag{16}$$

where

R = gas constant and

T = absolute temperature.

At $25^{o}C$

$$\Delta G = -1.364 \log Keq_{B}^{A}. \quad (17)$$

The estimated thermodynamic equilibrium constants and the free energies of adsorption are given in Appendix B.

4.0 RESULTS

The results and discussion of the evaluation of selected data sets emphasize the effectiveness of isotherms to model individual data sets, the influence of variables on the regression of isotherms, and the estimation of free energies of adsorption from isotherm parameters. Because the scope of this report was to illustrate the potential of the data base to develop isotherms and design future experiments, the authors chose to discuss results for a number of selected cases. These cases in their judgement represent the usefulness and potential of the data base. It is expected that an investigator involved in experimental design would look over specific results in accordance with his needs.

4.1 Modeling of Individual Sets

Individual data sets were modeled according to the four isotherm expressions; Linear, Langmuir, Freundlich, and Modified Freundlich; for adsorption (4.1.1) and desorption (4.1.2). In cases where the cation exchange capacity was not known, the Modified Freundlich expression was not modeled. For cations the CEC is assumed to be the maximum adsorption capacity of the tracer of interest.

4.1.1 Adsorption

<u>Statistical Parameters</u>

The statistical parameters associated with the four isotherm models are

given in Appendix B. Three examples that are representative of the results obtained from the modeling exercise are given in Table II. The data for the first set, cesium adsorption on the YM-22 tuff sample, indicate that the R^2 is very good for all models ranging from 0.9349 to 0.9983. The CV's are also good ranging from -5.5 for the Freundlich to 16.6 for the Langmuir. The sum of squared errors indicates that the Linear model has the lowest value (3.47E-2) with the Modified Freundlich having a similar value (4.6E-2) and the Langmuir having the largest value (23.1). These statistics suggest that all models represent the data very well with Langmuir being the least effective. However the plots of the data (Fig. 1) indicate that the above statistics could be misleading. For example, the data are distributed over eight orders of magnitude for the Freundlich and Modified Freundlich isotherms. But the distribution of data is essentially that of two data points for the Linear and the Langmuir isotherms; thus a best fit straight line will have very good statistics. These results demonstrate the importance of designing experiments for the models to be evaluated. In this case the experiments were more appropriate for evaluating the Freundlich and Modified Freundlich isotherm than for the Linear and Langmuir isotherms.

The second example given in Table II is the sorption of europium on the YM-22 tuff sample. The sorption data are graphically represented in Fig. 2 for the four models. Those graphs indicate a good distribution of data for all models, even though the Linear and Langmuir have "effectively" only three data points. The data in Table II indicate very good statistics for the Linear, Freundlich, and Modified Freundlich isotherms; the R^2 values range from 0.994 to 0.997, the CV values range from -0.8 to 4.8, and the SSE values

TABLE II
Statistical Parameter Estimates of
Isotherm Modeling for the Adsorption of
Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	Parameter	Isotherm Model: Linear	Langmuir	Freundlich	Modified Freundlich
YM-22 Cs 21 air	R^2	0.9976	0.9349	0.9979	0.9983
75-500 amb 58	CV	11.0	16.6	-5.53	-2.03
	SSE	3.47E-02	2.31E+01	8.20E-02	4.62E-02
YM-22 Eu 21 air	R^2	0.9994	0.7883	0.9997	0.9997
75-500 amb 58	CV	4.83	16.9	-1.52	-0.82
	SSE	1.89E-04	1.14E-02	4.81E-05	3.72E-05
GU3-433 Np 42 CO_2	R^2	0.8562	0.1282	0.9481	0.9481
75-500 amb 26	CV	99.7	178	-12.6	-9.17
	SSE	4.05E+04	3.64E+04	8.18E+05	5.28E+05

Refer to Tables B.VI, B.VIII and XVII for more detailed information. Graphical presentations are shown in Figures B.6, B.8 and B.17.

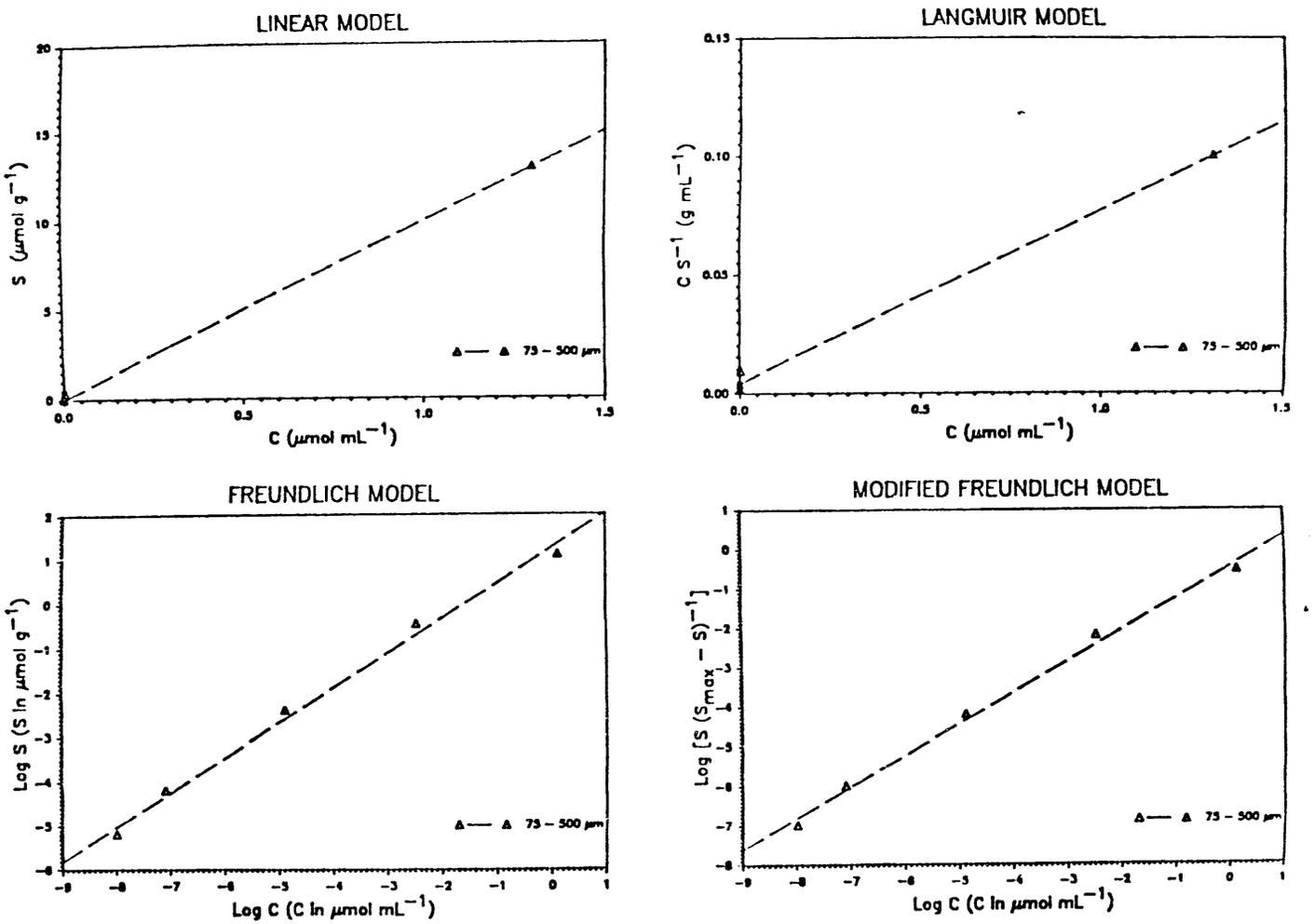

Figure 1. Isotherm plots of the adsorption of cesium on YM-22 tuff with a particle size of 75-500 μm and a cation exchange capacity of 58.0 μeq g^{-1} for a contact time of 21 days in an air atmosphere at ambient temperature.

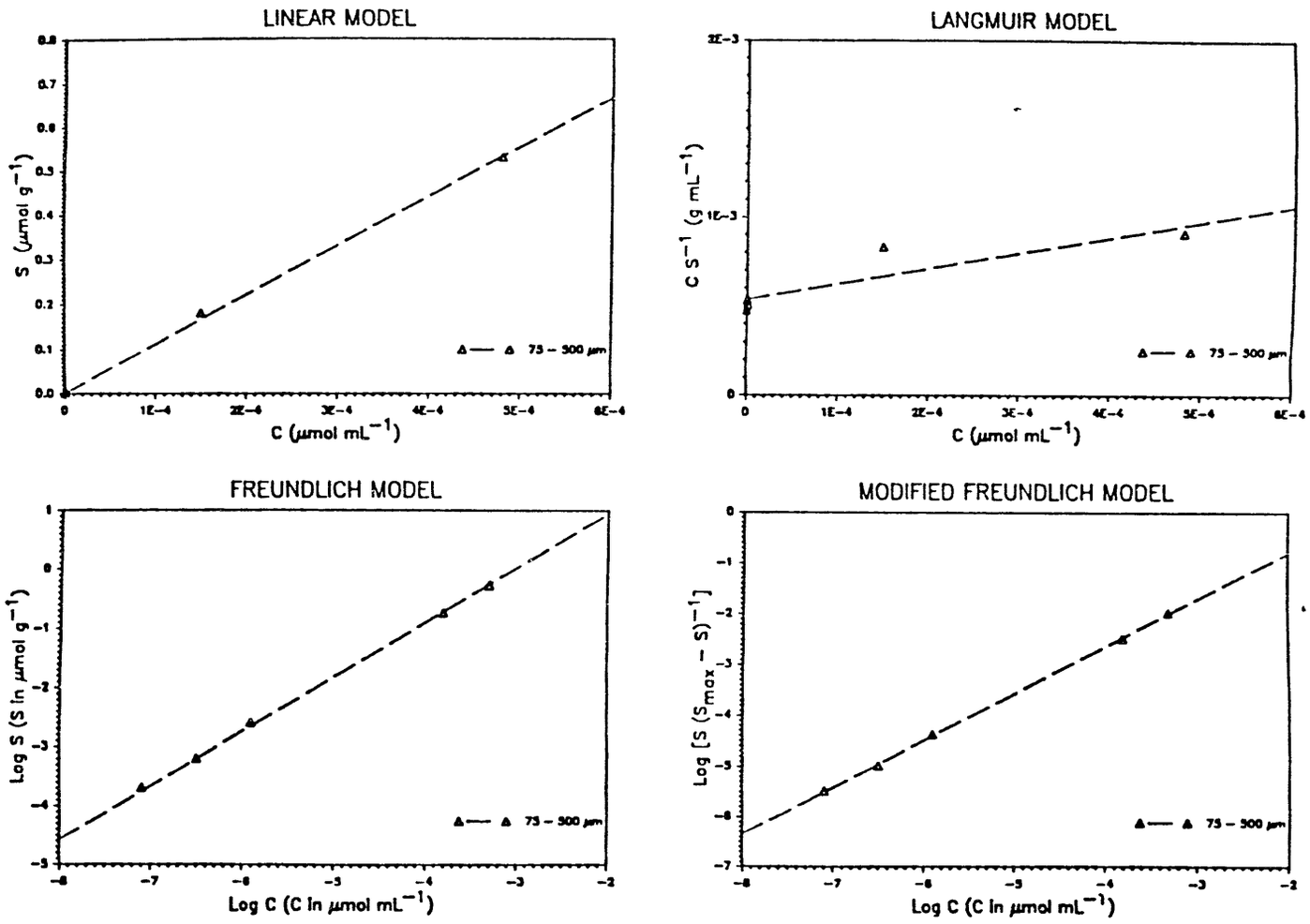

Figure 2. Isotherm plots of the adsorption of europium on YM-22 tuff with a particle size of 75-500 μm and a cation exchange capacity of 58.0 μeq g^{-1} for a contact time of 21 days in an air atmosphere at ambient temperature.

range from 1.9E-04 (Linear) to 3.7E-05 (Modified Freundlich). Although the statistics for the Langmuir are not as good as those for the other three models, they are still considered to be fair (R^2 = 0.7883, CV = 16.9, and SSE = 1.14E-02). Several factors may contribute to those less than ideal statistics. One factor is that the variability of the data increases as the concentration of the solute approaches zero. Therefore, as the concentrations of S and C decrease, the error associated with C/S is accentuated because of the relatively large errors associated with the analysis of low concentrations.

The third set of results in Table II, the sorption of neptunium on the GU3-433 tuff sample in a CO_2 environment, indicates good R^2 values for the Freundlich and Modified Freundlich models (0.9481); a fair R^2 for the Linear (0.8562) and a very poor R^2 for the Langmuir model (0.1282). The CV values are also good for the Freundlich and Modified Freundlich models (-12.6 and -10.4, respectively), but poor for both the Linear and Langmuir models (99.7 and 178, respectively). In contrast, the SSE are better for the Linear and Langmuir (4.05E+04 and 3.65E+04), respectively, than for the Freundlich and Modified Freundlich (8.18E+04 and 5.28E+05, respectively). It should be noted, however, that the CV's and SSE's are relatively large compared to those in the two previous cases for all of the models. Fig. 3 indicates that the distribution and variability of the data for the Langmuir plot are poorer than for the other three models as indicated by the poor R^2 value of the Langmuir isotherm. The higher SSE values for the Freundlich and Modified Freundlich models are due in a large part to two observations (one at the low range and one at the high range) as can be observed in Fig. 3. A Cook's D influence

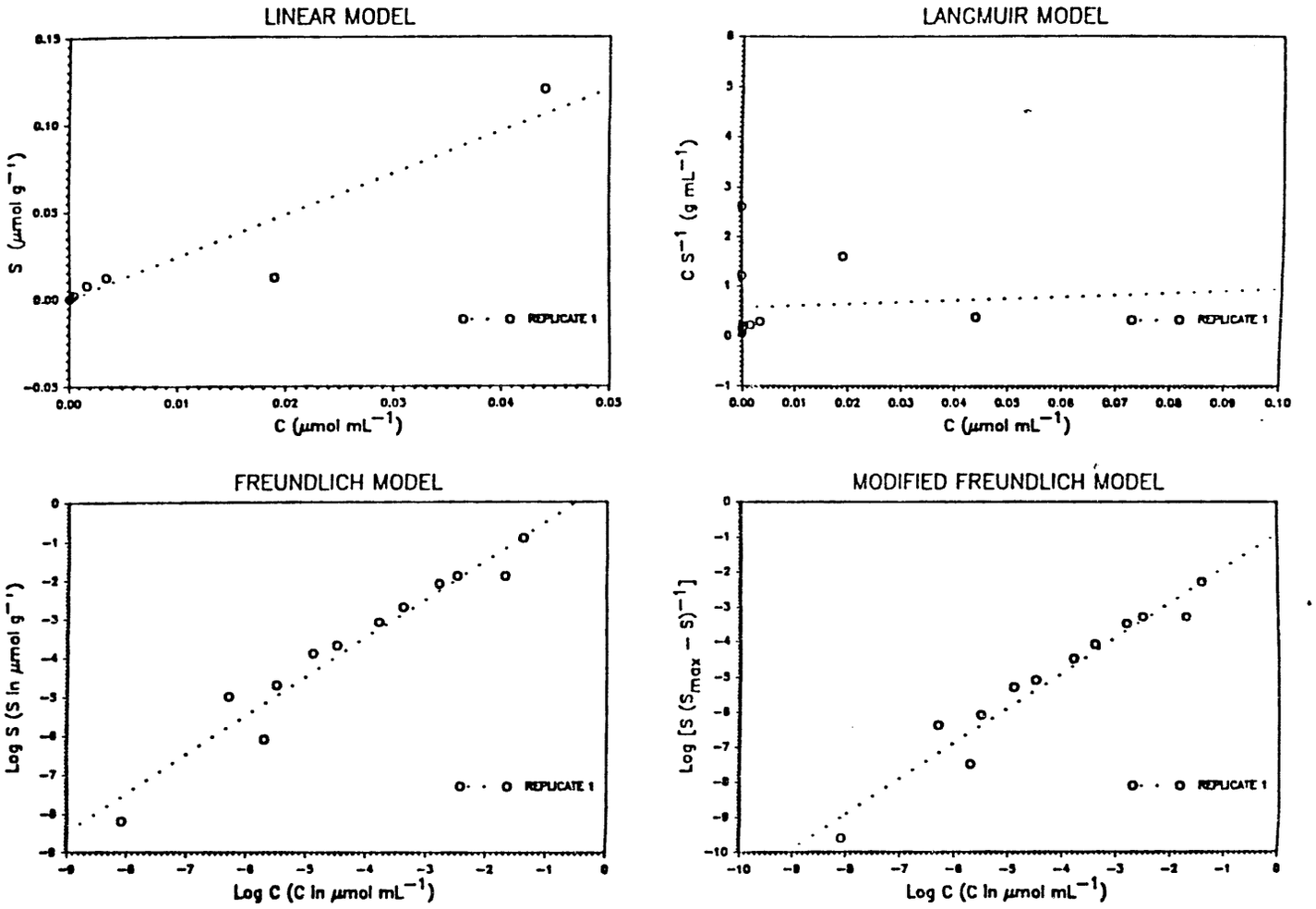

Figure 3. Isotherm plots of the adsorption of neptunium on GU3-433 tuff with a particle size of 75-500 μm and a cation exchange capacity of 26.0 μeq g^{-1} for a contact time of 42 days in a CO_2 atmosphere at ambient temperature.

statistic test (SAS 1985) indicates that those data points can be considered as outliers in all cases.

Equivalent Isotherm Parameters

The estimated equivalent parameters are given in Appendix B. The equivalent parameters are expressed as the K_d of the Linear model and the K_D and β of the Modified Freundlich model. Examples are given in Table III; these examples are for the same sorption data as those generating the statistical data given in Table II.

In the case of the sorption of cesium on YM-22 tuff, the K_d's are comparable for the Linear, Freundlich and Modified Freundlich models with the latter having the highest K_d (16.3 compared to 10.0 for the Linear and 12.9 for the Freundlich). The equivalent K_d for the Langmuir model was much higher (252). A similar trend occurred in the case of the equivalent K_D. The Linear model gave the lowest value (0.172) and the Langmuir giving the highest value (18.6). The equivalent β's were 1.0 for the Linear and Langmuir models and were estimated to be 0.79 and 0.80 for the Freundlich and Modified Freundlich models, respectively.

The differences in equivalent parameter values for the four isotherm models indicate that, regardless of the good overall correlation for all models, differences in correlation can result in different representations of adsorption when either model is arbitrarily selected. Using the parameters of the Modified Freundlich model as reference (these parameters show the highest correlation), retardation would be slightly underestimated (faster breakthrough) with the Linear and Freundlich compared to that with the Modified Freundlich model; the Langmuir model would significantly overestimate

TABLE III
Isotherm Parameters Equivalent to the K_d of the Linear Model and to the K_D and β of the Modified Freundlich Model for the Adsorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	Equivalent Parameter	Isotherm Model			
		Linear	Langmuir	Freundlich	Modified Freundlich
YM-22 Cs 21 air	K_d	10.0	252	12.9	16.3
75-500 amb 58	β	1.0	1.0	0.785	0.797
	K_D	0.172	18.6	0.222	0.281
YM-22 Eu 21 air	K_d	1110	1860	749	758
75-500 amb 58	β	1.0	1.0	0.922	0.922
	K_D	19.2	1630	12.9	13.1
GU3-433 Np 42 CO_2	K_d	1.4	1.82	1.86	1.86
75-500 amb 26	β	1.0	1.0	0.968	0.968
	K_D	0.054	65.1	0.071	0.071

(slower breakthrough) retardation. On the other hand, the Linear and Langmuir models would underestimate sorption heterogeneity, whereas the Freundlich would slightly overestimate heterogeneity compared to that estimated with the Modified Freundlich model.

In the case of the sorption of europium on YM-22 tuff samples the equivalent parameters are essentially the same for the Freundlich and Modified Freundlich models. The equivalent K_d's are 749 and 758, the equivalent K_D's are 12.9 and 13.1, and equivalent β's are both 0.922 for the Freundlich and Modified Freundlich models, respectively. The equivalent parameters for the Linear and Langmuir models are greater than those of the Freundlich and Modified Freundlich models with the Langmuir model having the largest values. Therefore based on the fundamental concepts of the Modified Freundlich the equivalent parameters indicate that the Freundlich model should predict similar retardation to those of the Modified Freundlich model for flow conditions. On the other hand, both the Linear and Langmuir models overestimate average retardation and sorption heterogeneity under flow conditions compared to those predicted with the Modified Freundlich model.

In the case of sorption of neptunium on the GU3-433 tuff samples, the equivalent parameters are the same for the Freundlich and Modified Freundlich models. The equivalent parameters for the Linear and Langmuir models approach the values of the first mentioned models; the one exception is the equivalent K_D. For example, the equivalent K_d's, K_D's and β are 1.86, 0.071 and 0.968, respectively, for both the Freundlich and Modified Freundlich models; equivalent parameter values for the Linear are 1.40, 0.054 and 1.0, respectively; and those for the Langmuir are 1.82, 65.1 and 1.0, respectively.

In this case, where the β value is close to 1 for the Modified Freundlich isotherm and the concentration is low the three special cases should have had similar parameter values (i.e., $S_{max} - S \cong S_{max}$ and $\beta = 1$). The fact that the equivalent K_D for the Langmuir does not have a similar value, indicates the importance of evaluating outliers in experiments. A look at the data in Fig. 3 suggest that one data point (the second largest C value) may be an outlier and, if so, pertubates the slopes of the Langmuir and Linear models. A Cook's D test indeed does suggest that that data point unduly influences the regression of the four isotherms; it has a much greater effect on the Langmuir regression than those of the Linear, Freundlich, and Modified Freundlich.

The elimination of that one data point would decrease the slope ($\frac{1}{b}$) in the Langmuir model, but would have only a minimal effect on the intercept ($\frac{1}{kb}$). Because the intercept is minimally affected by the outlier and because the equivalent K_d is equal to the reciprocal of the intercept, the elimination of the outlier should not change the equivalent K_d significantly. On the other hand, because the intercept ($\frac{1}{kb}$) is not significantly affected by the outlier, but the slope ($\frac{1}{b}$) is, $\frac{1}{k}$ or k must also be significantly affected by the outlier; when b varies, k must also vary in order to maintain $\frac{1}{bk}$ a constant. Likewise when k varies, the equivalent K_D will vary; equivalent K_D is equal to k. Thus the elimination of the outlier would bring the equivalent K_D in line with that predicted. Thus the discrepancy in the equivalent K_D values for the Langmuir model can be explained on the basis of an outlier in the data set.

4.1.2 Desorption

Statistical Parameters

Statistical parameter estimates are given in Table IV for the modeling of

TABLE IV
Statistical Parameter Estimates of Isotherm Modeling for Desorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	Parameter	Isotherm Model: Linear	Langmuir	Freundlich	Modified Freundlich
YM-48 Tc 63 air 106-500 amb 484	R^2	1.0000	0.0075	0.9991	0.9991
	CV	0.0519	33.2	-3.20	-1.98
	SSE	9.93E-08	8.26E+02	9.28E-03	9.50E-03
YM-49 Tc 63 air 106-500 amb 1170	R^2	1.0000	0.5735	0.9996	0.9996
	CV	0.0409	28.0	-2.21	-1.29
	SSE	4.53E-08	2.31	6.32E-04	6.13E-04

More detailed information is presented in Tables B.XXI and B.XXIV. Graphical representations are shown in Figures B.17 and B.21.

desorption of technetium on YM-48 and YM-49 tuff samples with the four isotherm expressions. The results indicate that the Linear model represents the data best, and the Langmuir represents the data the poorest. The Freundlich and Modified Freundlich models represent the data between two extremes. For example, the Linear model shows perfect correlation ($R^2 = 1$) with low CV's. On the other hand, the Langmuir model shows poorest correlation and large CV's. Figs. 4 and 5 give an indication as to the reason for the differences between the Linear and Langmuir models. In the case of the Linear model the data presents only two data points. Therefore perfect correlation and good CV and SSE are expected. On the other hand, the Langmuir model shows a cluster of three data points near a zero concentration (essentially one effective concentration) for three values of the dependent variable; that variable being CS^{-1}. At very low concentrations of C and S, the error tends to be relatively large and when one is divided by the other, then the errors are accentuated compared to dependent variables for the other models. The statistical parameter estimates for the Freundlich and Modified Freundlich models are more reliable because the data are more uniformly distributed over the range of concentrations than those of the Linear and Langmuir models.

Equivalent Isotherm Parameters

A comparison of equivalent isotherm parameters (K_d, K_D, and β) for the desorption of technetium on YM-48 and YM-49 tuff samples is given in Table V and shown in Figures 4 and 5. The data indicate that the equivalent parameter estimates for the four models are generally comparable. Those of the Langmuir

TABLE V
Isotherm Parameters Equivalent to the K_d of the Linear Model and to the K_D and β of the Modified Freundlich Model for the Desorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	Equivalent Parameter	Isotherm Model			
		Linear	Langmuir	Freundlich	Modified Freundlich
YM-22 Tc 63 air	K_d	1.505	1.577	1.296	1.300
106-500 amb 484	β	1.0	1.0	0.9870	0.9871
	K_D	0.00311	0.05123	0.00268	0.00269
YM-49 Tc 63 air	K_d	1.277	2.056	1.018	1.019
106-500 amb 1170	β	1.0	1.0	0.9653	0.9653
	K_D	0.00109	0.650	0.00087	0.00087

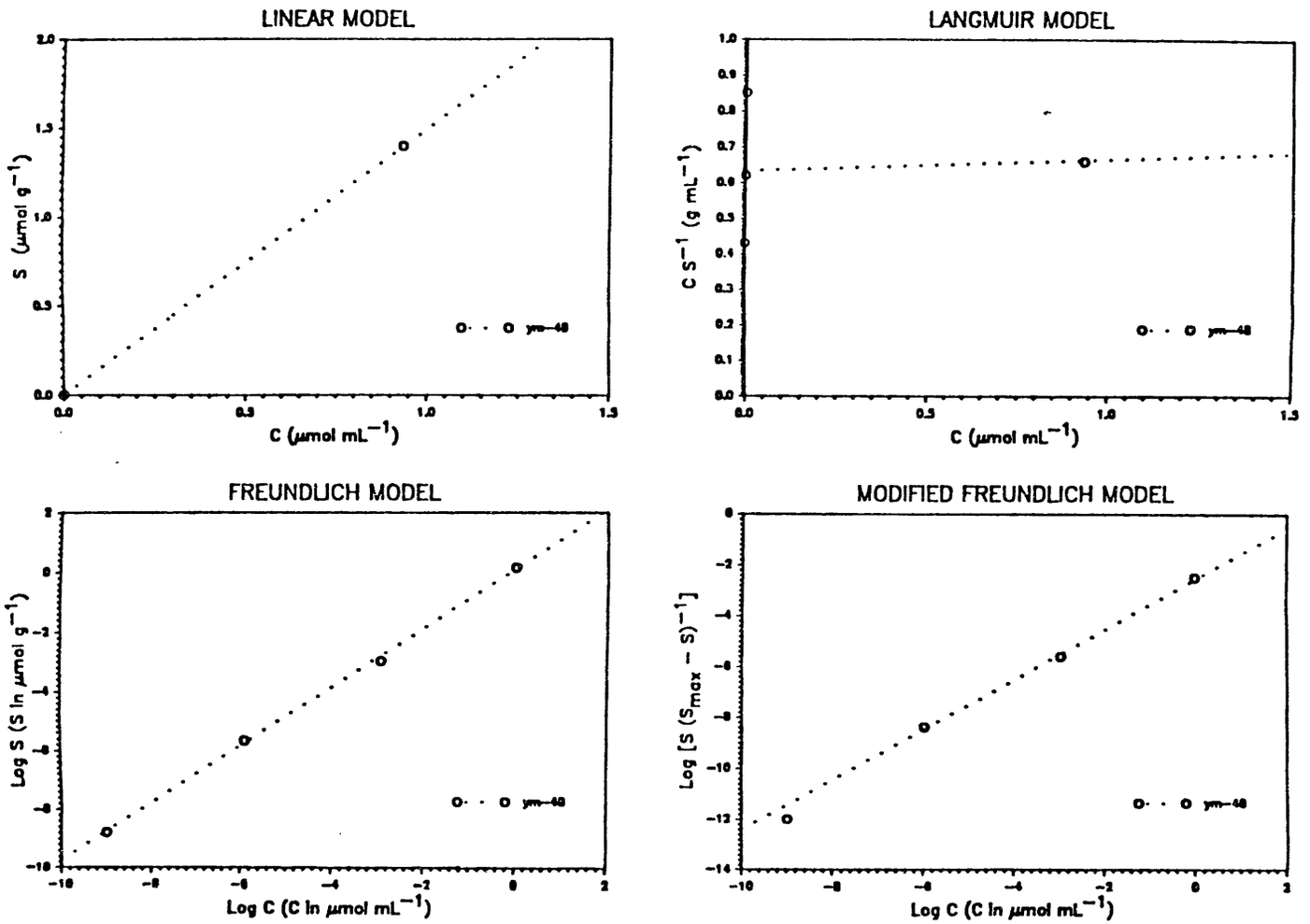

Figure 4. Isotherm plots of the desorption of technetium on YM-48 tuff with a particle size of 106-500 μm and a cation exchange capacity of 484.0 μeq g^{-1} for a contact time of 63 days in an air atmosphere at ambient temperature.

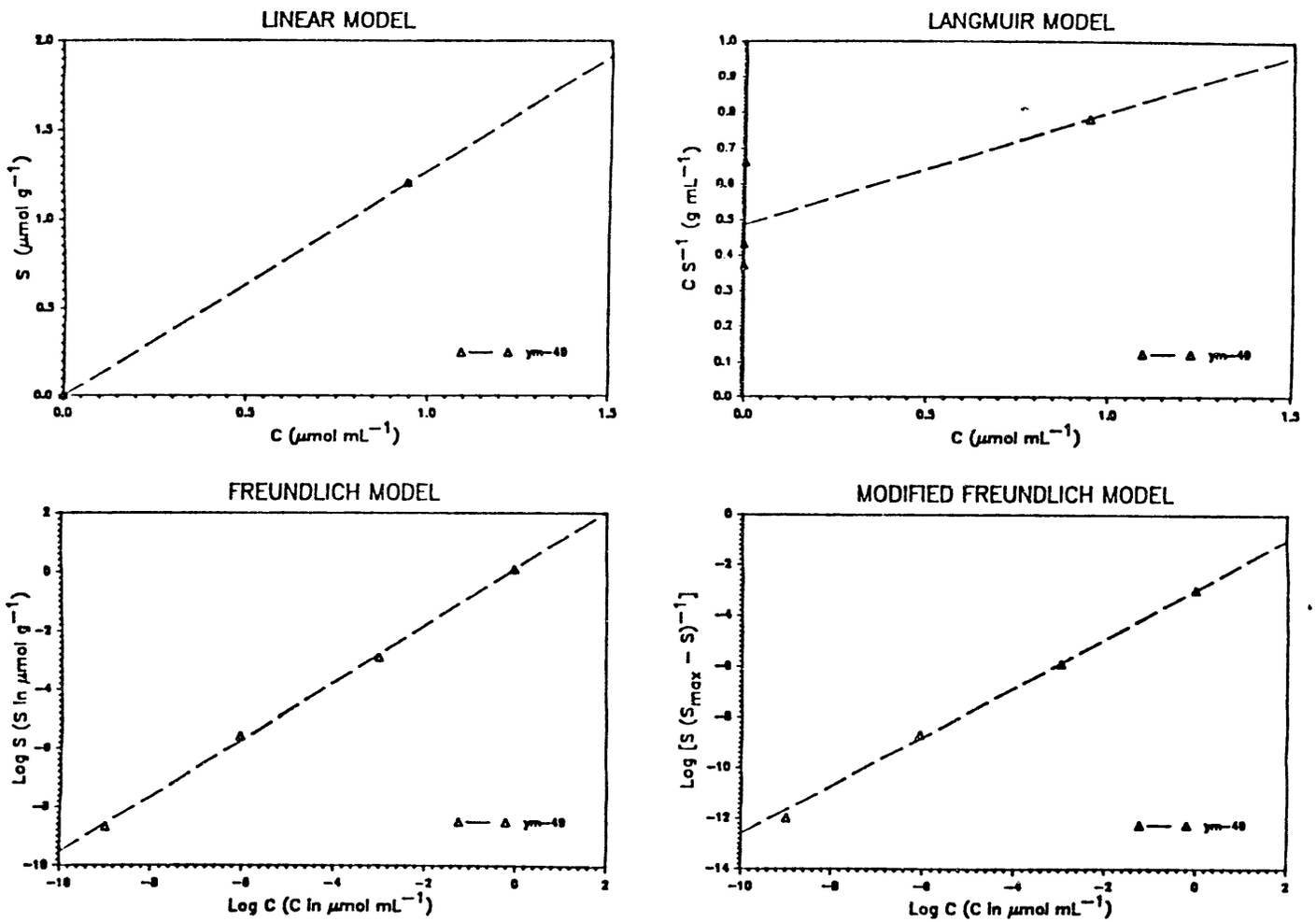

Figure 5. Isotherm plots of the desorption of technetium on YM-49 tuff with a particle size of 106-500 μm and a cation exchange capacity of 1170.0 μeq g^{-1} for a contact time of 63 days in an air atmosphere at ambient temperature.

being higher than the equivalent parameter estimates of the Linear model, and both being higher than those of the Freundlich and Modified Freundlich models. Parameter estimates were the same for the latter two models. This similarity of parameter estimates warrants the use of either isotherm in transport predictions with a minimum of differences. A larger value of 0.65 for the Langmuir model is likely a result of the larger statistical errors associated with the regression of the data.

4.2 Effects of Variables on Isotherms

Thomas (1987) investigated the sorption of radionuclides on Yucca Mountain area tuffs as a function of mineralogy, temperature, particle size, waste element concentration, water composition, sorption time, and other variables. It is also appropriate to examine the effects of these variables on parameters from the four isotherm models. It was not possible to evaluate all variables because sufficient data were not available. Those that could be evaluated were replication, particle size, mineralogy, and hysteresis.

Table VI gives the results of the evaluation of the effect of replication on the regression of the isotherm models for some sets. The results indicate that replication had no effect on the regression of the isotherm models with the exception of two cases of the regression of the Linear model. These two cases are the sorption of neptunium on the GU3-433 tuff (Fig. 6) and the sorption of protactinium on G4-1608 tuff (Fig. 7). The differences in regression lines for the Linear model in those two cases are mostly due to the difference in the amount of sorption occurring at the highest concentration of the radionuclide investigated. One of the two data points is an outlier because only one concentration is responsible for the difference in regression

TABLE VI
Effect of Replication on the Regression of the Isotherm Models for the Sorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	F-test (95% C.L.)	Isotherm Model: Linear	Langmuir	Freundlich	Modified Freundlich
G1-2840 Cs 21 air 75-500 amb 430 (Tables B.III and B.IV)*	Ft	3.52	3.52	3.52	3.52
	Fc	0.92	0.02	0.24	0.24
	Regression lines	same	same	same	same
G1-2840 Sr 21 air 75-500 amb 430 (Tables B.XI and B.XII)*	Ft	3.47	3.47	3.47	3.47
	Fc	0.00	0.45	0.12	0.13
	Regression lines	same	same	same	same
GU3-433 Np 42 CO_2 75-500 amb 26 (Tables B.XVII and B.XVIII)*	Ft	3.49	3.49	3.49	3.49
	Fc	5.52	0.48	0.12	0.12
	Regression lines	different	same	same	same
G4-1608 Np 42 CO_2 >5-500 amb n.a. (Tables B.XV and B.XVI)*	Ft	3.52	3.52	3.52	----
	Fc	0.51	0.40	0.33	----
	Regression lines	same	same	same	----
G4-1608 Pa 42 CO_2 75-500 amb n.a. (Tables B.IX and B.X)*	Ft	4.46	4.46	4.46	----
	Fc	10.20	0.64	0.49	----
	Regression lines	different	same	same	----

Ft = F value listed in F table
Fc = F value calculated
n.a. = not applicable
C.L. = confidence limit
*Refer to these tables for more detail.

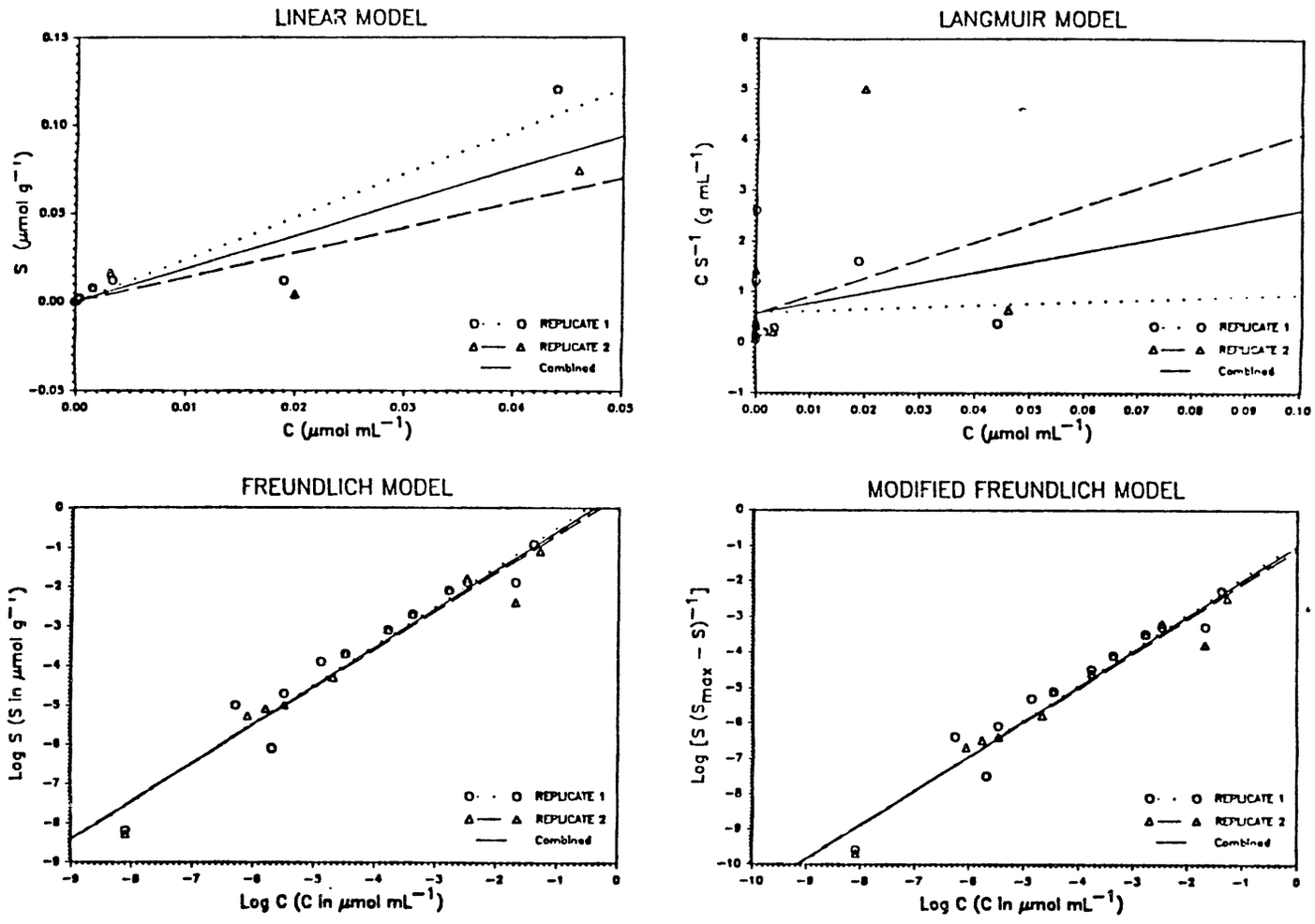

Figure 6. Isotherm plots that show the effect of replication on the adsorption of neptunium on GU3-433 tuff with a particle size of 75-500 μm and a cation exchange capacity of 26.0 μeq g^{-1} for a contact time of 42 days in a CO_2 atmosphere at ambient temperature.

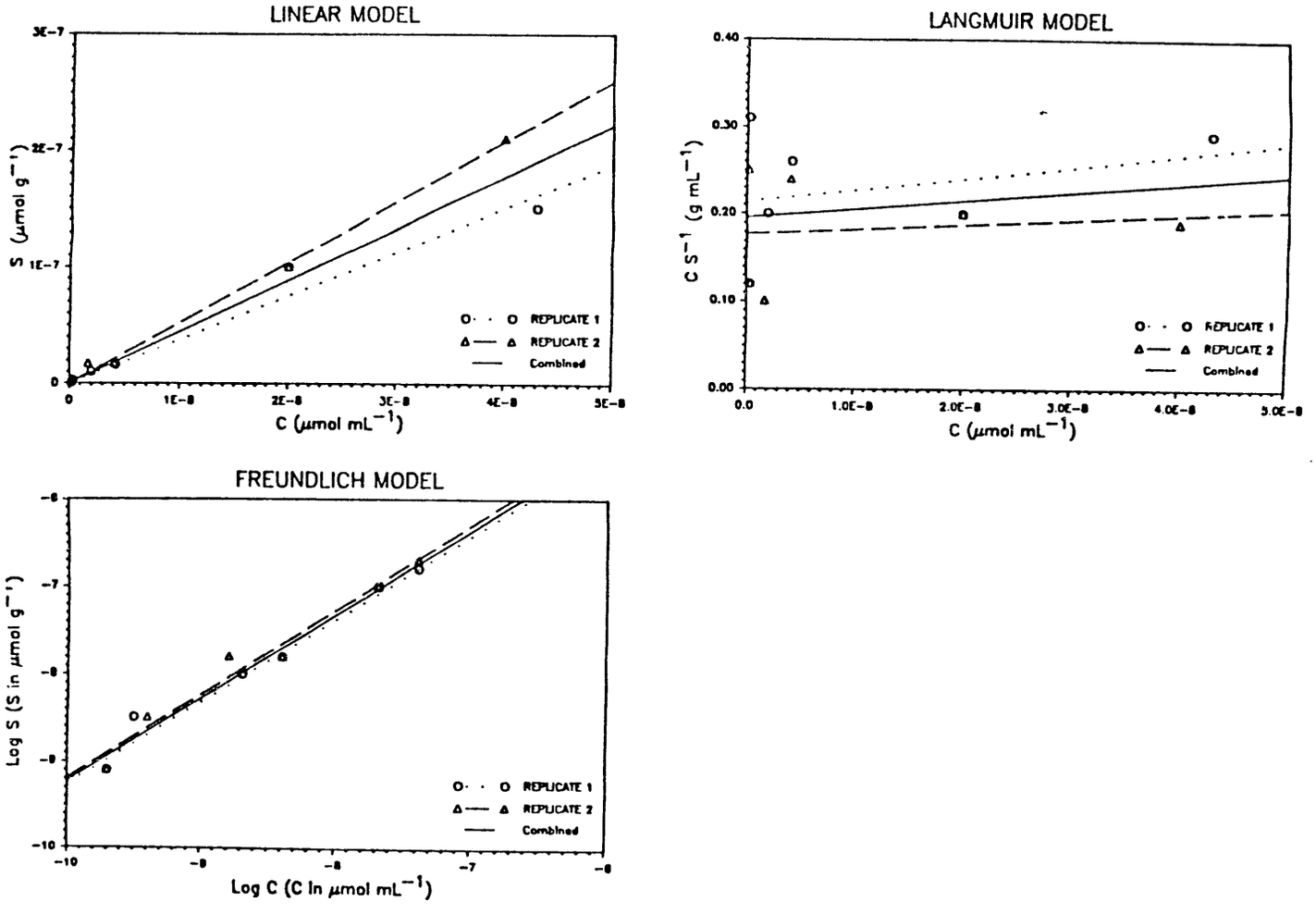

Figure 7. Isotherm plots that show the effect of replication on the adsorption of protactinium on G4-1608 tuff with a particle size of 75-500 μm for a contact time of 42 days in a CO_2 atmosphere at ambient temperature.

for replication. In general, the above results indicate that replication of data sets does not statistically affect the regression line for the isotherm models. Therefore the two data sets could be used as one data set. Combining the two data sets would improve the confidence in the data. These results also indicate that replication may not be necessary, thus potentially reducing laboratory effort.

The effect of particle size on the regression of the isotherm models was evaluated for the sorption of cesium, strontium, barium, and europium on YM-22 tuff (Table VII). The < 75 and 75-500 μm size ranges were compared. The result of those comparisons indicate that no difference in the regression lines was observed for the sorption of europium on the two size ranges of YM-22 tuff. In contrast, the sorption of barium on the two size fractions resulted in two statistically different regression lines for all four isotherm models. In the case of cesium sorption a difference in regression was observed only for the Linear model. In the case of strontium sorption a difference in regression was observed for the Linear and Langmuir models.

The results indicate that different regression lines occur for sorption on different particle size YM-22 tuff when: (1) the data set is not uniformly distributed over the concentration range of radionuclide in solution; and (2) the variability of the data about each regression line is small. The modeling of cesium sorption (Fig. 8) and of strontium sorption by the Linear and Langmuir isotherms (Fig. 9) is an example of poorly distributed sorption data. The differences in regression lines are due primarily to differences in sorption at the highest radionuclide concentration. Potential error in one or the other of the sorption data points would accentuate differences in the

TABLE VII
Effect of Particle Size on the Regression of the Isotherm Models for the Sorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	F-test (95% C.L.)	Isotherm Model: Linear	Langmuir	Freundlich	Modified Freundlich
YM-22 Cs 21 air (<75vs75-500) amb (44vs58) (Tables B.XXIX and B.XXX)*	Ft Fc Regression lines	5.14 30.4 different	5.14 4.54 same	5.14 0.05 same	5.14 0.73 same
YM-22 Sr 21 air (<75vs75-500) amb (44vs58) (Tables B.XIII and B.XIV)*	Ft Fc Regression lines	5.14 2380 different	5.14 46.9 different	5.14 1.72 same	---- ---- ----
YM-22 Ba 21 air (<75vs75-500) amb (44vs58) (Tables B.XXV and B.XXVI)*	Ft Fc Regression lines	5.14 9.16 different	5.14 682 different	5.14 11.6 different	5.14 36.8 different
YM-22 Eu 21 air (<75vs75-500) amb (44vs58) (Tables B.VII and B.VIII)*	Ft Fc Regression lines	5.79 0.03 same	5.79 1.79 same	5.79 0.20 same	5.79 0.71 same

Ft = F value listed in F table
Fc = F value calculated
C.L. = confidence limit
*Refer to these tables for more detail.

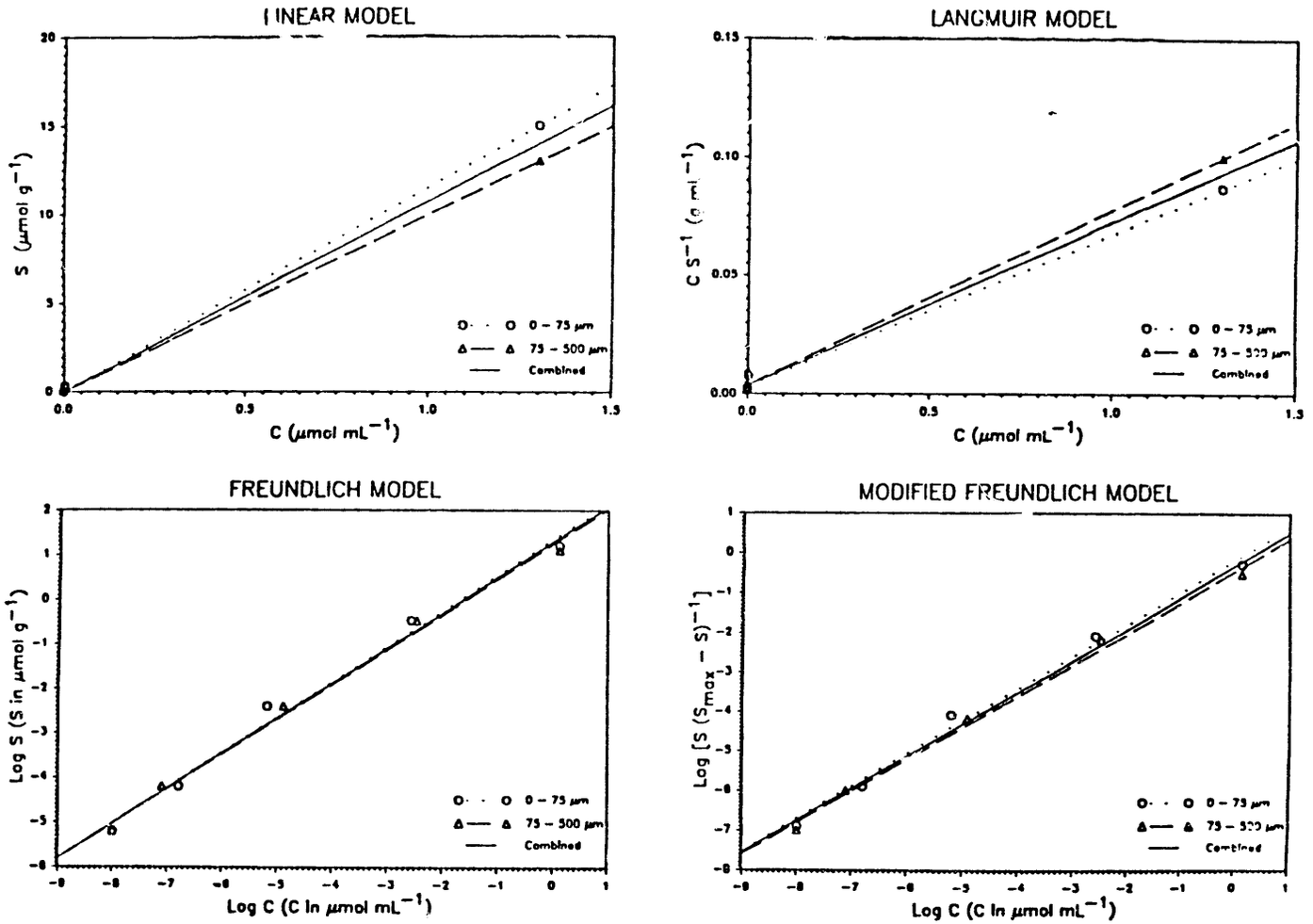

Figure 8. Isotherm plots that show the effect of particle size on the adsorption of cesium on YM-22 tuff for a contact time of 21 days in an air atmosphere at ambient temperature. A cation exchange capacity of 44.0 μeq g^{-1} for the < 75 μm tuff and 58.0 μeq g^{-1} for the 75-500 μm tuff were used for the Modified Freundlich isotherms.

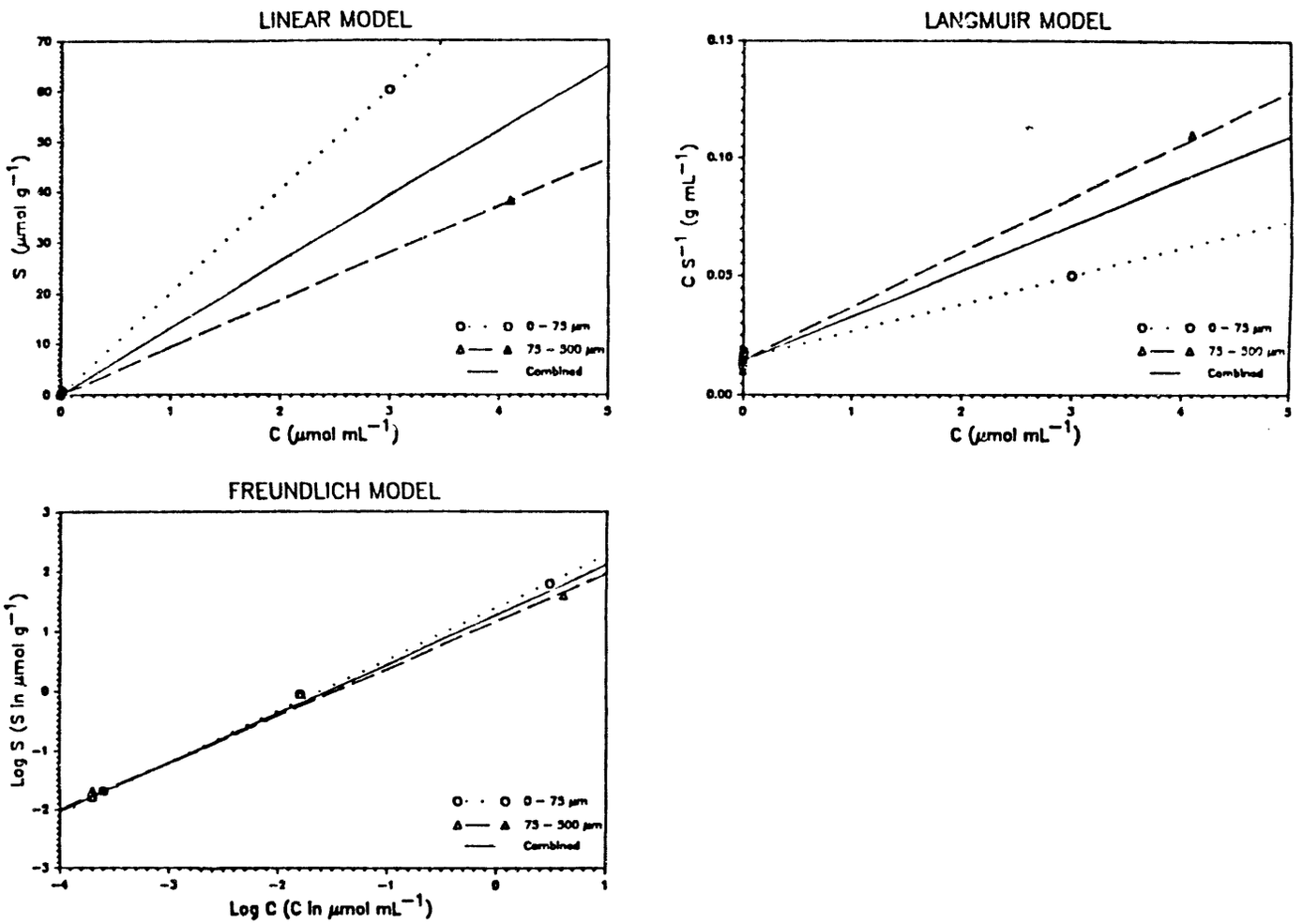

Figure 9. Isotherm plots that show the effect of particle size on the adsorption of strontium on YM-22 tuff for a contact time of 21 days in an air atmosphere at ambient temperature.

regression line. Therefore, additional data are needed in the higher concentration range in order to increase precision. The modeling of the sorption of barium by the four isotherms (Fig. 10) shows little variability about each of the regression lines. Thus apparently real differences do occur in the sorptive behavior of barium on YM-22 tuff between that of the < 75 μm and that of the 75-500 μm particle size range even though these differences may be small. In contrast, the modeling of the sorption of europium by the four isotherms (Fig. 11) shows greater variability of data about the regression line for sorption on the < 75 μm particle size range, so that any real difference may be masked by the large variability.

If the assumption is made that differences in the regression lines are due to differences in sorptive behavior of barium on YM-22 tuff, as opposed to experimental error, then the question should be asked as to the reason for this difference. The regression lines modeled by the Freundlich isotherm in Fig. 10 indicate that the < 75 μm particle size range has a higher sorptive capacity than does the 75-500 μm particle size range. This higher sorptive capacity could be due to a higher CEC. It should be noted that the CEC or maximum sorption is an integral part of the Freundlich K parameter. On the other hand, the CEC (maximum sorption) has been removed from the isotherm parameter K_D, and is included as a part of the dependent variable $(\frac{S}{S_{max} - S})$ in the Modified Freundlich model. Thus, if the difference in the regression lines for the Freundlich model is due to a difference in sorptive capacity between the two size fractions, then the F-test on the regression lines for the Modified Freundlich model should indicate the same line. The CEC of the two size fractions given by Thomas (1987) indicates that the 75-500 μm size

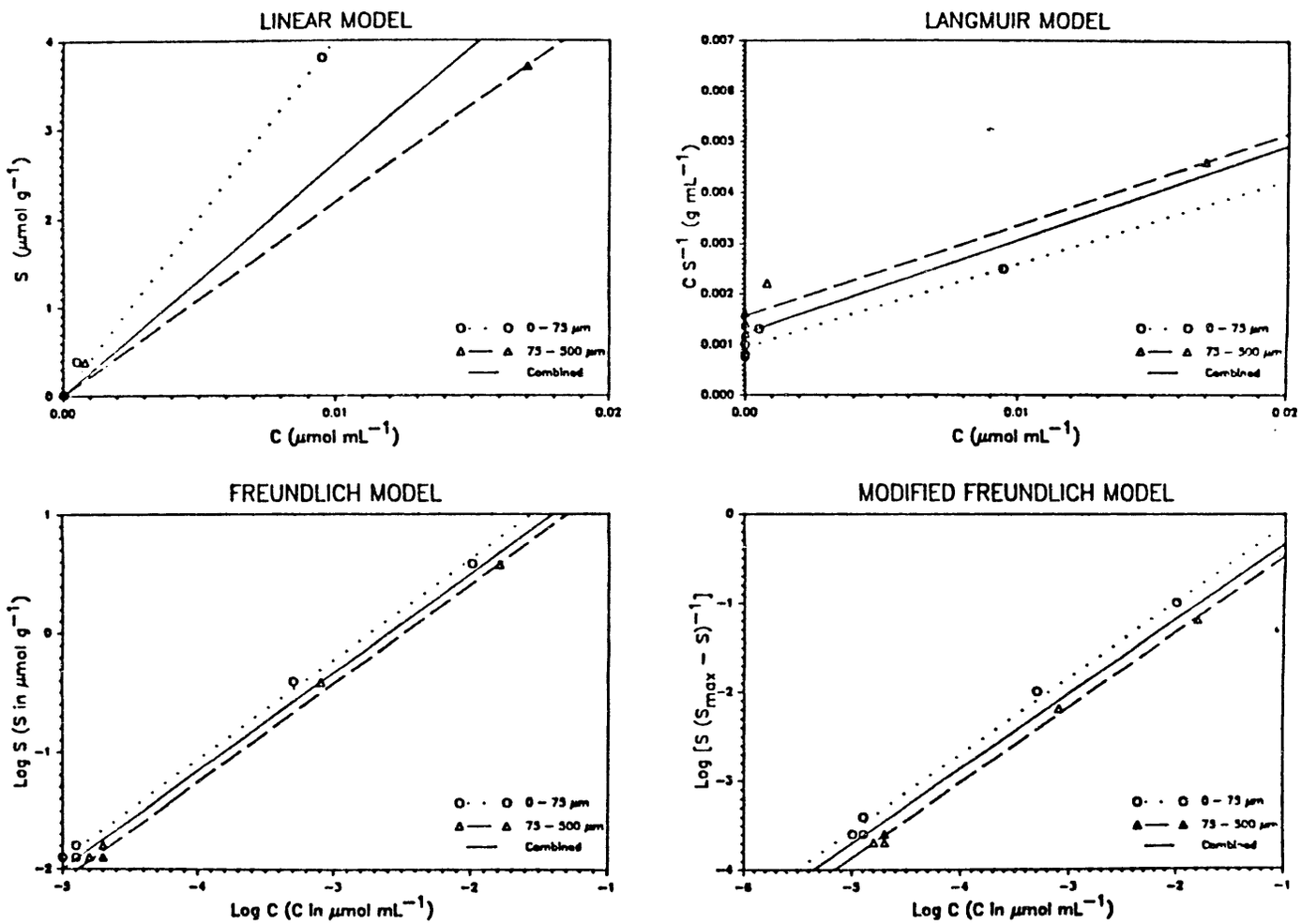

Figure 10. Isotherm plots that show the effect of particle size on the adsorption of barium on YM-22 tuff for a contact time of 21 days in an air atmosphere at ambient temperature. A cation exchange capacity of 44.0 μeq g^{-1} for the < 75 μm tuff and 58.0 μeq g^{-1} for the 75-500 μm tuff were used for S_{max} in the Modified Freundlich isotherm.

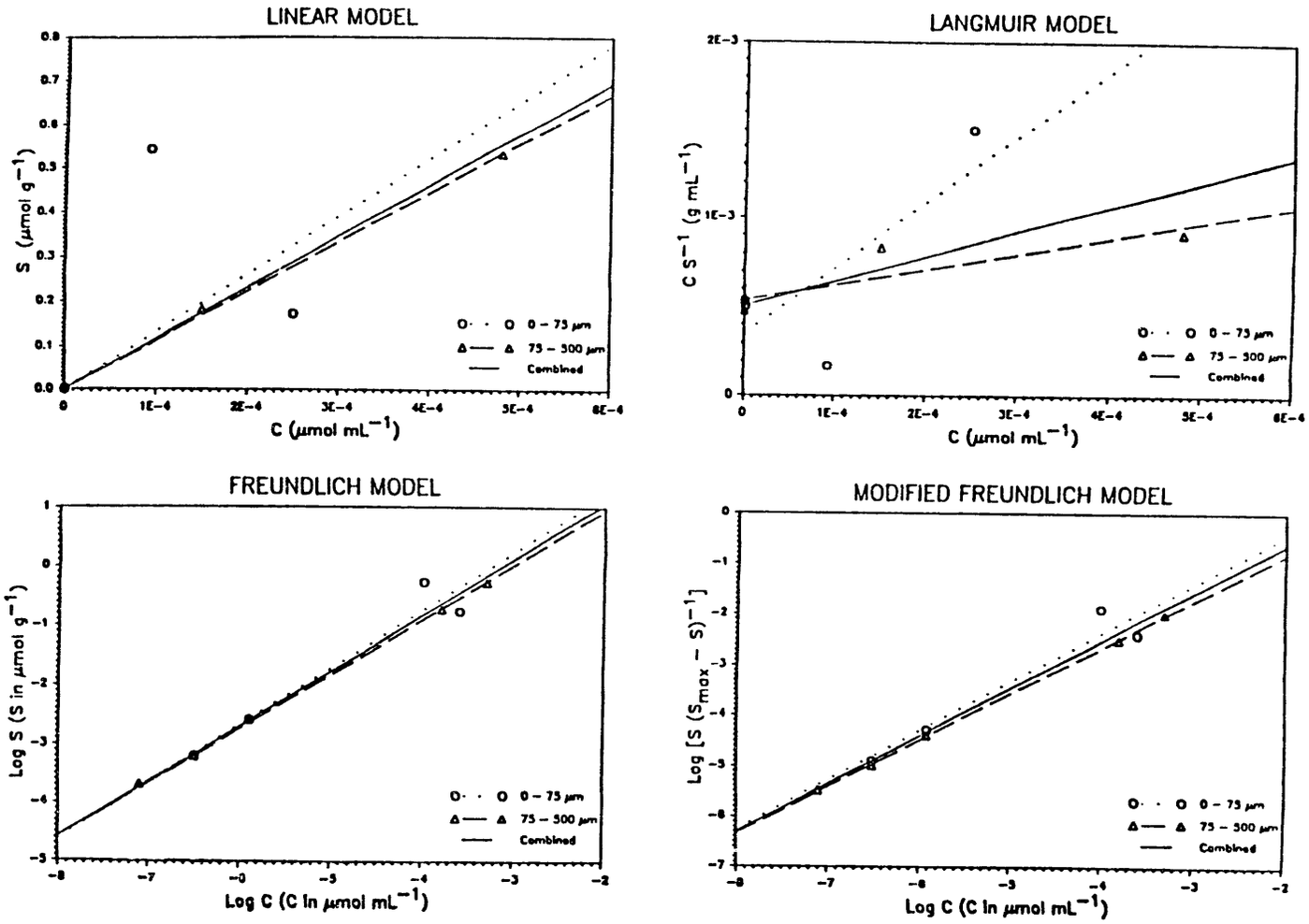

Figure 11. Isotherm plots that show the effect of particle size on the adsorption of europium on YM-22 tuff for a contact time of 21 days in an air atmosphere at ambient temperature. A cation exchange capacity of 44.0 μeq g^{-1} for the < 75 μm tuff and 58.0 μeq g^{-1} for the 75-500 μm tuff were used for S_{max} in the Modified Freundlich isotherms.

fraction has the higher CEC (58 μeq g^{-1} compared to 44 μeq g^{-1} for the < 75 μm size fraction). These CEC values were determined by the sum of cations method. CEC values determined by the NH_4OAC method were 8 μeq g^{-1} and 14 μeq g^{-1} for the 75-500 μm and < 75 μm size range, respectively. The latter appear to be reasonable in that the smaller size range has the higher CEC. On the other hand, these CEC values are less than the amount of cesium and strontium adsorbed on these tuff material. Therefore, the initial quoted values (58 and 44 μeq g^{-1}) were used in the Modified Freundlich model. For purposes of speculation, if a value of 58 μeq g^{-1} were used for the < 75 μm size fraction and 44 μeq g^{-1} for the 75-500 μm size fraction in the Modified Freundlich model, then the regression lines for sorption of barium on the tuffs of the two size fractions are not statistically different. These results would be consistent with the assumption that the finer size fraction has the greater CEC. Therefore, when the S_{max} (CEC) is included in the dependent variable of the Modified Freundlich model the sorption data are normalized with respect to the influence of CEC on the sorptive behavior of radionuclide in tuff. These results emphasize the importance of obtaining accurate values for maximum sorption capacities.

A comparison of adsorption and desorption regression lines for the isotherm models are given in Table VIII. The comparisons for the regression of technetium adsorption and desorption on YM-48 and YM-49 indicate that the adsorption regression lines are different from those of the desorption data. For both tuff samples the slope of the desorption regression line is greater than the slope of the adsorption regression line. The results coincide with those given by Thomas (1987) on retardation ratios. The comparison for the

TABLE VIII
Effect of Hysteresis on the Regression of the Isotherm
Models for the Sorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	F-test (95% C.L.)	Isotherm Model			
		Linear	Langmuir	Freundlich	Modified Freundlich
JA-37 U 7 air 335-500 amb n.a. (adsorption vs desorption)	Ft	6.94	6.94	6.94	----
	Fc	9.82	0.65	2.68	----
	Regression lines	different	same	same	----
YM-48 Tc 42-63 air 106-500 amb 484 (adsorption vs desorption)	Ft	6.94	6.94	6.94	6.94
	Fc	>1000	11.3	33.5	33.4
	Regression lines	different	different	different	different
YM-49 Tc 42-63 air 106-500 amb 1170 (adsorption vs desorption)	Ft	6.97	6.94	6.94	6.94
	Fc	>1000	33.9	86.9	86.9
	Regression lines	different	different	different	different

Ft = F value listed in F table
Fc = F value calculated
C.L. = confidence limit

sorption of uranium on JA-37 tuff indicates different regression lines when modeled by the Linear isotherm, but similar regression lines when modeled by the Langmuir and Freundlich isotherm. The variability associated the regression lines of the Langmuir and Freundlich isotherms is very large, thus statistically the regression lines should not be different. In the case of the Linear regression desorption is represented by two data points.

In evaluating the effect of major mineralogy on the regression of isotherm models the regression lines for the adsorption of technetium on YM-48 tuff was compared to the regression lines for the adsorption of technetium on YM-49 tuff (Table IX). The results indicate that major mineralogy has no significant effect on the regression lines. These results are similar to those when comparing sorption ratio for sorption of technetium on YM-48 and YM-49 tuffs (Thomas 1987). The results of the desorption comparisons indicate different regression lines for the Linear and Modified Freundlich models. The difference in regression lines with the Linear model can be explained by the fact that effectively only two data points are modeled in each case and thus even small variability would still show a difference. The regression lines for the Modified Freundlich model were just barely significant at the 95% confidence limit.

4.3 Thermodynamic Parameters

The next examples show that if experiments are properly designed, thermodynamic estimates can be made; these estimates provide a reference for comparison of adsorption of radionuclides on tuff materials and permit an estimation of their relative selectivity. The thermodynamic equilibrium constant and the Gibbs' free energy of adsorption are estimated. Assumptions

TABLE IX
Effect of Mineralogy on the Regression of the Isotherm Models for the Sorption of Radionuclides on Yucca Mountain Tuff Samples

Data Set Description	F-test (95% C.L.)	Isotherm Model			
		Linear	Langmuir	Freundlich	Modified Freundlich
(YM-48vsYM-49) Tc 42 air 106-500 amb (484vs1170) (adsorption)	Ft Fc Regression lines	6.94 0.00 same	6.94 2.44 same	6.94 1.36 same	6.94 1.20 same
(YM-48vsYM-49) Tc 63 air 106-500 amb (484vs1170) (desorption)	Ft Fc Regression lines	6.94 <1000 different	6.94 0.57 same	6.94 0.69 same	6.94 7.53 different

Mineralogy (Thomas, 1987; Bish and Chipera, 1986)

YM-48: CEC-484 μeq g^{-1}, zeolitic (50 ± 14% clinoptilolite, 18 ± 5% Mordenite, 15 ± 3% Opal-CT, 14 ± 4% Alkali-Feldspar, 1 ± 1% smectite)

YM-49: CEC-1170 μeq g^{-1}, glassy (69 ± 3% glass, 17 ± 2% alkali-feldspar, 11 ± 1% clinoptilolite, 3 ± 1% smectite)

are made in these calculations and are based on the information reported by Fuentes et al. (1988). This section is only presented to scope the feasibility of generating thermodynamic properties from isotherms.

Free energy data are presented in Tables X and XI as illustration of estimated free energies of adsorption based on the assumption that sodium is being replaced by the tracer radionuclides. Table X gives estimated ΔG values for the adsorption of cesium, barium, and europium on YM-22 Tuff for 75 μm and 75-500 μm particle sizes. Table XI gives estimates for the adsorption of cesium and strontium on G1-2840 tuff having a particle size of 75-500 μm for replicate experiments. All estimates of ΔG are given in Appendix B for mixtures of sodium and calcium being replaced by the radionuclides; the effective valences of these mixtures are assumed to be 1.0, 1.2, 1.5 and 2.0.

Estimated ΔG values based on theoretical considerations (Eisenman, 1962; Truesdell, 1972) indicate that there is a slight higher preference of feldspar for cesium than for sodium. The ΔG values estimated for the adsorption of cesium on YM-22 tuff (primarily quartz and feldspar) suggest that YM-22 tuff prefers cesium over sodium; ΔG values differ from zero by $\pm$ 0.1 kcal mole^{-1} or less which is probably within the experimental error. The data in Table X indicate that YM-22 has the greatest preference for europium (greatest negative value) and the least preference for cesium (least negative value); the preference for barium is intermediate. The data also indicate slightly greater negative values for the <75 μm particle size than for the 75-500 μm particle size; however, those differences are probably within experimental error. The data in Table XI suggest that the G1-2840 tuff prefers strontium over sodium; on the other hand, sodium and cesium tend to be equally preferred.

TABLE X
Estimated Free Energies of Adsorption for the Sorption of Radionuclides on Two Size Fractions of YM-22 Tuff

	ΔG (kcal mole^{-1})[1]	
	<75 μm	75-500 μm
Cs	-0.12	-0.10
Ba	-2.80	-2.52
Eu	-4.82	-4.38

[1]These estimates assume that the radionuclide replaces a univalent cation on the adsorption site.
Refer to Tables D.XXV, D.XXVI, D.XXIX, D.XXX, D.XXXI and D.XXXII for more details.

TABLE XI
Estimated Free Energies of Adsorption for the Sorption of Radionuclides on 75-500 μm Sized G1-2840 Tuff

	ΔG (kcal $mole^{-1}$)[1]	
	Replicate 1	Replicate 2
Cs	1.34	1.25
Sr	-0.99	-1.07

[1]These estimates assume that the radionuclide replaces a univalent cation on the adsorption site. Refer to Tables D.III, D.IV, D.XI and D.XII for more details.

5.0 CONCLUSIONS

Only a limited number of data sets (15% of total entries) met our requirements for modeling of isotherms and evaluation of variable effects on isotherms. However the results from these sets provide insight into the importance of proper planning of experiments designed for isotherm modeling of sorption data. The limited number of data sets reflects the fact that the inventoried data bases correspond to experiments that were designed to scope the effects of variables on sorption and were not designed for the development of isotherms. No effort was made to provide an exhaustive analysis of each data set, nor to provide specific recommendations for future laboratory work; such aspects were not within the scope of this analysis. The following conclusions are based on the limited number of data sets.

1. If isotherms are required, sorption experiments should be designed with a specific isotherm equation or equations in mind. A set of data may be appropriate for representation by one isotherm equation but not another. In general, the sorption data modeled in this report tended to be appropriate for the Freundlich and Modified Frendlich equations, but less appropriate for the Linear and Langmuir equations.
2. One sorption model may be compared to another model using a number of statistical parameters; however, one statistical criterion may give a conclusion contradictory to another statistical criterion. Therefore one should be concerned that the experimental design was appropriate for each of the models and that one should be aware of the shortcomings of each

statistical criterion. For example, the data used in the regression for each model should be uniformly distributed over the regression. Also, if the data are uniformly distributed over the regression of each of the models, the sums of squared errors from the regressions should provide an appropriate criterion when the errors apply to the same dependent variable.

3. Even though various models may represent the sorption data well from a statistical evaluation, each model may represent sorption differently depending on its extent of correlation.

4. The particle size of tuff material could affect the isotherm parameters derived from the regression of sorption data, if the maximum sorption (e.g., CEC) is a function of particle size. This concept can be tested, for example, by evaluating the effect ofFreundlich model and for the Modified Freundlich model. The Modified Freundlich incorporates the differences in CEC; the Freundlich does not. Thus the regression lines of the sorption data for the two particle sizes should be different when the Freundlich model is used; whereas the regression of that data should be the same when the Modified Freundlich is used. The above evaluation is based on the assumption that the variability of data about the regression lines is less than the effect of a different CEC.

5. The evaluation of the effects of the variables replication, particle size, mineralogy, and hysteresis <u>for the limited number of data sets</u> indicates the following:

   (a) Replication had no affect on the regression lines of the four isotherms.

(b) Particle size did affect the regression lines for the sorption of barium on YM-22 tuff; but did not affect the regression lines for other radionucles, cesium, strontium, and europium. The variability associated with sorption of the latter radionuclides was too great.

(c) No difference was observed in the regression of isotherms as a function of major mineralogy. However, data points were few.

(d) The regression of the adsorptive data was different from that of the desorptive data, suggesting hysteresis. However, a minimum of data was available for evaluation of hysteresis.

Clearly, the above findings are limited to the analyzed sets, and therefore can not be extrapolated to other data sets. Nevertheless, they can be useful in either emphasizing or deemphasizing certain aspects of the design of future experiments. For example, less emphasis may be placed on experiments to test reproducibility (effectiveness of replication) and more emphasis placed on experiments to test hysteresis.

6. The estimated thermodynamic free energies of adsorption for the exchange of monovalent radionuclide (cesium) for a sodium in tuff material are in good agreement with estimated theoretical free energies of adsorption. Free energies of adsorption estimated from sorption data should provide a reference for comparing adsorption of radionuclide and also give an indication of the selectivity of radionuclides for Yucca Mountain tuff materials.

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Appendix A

Adsorption and Desorption Data Sets Used in Modeling and Comparison Tests

Appendix A is a compilation of adsorption and desorption data sets (best sets) that were used (1) for modeling according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherms and (2) for the statistical evaluation of the effect of replication, particle size, mineralogy, and hysteresis on the regression line, intercept, and slope of the four isotherms. A description of the data sets include tuff sample (CORE), radionuclide (EL), sorption ratio (R_d in mL g^{-1}), time of contact (TI in days), atmosphere (ATM as air, controlled, or CO_2), particle size (SIZE in μm), initial concentration (C_0 in mol L^{-1}), equilibrium concentration (C in μmol mL^{-1}), amount sorbed (S in μmol g^{-1}), and stratigraphic unit mineralogy (UNIT-MINER). The stratigraphic units include Topopah Spring (Tpt), Calico Hills (Tht), Prow Pass (Tcp), and Tram (Tct). The mineralogy classification includes devitified, zerolitized, glass, and clays; a description of each is given by Thomas (1987).

TABLE A.I
ADSORPTION DATA SETS USED FOR MODELING AND COMPARISON

CORE	EL	R_d	TI	ATM	SIZE	C_o	C	S	UNIT - MINER
ym-22	ba	760.0	21	air	- 75	0.10E-04	0.51E-03	0.39E+00	Tpt - Devitrified
ym-22	ba	400.0	21	air	- 75	0.10E-03	0.95E-02	0.38E+01	
ym-22	ba	1200.0	21	air	- 75	0.40E-06	0.13E-04	0.16E-01	
ym-22	ba	1300.0	21	air	- 75	0.30E-06	0.91E-05	0.12E-01	
ym-22	ba	1000.0	21	air	- 75	0.30E-06	0.12E-04	0.12E-01	
ym-22	ba	670.0	21	air	75-500	0.30E-06	0.17E-04	0.12E-01	Tpt - Devitrified
ym-22	ba	600.0	21	air	75-500	0.30E-06	0.19E-04	0.12E-01	
ym-22	ba	790.0	21	air	75-500	0.40E-06	0.20E-04	0.16E-01	
ym-22	ba	210.0	21	air	75-500	0.10E-03	0.17E-01	0.37E+01	
ym-22	ba	470.0	21	air	75-500	0.10E-04	0.82E-03	0.38E+00	
gl-2840	cs	1430.0	21	air	75-500	0.18E-08	0.25E-07	0.36E-04	Tpt - Devitrified
gl-2840	cs	1130.0	21	air	75-500	0.18E-08	0.31E-07	0.35E-04	
gl-2840	cs	2400.0	21	air	75-500	0.50E-08	0.41E-07	0.99E-04	
gl-2840	cs	65.0	21	air	75-500	0.16E-04	0.38E-02	0.25E+00	
gl-2840	cs	68.0	21	air	75-500	0.16E-04	0.36E-02	0.25E+00	
gl-2840	cs	1330.0	21	air	75-500	0.70E-08	0.10E-06	0.14E-03	
gl-2840	cs	1580.0	21	air	75-500	0.70E-08	0.87E-07	0.14E-03	
gl-2840	cs	31.0	21	air	75-500	0.16E-03	0.63E-01	0.20E+01	
gl-2840	cs	32.0	21	air	75-500	0.16E-03	0.62E-01	0.20E+01	
gl-2840	cs	19.0	21	air	75-500	0.13E-02	0.67E+00	0.13E+02	
gl-2840	cs	21.0	21	air	75-500	0.13E-02	0.63E+00	0.13E+02	
gl-2840	cs	371.0	21	air	75-500	0.63E-06	0.32E-04	0.12E-01	
gl-2840	cs	366.0	21	air	75-500	0.63E-06	0.33E-04	0.12E-01	
gl-2840	cs	182.0	21	air	75-500	0.16E-05	0.16E-03	0.29E-01	
gl-2840	cs	179.0	21	air	75-500	0.16E-05	0.16E-03	0.29E-01	
gl-2840	cs	24.0	21	air	75-500	0.63E-03	0.29E+00	0.69E+01	
gl-2840	cs	25.0	21	air	75-500	0.63E-03	0.28E+00	0.70E+01	
gl-2840	cs	78.0	21	air	75-500	0.63E-05	0.13E-02	0.10E+00	
gl-2840	cs	81.0	21	air	75-500	0.63E-05	0.12E-02	0.10E+00	
gl-2840	cs	49.0	21	air	75-500	0.63E-04	0.18E-01	0.89E+00	
gl-2840	cs	45.0	21	air	75-500	0.63E-04	0.19E-01	0.87E+00	
gl-2840	cs	1170.0	21	air	75-500	0.63E-07	0.11E-05	0.12E-02	
gl-2840	cs	1060.0	21	air	75-500	0.63E-07	0.12E-05	0.12E-02	
ym-22	cs	130.0	21	air	- 75	0.20E-04	0.27E-02	0.35E+00	Tpt - Devitrified
ym-22	cs	610.0	21	air	- 75	0.20E-06	0.64E-05	0.39E-02	
ym-22	cs	610.0	21	air	- 75	0.30E-09	0.95E-08	0.58E-05	
ym-22		12.0	21	air	- 75	0.20E-02	0.13E+01	0.15E+02	
ym-22	cs	380.0	21	air	- 75	0.30E-08	0.15E-06	0.57E-04	
ym-22	cs	550.0	21	air	75-500	0.30E-09	0.10E-07	0.58E-05	Tpt - Devitrified
ym-22	cs	660.0	21	air	75-500	0.30E-08	0.88E-07	0.58E-04	

TABLE A.I (cont.)
ADSORPTION DATA SETS USED FOR MODELING AND COMPARISON

CORE	EL	R_d	TI	ATM	SIZE	C_o	C	S	UNIT - MINER
ym-22	cs	260.0	21	air	75-500	0.20E-06	0.14E-04	0.37E-02	
ym-22	cs	10.0	21	air	75-500	0.20E-02	0.13E+01	0.13E+02	
ym-22	cs	110.0	21	air	75-500	0.20E-04	0.31E-02	0.34E+00	
ym-22	eu	5800.0	21	air	- 75	0.90E-05	0.93E-04	0.54E+00	Tpt - Devitrified
ym-22	eu	690.0	21	air	- 75	0.30E-05	0.25E-03	0.17E+00	
ym-22	eu	1900.0	21	air	- 75	0.40E-07	0.12E-05	0.24E-02	
ym-22	eu	1900.0	21	air	- 75	0.10E-07	0.31E-06	0.59E-03	
ym-22	eu	1100.0	21	air	75-500	0.90E-05	0.48E-03	0.53E+00	Tpt - Devitrified
ym-22	eu	2100.0	21	air	75-500	0.30E-08	0.85E-07	0.18E-03	
ym-22	eu	1900.0	21	air	75-500	0.10E-07	0.31E-06	0.59E-03	
ym-22	eu	1900.0	21	air	75-500	0.40E-07	0.12E-05	0.24E-02	
ym-22	eu	1200.0	21	air	75-500	0.30E-05	0.15E-03	0.18E+00	
g4-1608	np	3.5	42	co2	75-500	0.70E-04	0.60E-01	0.21E+00	Tht - Zeolitized
g4-1608	np	3.2	42	co2	75-500	0.70E-04	0.60E-01	0.19E+00	
g4-1608	np	5.2	42	co2	75-500	0.20E-10	0.16E-07	0.83E-07	
g4-1608	np	5.6	42	co2	75-500	0.20E-10	0.16E-07	0.87E-07	
g4-1608	np	6.0	42	co2	75-500	0.40E-07	0.31E-04	0.18E-03	
g4-1608	np	4.7	42	co2	75-500	0.40E-07	0.32E-04	0.15E-03	
g4-1608	np	5.2	42	co2	75-500	0.70E-06	0.56E-03	0.29E-02	
g4-1608	np	4.7	42	co2	75-500	0.70E-06	0.57E-03	0.27E-02	
g4-1608	np	4.4	42	co2	75-500	0.40E-06	0.33E-03	0.14E-02	
g4-1608	np	5.9	42	co2	75-500	0.40E-06	0.31E-03	0.18E-02	
g4-1608	np	2.0	42	co2	75-500	0.60E-03	0.55E+00	0.11E+01	
g4-1608	np	2.7	42	co2	75-500	0.60E-03	0.53E+00	0.14E+01	
g4-1608	np	3.4	42	co2	75-500	0.30E-04	0.26E-01	0.87E-01	
g4-1608	np	3.1	42	co2	75-500	0.30E-04	0.26E-01	0.80E-01	
g4-1608	np	1.3	42	co2	75-500	0.30E-03	0.28E+00	0.37E+00	
g4-1608	np	0.6	42	co2	75-500	0.30E-03	0.29E+00	0.17E+00	
g4-1608	np	3.0	42	co2	75-500	0.40E-08	0.35E-05	0.10E-04	
g4-1608	np	7.8	42	co2	75-500	0.40E-08	0.29E-05	0.22E-04	
g4-1608	np	4.8	42	co2	75-500	0.70E-07	0.57E-04	0.27E-03	
g4-1608	np	-1.5	42	co2	75-500	0.70E-07	0.76E-04	-0.11E-03	
g4-1608	np	4.7	42	co2	75-500	0.80E-05	0.65E-02	0.30E-01	
g4-1608	np	5.1	42	co2	75-500	0.80E-05	0.64E-02	0.32E-01	
g4-1608	np	4.5	42	co2	75-500	0.30E-05	0.25E-02	0.11E-01	
g4-1608	np	5.4	42	co2	75-500	0.30E-05	0.24E-02	0.13E-01	
gu3-433	np	19.0	42	co2	75-500	0.10E-08	0.51E-06	0.97E-05	Tpt - Devitrified
gu3-433	np	7.3	42	co2	75-500	0.10E-08	0.73E-06	0.53E-05	
gu3-433	np	6.4	42	co2	75-500	0.40E-08	0.30E-05	0.19E-04	
gu3-433	np	3.0	42	co2	75-500	0.40E-08	0.35E-05	0.10E-04	
gu3-433	np	0.6	42	co2	75-500	0.20E-04	0.19E-01	0.12E-01	

TABLE A.I (cont.)

ADSORPTION DATA SETS USED FOR MODELING AND COMPARISON

CORE	EL	R_d	TI	ATM	SIZE	C_o	C	S	UNIT - MINER
gu3-433	np	0.2	42	co2	75-500	0.20E-04	0.20E-01	0.40E-02	
gu3-433	np	5.5	42	co2	75-500	0.20E-06	0.16E-03	0.86E-03	
gu3-433	np	4.3	42	co2	75-500	0.20E-06	0.17E-03	0.71E-03	
gu3-433	np	6.3	42	co2	75-500	0.40E-07	0.30E-04	0.19E-03	
gu3-433	np	6.1	42	co2	75-500	0.40E-07	0.31E-04	0.19E-03	
gu3-433	np	2.6	42	co2	75-500	0.50E-04	0.44E-01	0.12E+00	
gu3-433	np	1.6	42	co2	75-500	0.50E-04	0.46E-01	0.74E-01	
gu3-433	np	5.3	42	co2	75-500	0.50E-06	0.40E-03	0.21E-02	
gu3-433	np	5.1	42	co2	75-500	0.50E-06	0.40E-03	0.20E-02	
gu3-433	np	4.6	42	co2	75-500	0.20E-05	0.16E-02	0.75E-02	
gu3-433	np	5.0	42	co2	75-500	0.20E-05	0.16E-02	0.80E-02	
gu3-433	np	0.8	42	co2	75-500	0.80E-11	0.77E-08	0.62E-08	
gu3-433	np	0.7	42	co2	75-500	0.80E-11	0.77E-08	0.54E-08	
gu3-433	np	0.4	42	co2	75-500	0.20E-08	0.20E-05	0.78E-06	
gu3-433	np	4.5	42	co2	75-500	0.20E-08	0.16E-05	0.74E-05	
gu3-433	np	3.4	42	co2	75-500	0.40E-05	0.34E-02	0.12E-01	
gu3-433	np	4.9	42	co2	75-500	0.40E-05	0.32E-02	0.16E-01	
gu3-433	np	9.6	42	co2	75-500	0.20E-07	0.14E-04	0.13E-03	
gu3-433	np	2.6	42	co2	75-500	0.20E-07	0.18E-04	0.46E-04	
g4-1608	pa	3.4	42	co2	75-500	0.10E-10	0.43E-07	0.15E-06	Tht - Zeolitized
g4-1608	pa	5.3	42	co2	75-500	0.10E-10	0.40E-07	0.21E-06	
g4-1608	pa	5.0	42	co2	75-500	0.50E-11	0.20E-07	0.10E-06	
g4-1608	pa	5.0	42	co2	75-500	0.50E-11	0.20E-07	0.10E-06	
g4-1608	pa	3.3	42	co2	75-500	0.50E-13	0.22E-09	0.71E-09	
g4-1608	pa	4.1	42	co2	75-500	0.50E-13	0.21E-09	0.85E-09	
g4-1608	pa	8.4	42	co2	75-500	0.10E-12	0.35E-09	0.30E-08	
g4-1608	pa	8.0	42	co2	75-500	0.10E-12	0.36E-09	0.29E-08	
g4-1608	pa	3.8	42	co2	75-500	0.10E-11	0.42E-08	0.16E-07	
g4-1608	pa	4.1	42	co2	75-500	0.10E-11	0.41E-08	0.17E-07	
g4-1608	pa	5.3	42	co2	75-500	0.50E-12	0.20E-08	0.10E-07	
g4-1608	pa	10.1	42	co2	75-500	0.50E-12	0.17E-08	0.17E-07	
g1-2840	sr	59.0	21	air	75-500	0.81E-06	0.41E-03	0.24E-01	Tct - Devitrified
g1-2840	sr	57.0	21	air	75-500	0.81E-06	0.42E-03	0.24E-01	
g1-2840	sr	46.6	21	air	75-500	0.83E-04	0.50E-01	0.23E+01	
g1-2840	sr	47.3	21	air	75-500	0.83E-04	0.49E-01	0.23E+01	
g1-2840	sr	47.0	21	air	75-500	0.77E-04	0.46E-01	0.22E+01	
g1-2840	sr	51.0	21	air	75-500	0.77E-04	0.43E-01	0.22E+01	
g1-2840	sr	55.3	21	air	75-500	0.24E-04	0.13E-01	0.70E+00	
g1-2840	sr	56.4	21	air	75-500	0.24E-04	0.13E-01	0.71E+00	
g1-2840	sr	30.5	21	air	75-500	0.33E-03	0.26E+00	0.80E+01	
g1-2840	sr	30.7	21	air	75-500	0.33E-03	0.26E+00	0.80E+01	
g1-2840	sr	39.5	21	air	75-500	0.21E-03	0.14E+00	0.56E+01	

TABLE A.I (cont.)
ADSORPTION DATA SETS USED FOR MODELING AND COMPARISON

CORE	EL	R_d	TI	ATM	SIZE	C_o	C	S	UNIT - MINER
g1-2840	sr	38.1	21	air	75-500	0.21E-03	0.14E+00	0.55E+01	
g1-2840	sr	160.0	21	air	75-500	0.10E-05	0.22E-03	0.36E-01	
g1-2840	sr	59.6	21	air	75-500	0.14E-05	0.70E-03	0.42E-01	
g1-2840	sr	63.6	21	air	75-500	0.14E-05	0.67E-03	0.43E-01	
g1-2840	sr	21.9	21	air	75-500	0.60E-03	0.57E+00	0.13E+02	
g1-2840	sr	19.9	21	air	75-500	0.60E-03	0.60E+00	0.12E+02	
g1-2840	sr	9.2	21	air	75-500	0.14E-02	0.19E+01	0.18E+02	
g1-2840	sr	9.7	21	air	75-500	0.14E-02	0.19E+01	0.18E+02	
g1-2840	sr	14.8	21	air	75-500	0.85E-03	0.98E+00	0.15E+02	
g1-2840	sr	15.9	21	air	75-500	0.85E-03	0.95E+00	0.15E+02	
g1-2840	sr	61.7	21	air	75-500	0.28E-05	0.14E-02	0.85E-01	
g1-2840	sr	61.2	21	air	75-500	0.28E-05	0.14E-02	0.84E-01	
g1-2840	sr	56.7	21	air	75-500	0.12E-04	0.63E-02	0.35E+00	
g1-2840	sr	57.1	21	air	75-500	0.12E-04	0.62E-02	0.35E+00	
g1-2840	sr	159.0	42	air	75-500	0.10E-05	0.22E-03	0.36E-01	
ym-22	sr	70.0	21	air	- 75	0.60E-06	0.27E-03	0.19E-01	Tpt - Devitrified
ym-22	sr	54.0	21	air	- 75	0.30E-04	0.16E-01	0.88E+00	
ym-22	sr	81.0	21	air	- 75	0.50E-06	0.20E-03	0.16E-01	
ym-22	sr	20.0	21	air	- 75	0.30E-02	0.30E+01	0.60E+02	
ym-22	sr	65.0	21	air	- 75	0.60E-06	0.28E-03	0.18E-01	
ym-22	sr	95.0	21	air	75-500	0.60E-06	0.21E-03	0.20E-01	Tpt - Devitrified
ym-22	sr	65.0	21	air	75-500	0.60E-06	0.28E-03	0.18E-01	
ym-22	sr	55.0	21	air	75-500	0.30E-04	0.16E-01	0.88E+00	
ym-22	sr	9.4	21	air	75-500	0.30E-02	0.41E+01	0.38E+02	
ym-22	sr	71.0	21	air	75-500	0.50E-06	0.22E-03	0.16E-01	
ym-22	tc	0.2	42	air	106-500	0.10E-05	0.99E-03	0.20E-03	Tpt - Devitrified
ym-22	tc	0.2	42	air	106-500	0.10E-08	0.99E-06	0.20E-06	
ym-22	tc	0.7	42	air	106-500	0.10E-11	0.97E-09	0.68E-09	
ym-22	tc	0.1	42	air	106-500	0.10E-02	0.10E+01	0.10E+00	
ym-48	tc	0.2	42	air	106-500	0.10E-02	0.99E+00	0.20E+00	Tcp - Zeolitized
ym-48	tc	0.1	42	air	106-500	0.10E-05	0.10E-02	0.10E-03	
ym-48	tc	0.1	42	air	106-500	0.10E-08	0.10E-05	0.99E-07	
ym-48	tc	0.2	42	air	106-500	0.10E-11	0.99E-09	0.20E-09	
ym-49	tc	0.2	42	air	106-500	0.10E-02	0.99E+00	0.20E+00	Tcp - Glass
ym-49	tc	0.3	42	air	106-500	0.10E-08	0.99E-06	0.30E-06	
ym-49	tc	0.2	42	air	106-500	0.10E-05	0.99E-03	0.20E-03	
ym-49	tc	0.2	42	air	106-500	0.10E-11	0.99E-09	0.20E-09	
ja-37	u	5.0	7	air	355-500	0.20E-05	0.64E-02	0.32E-01	Tct - Clays

TABLE A.I (cont.)

ADSORPTION DATA SETS USED FOR MODELING AND COMPARISON

CORE	EL	R_d	TI	ATM	SIZE	C_o	C	S	UNIT - MINER
ja-37	u	0.5	7	air	355-500	0.20E-05	0.78E-02	0.39E-02	
ja-37	u	6.0	7	air	355-500	0.20E-05	0.61E-02	0.37E-01	
ja-37	u	2.6	7	air	355-500	0.10E-06	0.35E-03	0.92E-03	

TABLE A.I (cont.)

DESORPTION DATA SETS USED FOR MODELING AND COMPARISON

CORE	EL	R_d	TI	ATM	SIZE	C_o	C	S	UNIT - MINER
ym-22	tc	1.9	63	air	106-500	0.10E-08	0.91E-06	0.17E-05	Tpt - Devitrified
ym-22	tc	1.2	63	air	106-500	0.10E-11	0.94E-09	0.11E-08	
ym-22	tc	0.5	63	air	106-500	0.10E-02	0.98E+00	0.49E+00	
ym-22	tc	1.2	63	air	106-500	0.10E-05	0.94E-03	0.11E-02	
ym-48	tc	1.2	63	air	106-500	0.10E-05	0.94E-03	0.11E-02	Tcp - Zeolitized
ym-48	tc	2.3	63	air	106-500	0.10E-08	0.90E-06	0.21E-05	
ym-48	tc	1.6	63	air	106-500	0.10E-11	0.93E-09	0.15E-08	
ym-48	tc	1.5	63	air	106-500	0.10E-02	0.93E+00	0.14E+01	
ym-49	tc	2.7	63	air	106-500	0.10E-08	0.88E-06	0.24E-05	Tcp - Glass
ym-49	tc	1.5	63	air	106-500	0.10E-05	0.93E-03	0.14E-02	
ym-49	tc	2.3	63	air	106-500	0.10E-11	0.90E-09	0.21E-08	
ym-49	tc	1.3	63	air	106-500	0.10E-02	0.94E+00	0.12E+01	
gl-1982	u	4.1	42	air	75-500	0.27E-05	0.90E-02	0.37E-01	Tcp - Devitrified
gl-1982	u	4.1	42	air	75-500	0.27E-05	0.90E-02	0.37E-01	
gl-1982	u	0.0	42	air	75-500	0.27E-05	0.11E-01	0.00E+00	
gl-1982	u	4.1	42	air	75-500	0.27E-05	0.90E-02	0.37E-01	
gl-1982	u	0.0	42	air	75-500	0.27E-05	0.11E-01	0.00E+00	
ja-37	u	13.0	7	air	355-500	0.20E-05	0.49E-02	0.63E-01	Tct - Clays
ja-37	u	13.0	7	air	355-500	0.20E-05	0.49E-02	0.63E-01	
ja-37	u	13.0	7	air	355-500	0.20E-05	0.49E-02	0.63E-01	
ja-37	u	12.0	7	air	355-500	0.10E-06	0.25E-03	0.30E-02	

Appendix B

Statistical, Isotherm, Equivalent Isotherm, and Thermodynamic Parameters Estimated from the Regression of Sorption Data for Isotherm Models

Appendix B is a compilation of tabulated parameters and plots of sorption data modeled according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherms. Statistical parameters include the index of determination (R^2), coefficient of variation (CV), error sum of squares (SSE), standard error of the intercept (SE Int), and standard error of the slope (SE Slope). All statistical parameters with the exception of SSE were calculated using the SAS statistical code; the SSE was calculated for the amount of the radionuclide sorbed (S) from the sum of squared deviations of the difference between the observed and predicted S values and then taking the square root of that sum. The SSE was calculated for the regression of each model so that a valid comparison for the amount adsorbed could be made among the four isotherm models. The SE is not an appropriate parameter for this comparison because the sum of the squared errors may be for S in one model (e.g., Linear) and for log S in another (e.g., Freundlich).

The calculated isotherm parameters include K_d for the Linear model, k and b for the Langmuir model, K and N for the Freundlich model, and K_D and β for the Modified Freundlich model. A SE was also calculated and tabulated for each of the isotherm parameters. In those cases where a parameter was equal to either the slope or the intercept, the value of the respective SE Slope or SE Int was equal to the SE of the parameter. In those cases where the parameter was not equal to either the slope or the intercept, the error was

propagated. The parameters for each of the four isotherm models were converted to equivalent parameters of the Linear (K_d) and Modified Freundlich (K_D and B) isotherm models. The relation between isotherm parameters and equivalent isotherm parameters are given by Fuentes et al. (1989).

Thermodynamic parameters are also tabulated in Appendix B. The Gibb's free energy of adsorption is denoted as G and the thermodynamic equilibrium constant is noted as Keq. The z_B symbol denotes the valence of the ion being replaced from the adsorption sites; hypothetical ions with composite valences of 1.0, 1.2, 1.5 and 2.0 were assumed for the calculation of thermodynamic parameters. The rationale for this assumption is presented in the text. See Fuentes et al. (1989) for a more detailed discussion.

The notation n.a. in the tables indicates not applicable.

TABLE B.I

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Ba 21 air - 75 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9976	0.9349	0.9979	0.9983
C.V.	11.01	16.57	-5.525	-2.029
SSE	3.47E-02	2.31E+01	8.20E-02	4.62E-02
SE Slope	9.795	0.02521	0.02263	0.02073
SE Int.	n.a.	0.0001073	0.09518	0.08720
Isotherm Parameters				
Kd	401.1 +/- 9.8	n.a.	n.a.	n.a.
k	n.a.	175.3 +/-2242000.0	n.a.	n.a.
b	n.a.	6.046 +/- 0.921	n.a.	n.a.
K	n.a.	n.a.	211.5 +/- 0.1	n.a.
N	n.a.	n.a.	0.8478 +/- 0.0226	n.a.
KD	n.a.	n.a.	n.a.	7.201 +/- 0.193
B	n.a.	n.a.	n.a.	0.8592 +/- 0.0207
Equivalent Isotherm Parameters				
Kd	401.1	1060.0	280.4	316.8
KD	9.115	175.3	6.373	7.201
B	1.0	1.0	0.8478	0.8592
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-2.89	-3.13	-3.52	-4.18
Keq	1.31E+02	1.97E+02	3.79E+02	1.17E+03

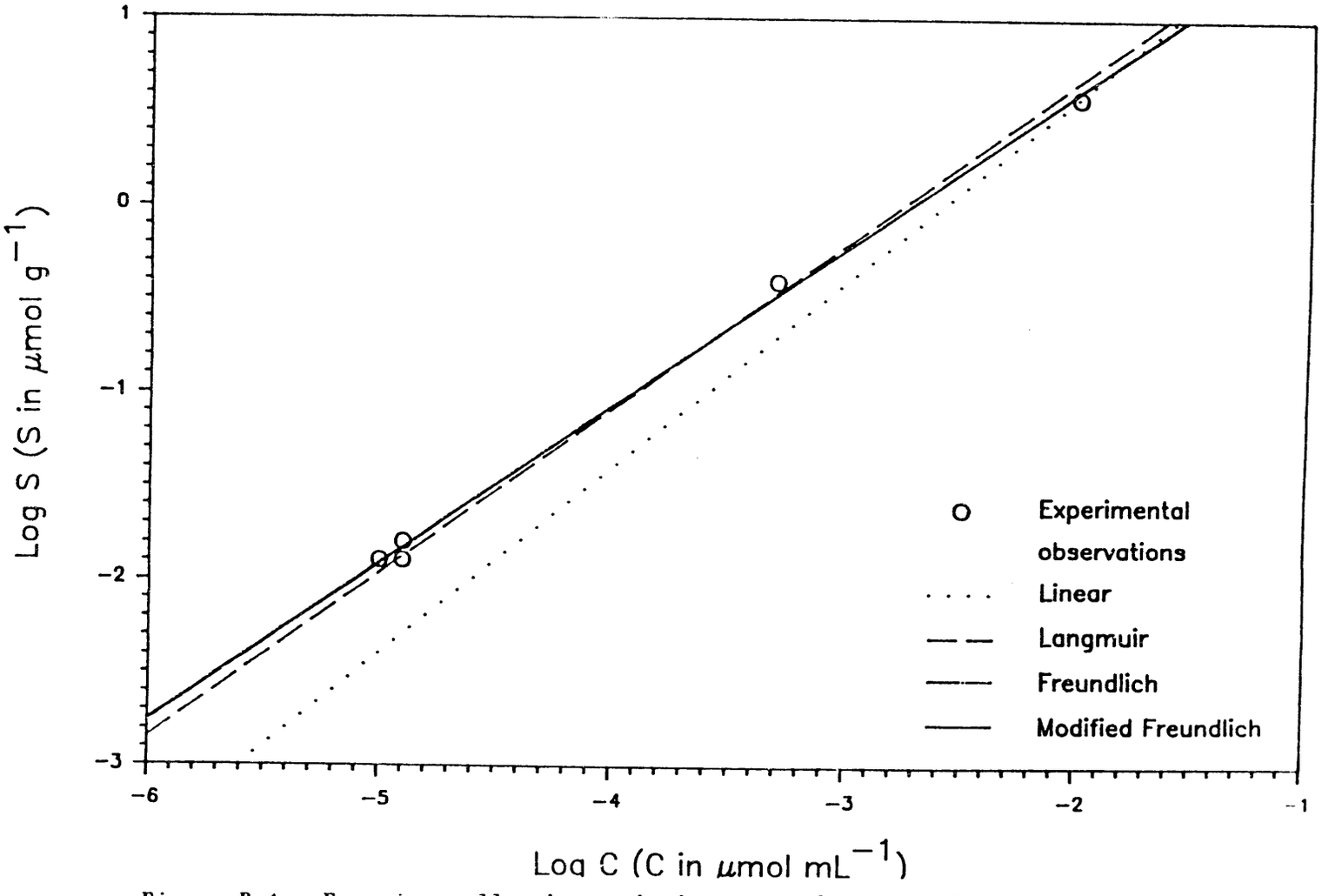

Figure B.1. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM 22 Ba 21 air -75 amb 44.0.

TABLE B.II

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Ba 21 air 75-500 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9971	0.9576	0.9974	0.9978
C.V.	12.25	14.92	-6.006	-2.144
SSE	4.08E-02	1.76E+01	1.37E-01	1.03E-01
SE Slope	5.933	0.02186	0.02452	0.02276
SE Int.	n.a.	0.0001664	0.09796	0.0903
Isotherm Parameters				
Kd	218.2 +/- 5.9	n.a.	n.a.	n.a.
k	n.a.	115.5 +/- 22.6	n.a.	n.a.
b	n.a.	5.558 +/- 0.675	n.a.	n.a.
K	n.a.	n.a.	123.1 +/- 0.1	n.a.
N	n.a.	n.a.	0.8370 +/- 0.0245	n.a.
KD	n.a.	n.a.	n.a.	2.701 +/- 0.149
B	n.a.	n.a.	n.a.	0.8453 +/- 0.0223
Equivalent Isotherm Parameters				
Kd	218.3	642.2	142.5	156.7
KD	3.762	115.5	2.457	2.701
B	1.0	1.0	0.8370	0.8453
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-2.43	-2.54	-2.74	-3.10
Keq	6.03E+01	7.34E+01	1.03E+02	1.88E+02

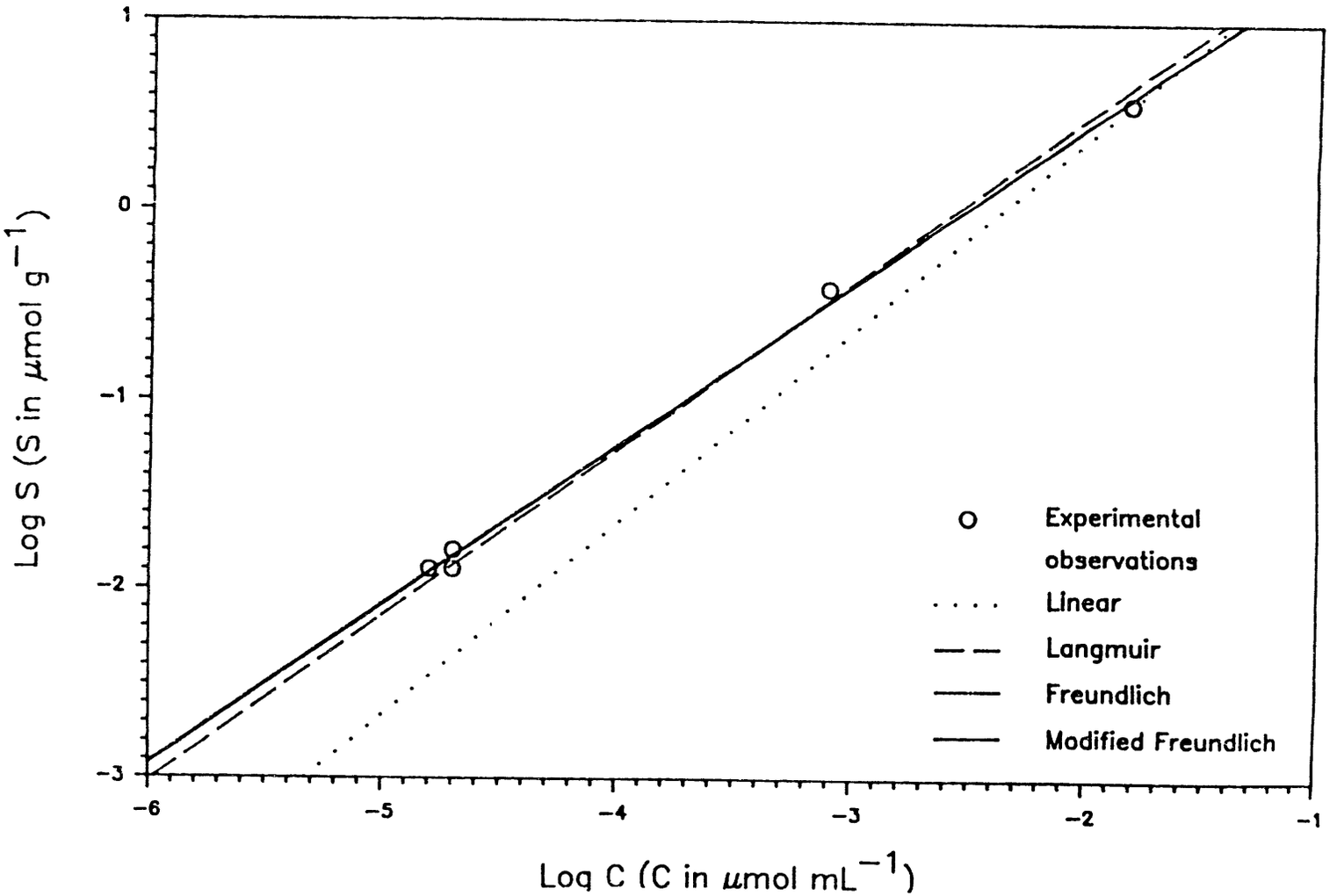

Figure B.2. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Ba 21 air 75-500 amb 58.0.

TABLE B.III

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g1-2840 Cs 21 air 75-500 amb 430.0

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9900	0.7146	0.9975	0.9974
C.V.	23.22	64.37	-6.809	-2.497
SSE	2.21E+00	5.31E+02	1.74E+00	2.43E+00
SE Slope	0.6120	0.07412	0.01146	0.01154
SE Int.	n.a.	0.003134	0.05234	0.05271
Isotherm Parameters				
Kd	20.20 +/- 0.61	n.a.	n.a.	n.a.
k	n.a.	8.323 +/- 3.920	n.a.	n.a.
b	n.a.	13.49 +/- 2.70	n.a.	n.a.
K	n.a.	n.a.	15.68 +/- 0.05	n.a.
N	n.a.	n.a.	0.7174 +/- 0.0115	n.a.
KD	n.a.	n.a.	n.a.	0.01014 +/- 0.01381
B	n.a.	n.a.	n.a.	0.7183 +/- 0.0115
Equivalent Isotherm Parameters				
'd	20.20	112.3	4.255	4.360
KD	0.04698	8.323	0.009895	0.01014
B	1.0	1.0	0.7174	0.7183
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	1.34	1.98	2.92	4.45
Keq	1.04E-01	3.53E-02	7.25E-03	5.48E-04

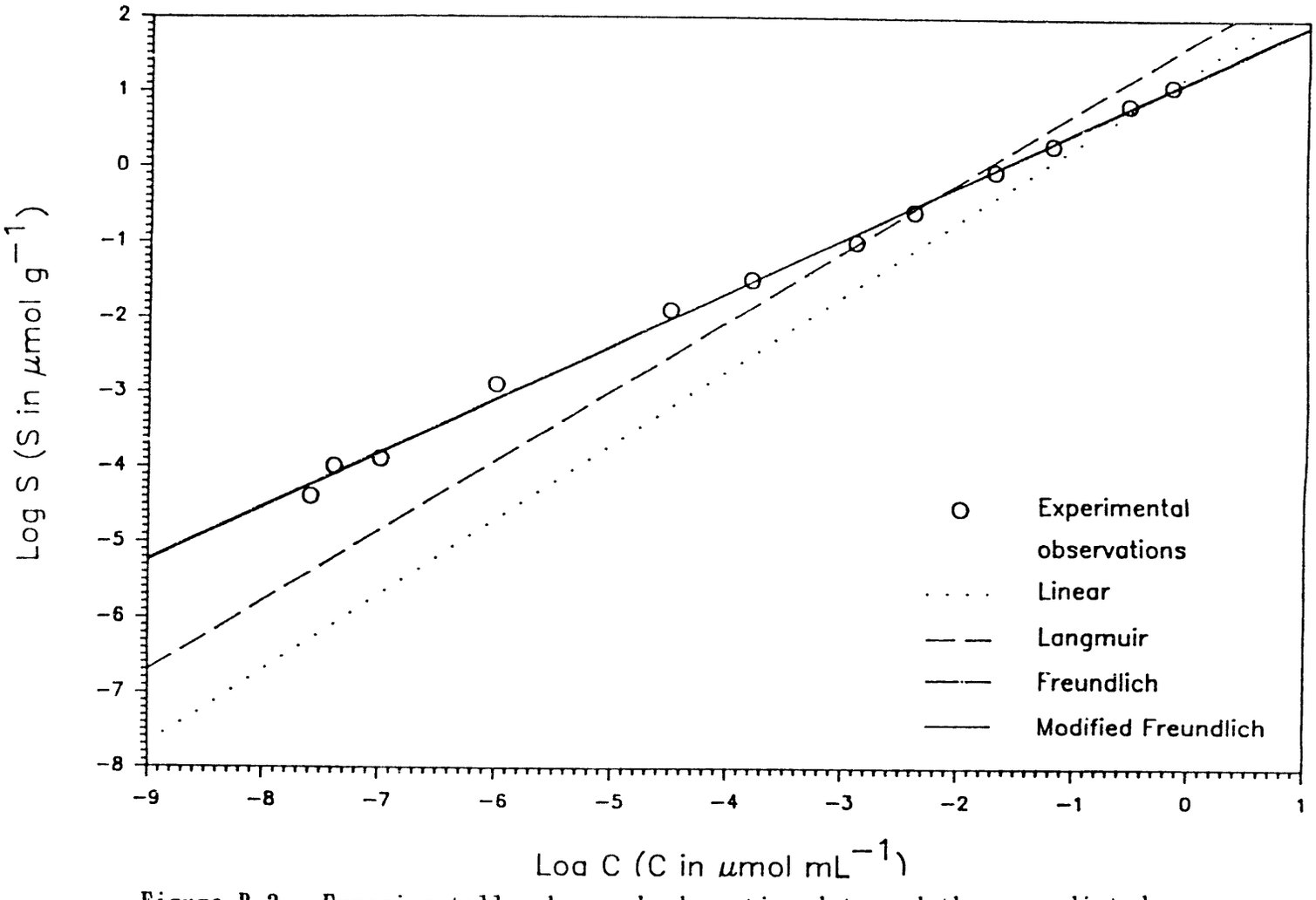

Figure B.3. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 1.

TABLE B.IV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

gl-2840 Cs 21 air 75-500 amb 430.0

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9912	0.6974	0.9969	0.9969
C.V.	20.88	60.67	-8.519	-2.804
SSE	1.99E+00	5.57E+02	1.27E+00	1.78E+00
SE Slope	0.6378	0.01578	0.01353	0.01360
SE Int.	n.a.	0.003294	0.05697	0.05728
Isotherm Parameters				
Kd	21.46 +/- 0.64	n.a.	n.a.	n.a.
k	n.a.	7.393 +/- 3.527	n.a.	n.a.
b	n.a.	13.92 +/- 3.06	n.a.	n.a.
K	n.a.	n.a.	16.75 +/- 0.06	n.a.
N	n.a.	n.a.	0.7287 +/- 0.0135	n.a.
KD	n.a.	n.a.	n.a.	0.01193 +/- 0.01603
B	n.a.	n.a.	n.a.	0.7298 +/- 0.0136
Equivalent Isotherm Parameters				
Kd	21.46	102.9	5.003	5.130
KD	0.04991	7.393	0.01164	0.01193
B	1.0	1.0	0.7287	0.7298
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	1.25	1.87	2.77	4.26
Keq	1.22E-01	4.29E-02	9.25E-03	7.59E-04

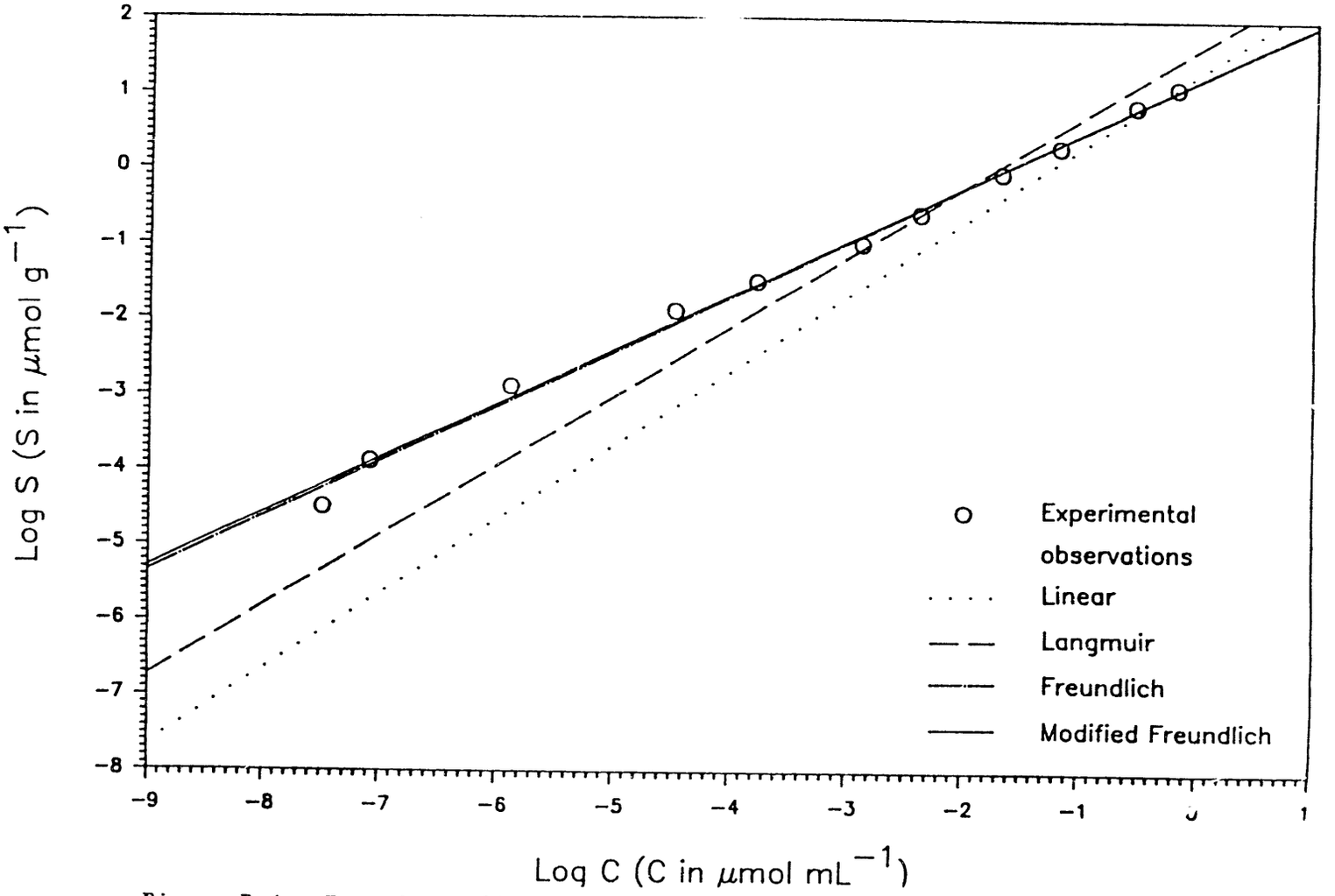

Figure B.4. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1-2840 Cs 21 75-500 amb 430.0 Replicate 2.

TABLE B.V

ST .TISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Cs 21 air - 75 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9995	0.9957	0.9880	0.9915
C.V.	5.192	14.08	-14.95	-7.493
SSE	1.02E-01	1.99E+02	1.65E+02	9.15E+01
SE Slope	0.1226	0.002431	0.05074	0.04373
SE Int.	n.a.	0.001413	0.2728	0.2351
Isotherm Parameters				
Kd	11.54 +/- 0.12	n.a.	n.a.	n.a.
k	n.a.	19.70 +/- 8.37	n.a.	n.a.
b	n.a.	15.60 +/- 0.59	n.a.	n.a.
K	n.a.	n.a.	22.59 +/- 0.27	n.a.
N	n.a.	n.a.	0.7975 +/- 0.0507	n.a.
KD	n.a.	n.a.	n.a.	0.6278 +/- 0.2425
B	n.a.	n.a.	n.a.	0.8169 +/- 0.0437
Equivalent Isotherm Parameters				
Kd	11.54	307.4	19.07	27.62
KD	0.2622	19.70	0.4335	0.6278
B	1.0	1.0	0.7975	0.8169
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-0.32	-0.22	-0.07	0.16
Keq	1.71E+00	1.44E+00	1.13E+00	7.65E-01

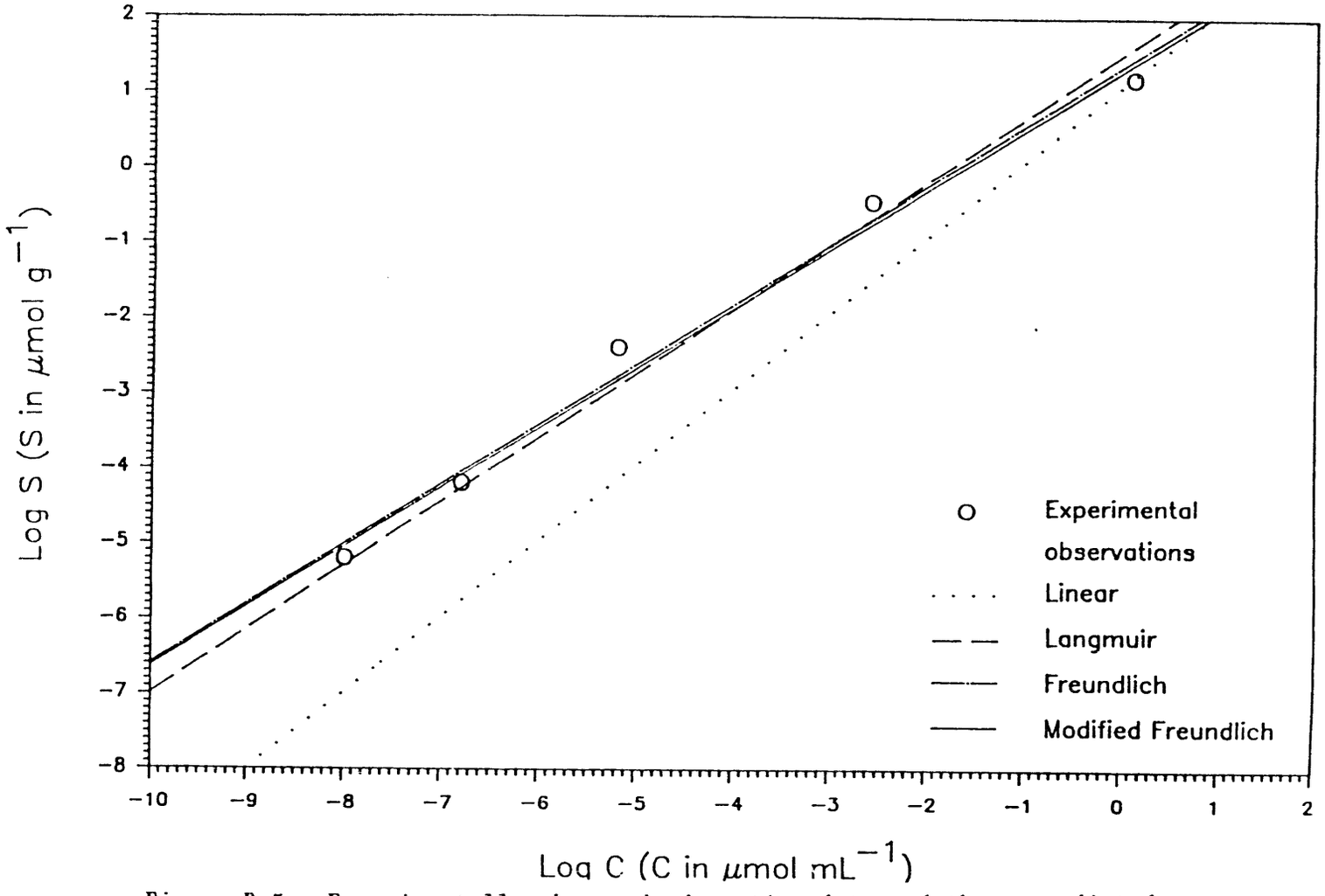

Figure B.5. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Cs 21 air -75 amb 44.0.

TABLE B.VI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Cs 21 air 75-500 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9994	0.9952	0.9936	0.9954
C.V.	5.790	14.76	-10.74	-5.231
SSE	9.55E-02	1.45E+02	7.85E+01	5.15E+01
SE Slope	0.1189	0.002951	0.03641	0.03144
SE Int.	n.a.	0.001716	0.1952	0.1685
Isotherm Parameters				
Kd	10.00 +/- 0.12	n.a.	n.a.	n.a.
k	n.a.	18.58 +/- 8.38	n.a.	n.a.
b	n.a.	13.54 +/- 0.54	n.a.	n.a.
K	n.a.	n.a.	17.79 +/- 0.20	n.a.
N	n.a.	n.a.	0.7851 +/- 0.0364	n.a.
KD	n.a.	n.a.	n.a.	0.2810 +/- 0.1325
B	n.a.	n.a.	n.a.	0.7966 +/- 0.0314
Equivalent Isotherm Parameters				
Kd	10.00	251.6	12.87	16.30
KD	0.1724	18.58	0.2220	0.2810
B	1.0	1.0	0.7851	0.7966
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	0.10	0.30	0.59	1.07
Keq	8.49E-01	6.02E-01	3.66E-01	1.64E-01

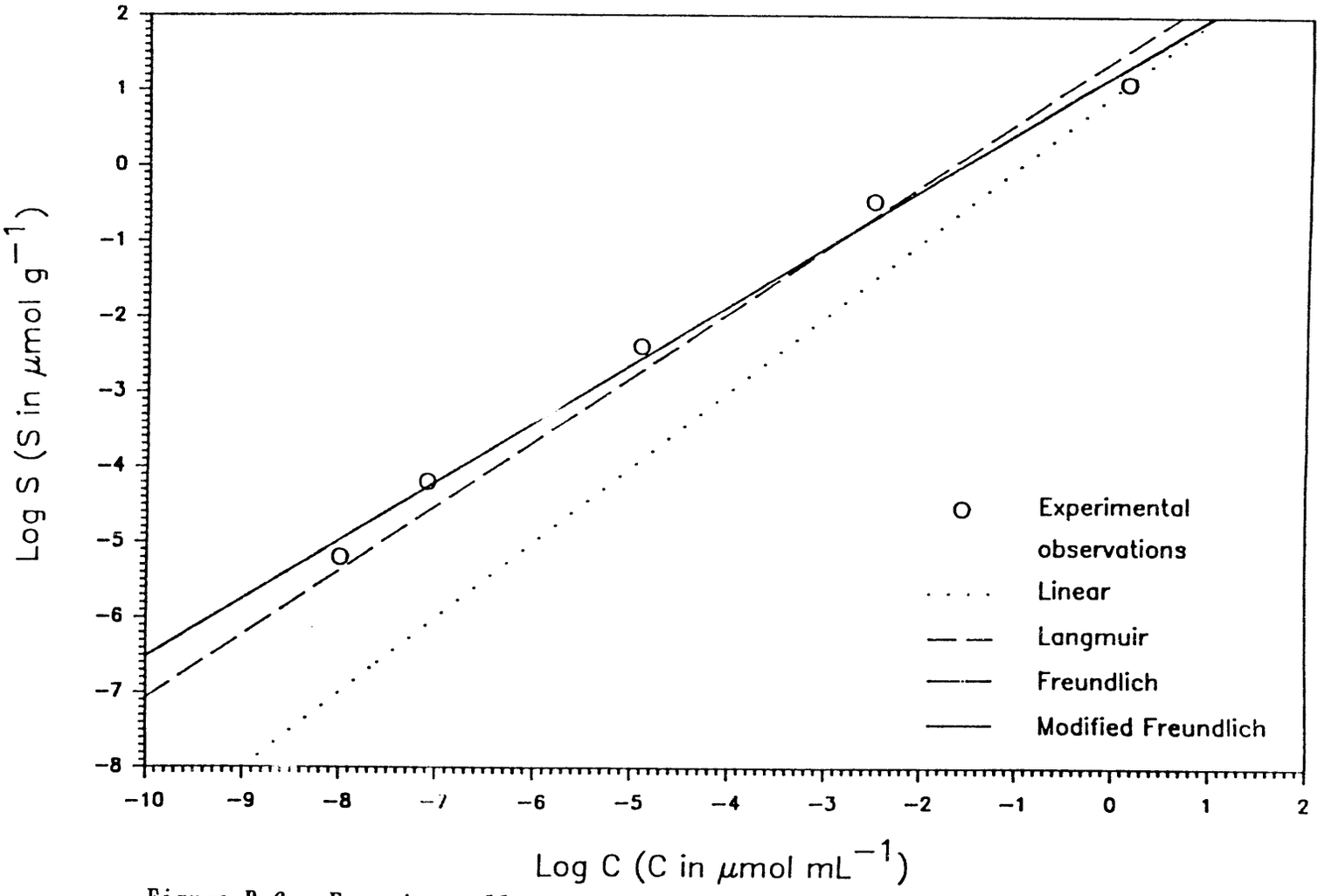

Figure B.6. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM 22 Cs 21 air 75-500 amb 58.0.

TABLE B.VII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Eu 21 air - 75 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.3770	0.6141	0.9297	0.9292
C.V.	144.7	63.79	-26.90	-13.83
SSE	2.00E-01	2.88E-01	2.13E-01	2.15E-01
SE Slope	967.2	2.089	0.1888	0.1897
SE Int.	n.a.	0.0002787	0.9750	0.9795
Isotherm Parameters				
Kd	1303.0 +/- 967.2	n.a.	n.a.	n.a.
k	n.a.	10770.0 +/- 13390.0	n.a.	n.a.
b	n.a.	0.2683 +/- 0.1504	n.a.	n.a.
K	n.a.	n.a.	1408.0 +/- 1.0	n.a.
N	n.a.	n.a.	0.9710 +/- 0.1888	n.a.
KD	n.a.	n.a.	n.a.	36.02 +/- 3.40
B	n.a.	n.a.	n.a.	0.9722 +/- 0.1897
Equivalent Isotherm Parameters				
Kd	1303.0	2890.0	1562.0	1585.0
KD	29.62	10770.0	35.50	36.02
B	1.0	1.0	0.9710	0.9722
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-4.80	-5.27	-5.99	-7.22
Keq	3.32E+03	7.24E+03	2.45E+04	1.97E+05

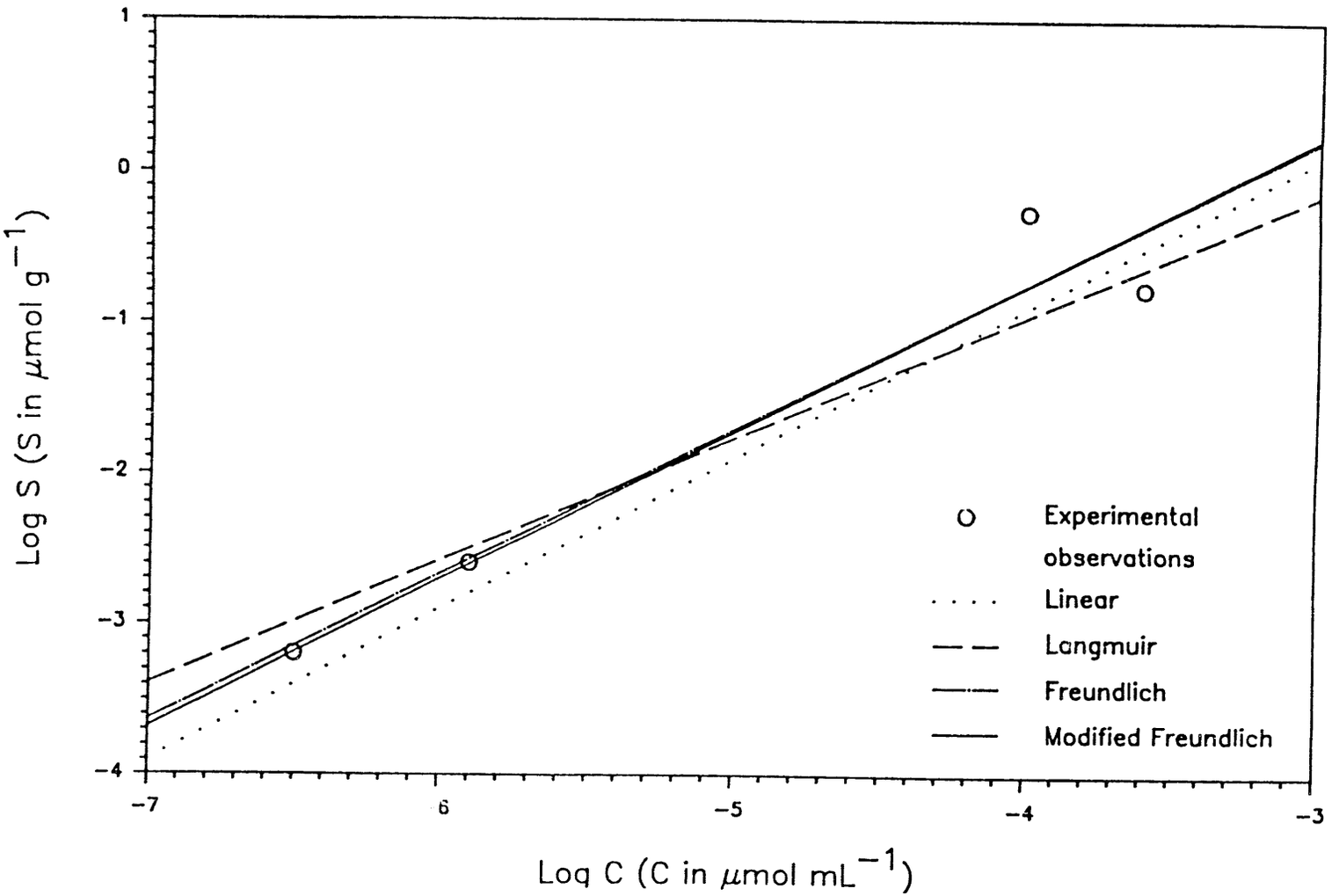

Figure B.7. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Eu 21 air -75 amb 44.0.

TABLE B.VIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 £u 21 air 75-500 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9994	0.7883	0.9997	0.9997
C.V.	4.825	16.85	-1.517	-0.8211
SSE	1.89E-04	1.14E-02	4.81E-05	3.72E-05
SE Slope	13.69	0.2621	0.009673	0.009584
SE Int.	n.a.	0.00005895	0.05351	0.05302
Isotherm Parameters				
Kd	1123.0 +/- 13.7	n.a.	n.a.	n.a.
k	n.a.	1633.0 +/- 607.5	n.a.	n.a.
b	n.a.	1.141 +/- 0.342	n.a.	n.a.
K	n.a.	n.a.	612.8 +/- 0.1	n.a.
N	n.a.	n.a.	0.9215 +/- 0.0097	n.a.
KD	n.a.	n.a.	n.a.	13.07 +/- 0.14
B	n.a.	n.a.	n.a.	0.9224 +/- 0.0096
Equivalent Isotherm Parameters				
Kd	1113.0	1863.0	749.1	758.3
KD	19.18	1633.0	12.92	13.07
B	1.0	1.0	0.9215	0.9224
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-4.39	-4.71	-5.23	-6.14
Kzq	1.65E+03	2.84E+03	6.84E+03	3.17E+04

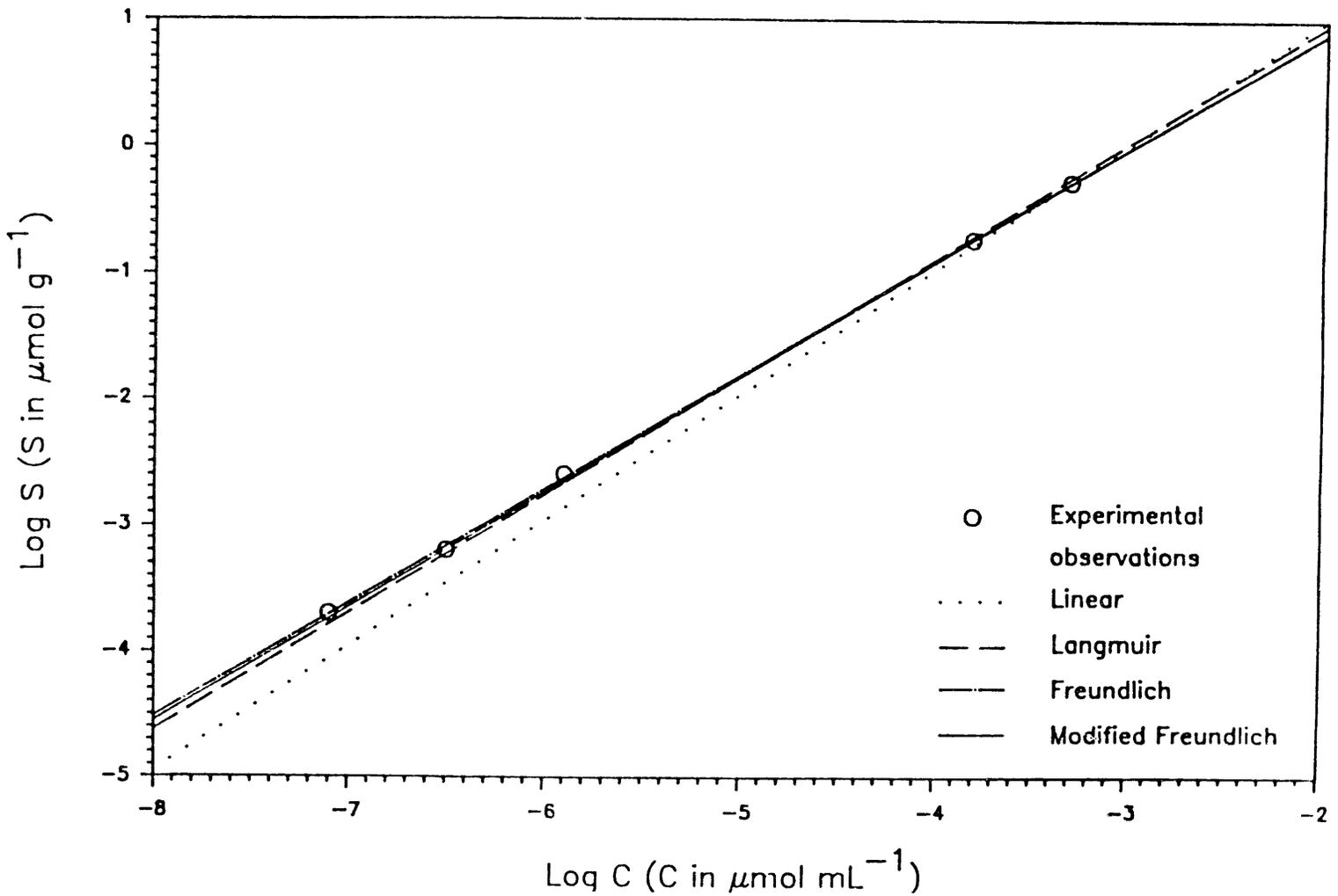

Figure B.8. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Eu 21 air 75-500 amb 58.0.

TABLE B.IX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g4-1608 Pa 42 CO2 75-500 amb n.a.

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9769	0.1021	0.9719	n.a.
C.V.	26.46	32.86	-2.109	n.a.
SSE	7.61E-16	3.29E-14	7.98E-16	n.a.
SE Slope	0.2588	1972000.0	0.08087	n.a.
SE Int.	n.a.	0.03837	0.6942	n.a.
Isotherm Parameters				
Kd	3.760 +/- 0.259	n.a.	n.a.	n.a.
k	n.a.	6220.0 +/- 9931000.0	n.a.	n.a.
b	n.a.	0.75E-6 +/- 1.12E-6	n.a.	n.a.
K	n.a.	n.a.	1.760 +/- 0.694	n.a.
N	n.a.	n.a.	0.9514 +/- 0.0809	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

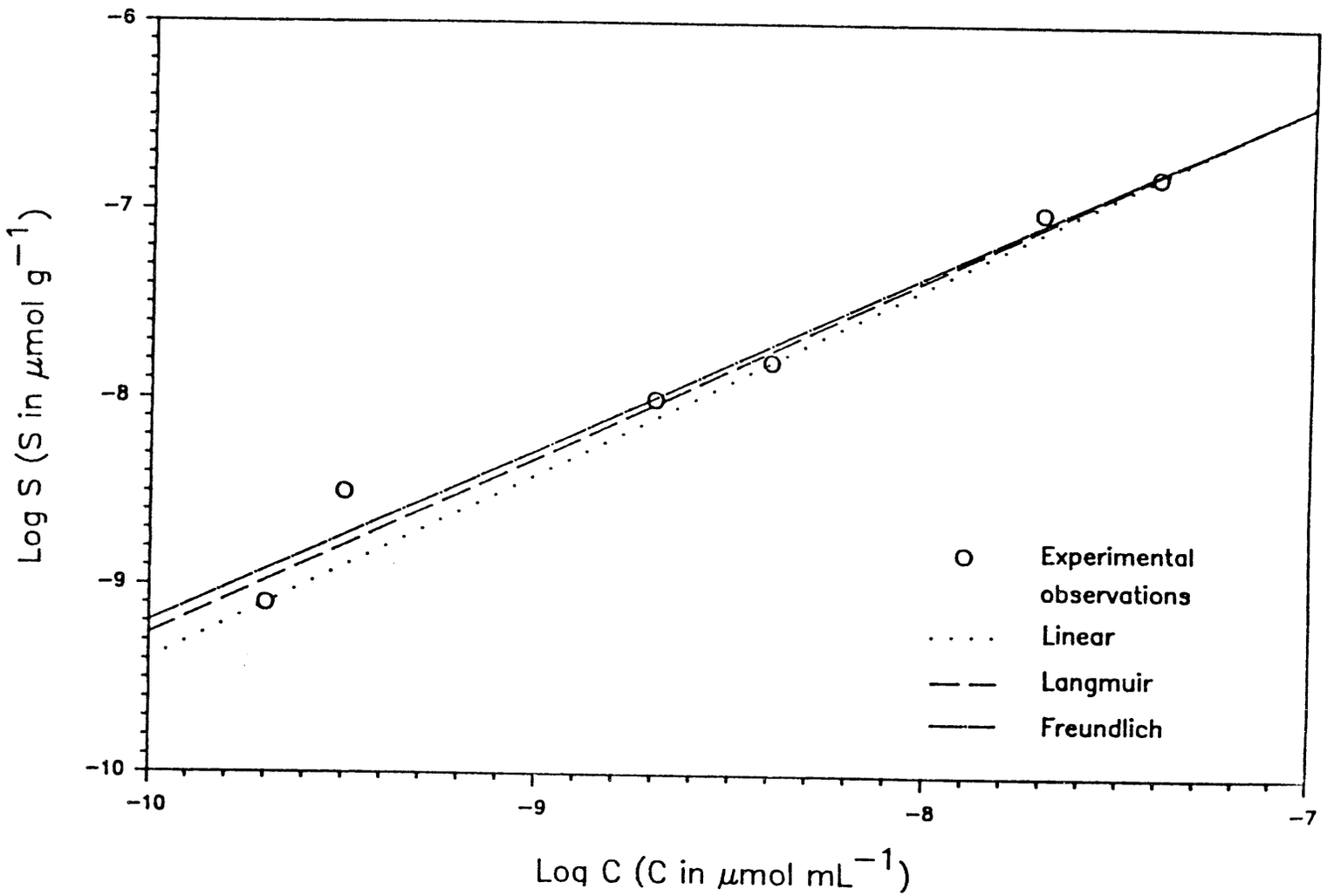

Figure B.9. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 1.

TABLE B.X

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g4-1608 Pa 42 CO2 75-500 amb n.a.

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9981	0.0195	0.9695	n.a.
C.V.	7.958	36.32	-2.253	n.a.
SSE	1.06E-16	5.47E-14	1.50E-16	n.a.
SE Slope	0.1026	1862000.0	0.08585	n.a.
SE Int.	n.a.	0.03416	0.7386	n.a.
Isotherm Parameters				
Kd	5.198 +/- 0.103	n.a.	n.a.	n.a.
k	n.a.	2.95E+6 +/- 10.81E+6	n.a.	n.a.
b	n.a.	1.9E-6 +/- 6.8E-6	n.a.	n.a.
K	n.a.	n.a.	3.082 +/- 0.739	n.a.
N	n.a.	n.a.	0.9685 +/- 0.0859	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

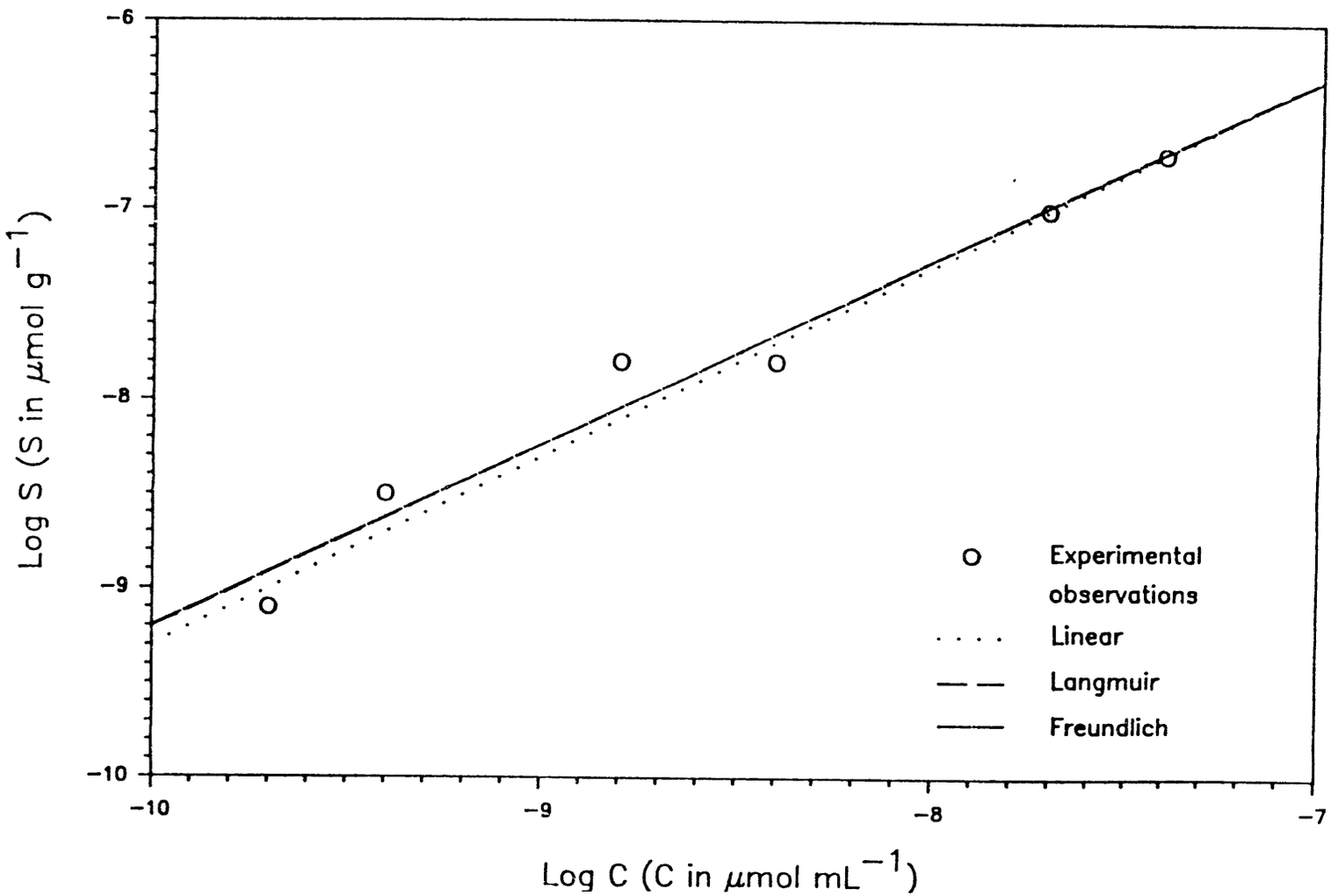

Figure B.10. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 2.

TABLE B.XI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g1-2840 Sr 21 air 75-500 amb 430.0

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.8585	0.9831	0.9827	0.9833
C.V.	62.02	11.65	-867.9	-5.497
SSE	1.17E+02	2.24E+03	2.04E+02	1.93E+02
SE Slope	1.396	0.001880	0.03181	0.03136
SE Int.	n.a.	0.001165	0.06605	0.06512
Isotherm Parameters				
Kd	11.91 +/- 1.40	n.a.	n.a.	n.a.
k	n.a.	2.820 +/- 0.268	n.a.	n.a.
b	n.a.	21.04 +/- 0.83	n.a.	n.a.
K	n.a.	n.a.	18.96 +/- 0.07	n.a.
N	n.a.	n.a.	0.7943 +/- 0.0318	n.a.
KD	n.a.	n.a.	n.a.	0.02079 +/- 0.02595
B	n.a.	n.a.	n.a.	0.7986 +/- 0.0314
Equivalent Isotherm Parameters				
Kd	11.91	59.32	8.450	8.939
KD	0.02770	2.820	0.01965	0.02079
B	1.0	1.0	0.7943	0.7986
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-0.99	-0.45	0.33	1.55
Keq	5.32E+00	2.13E+00	5.77E-01	7.33E-02

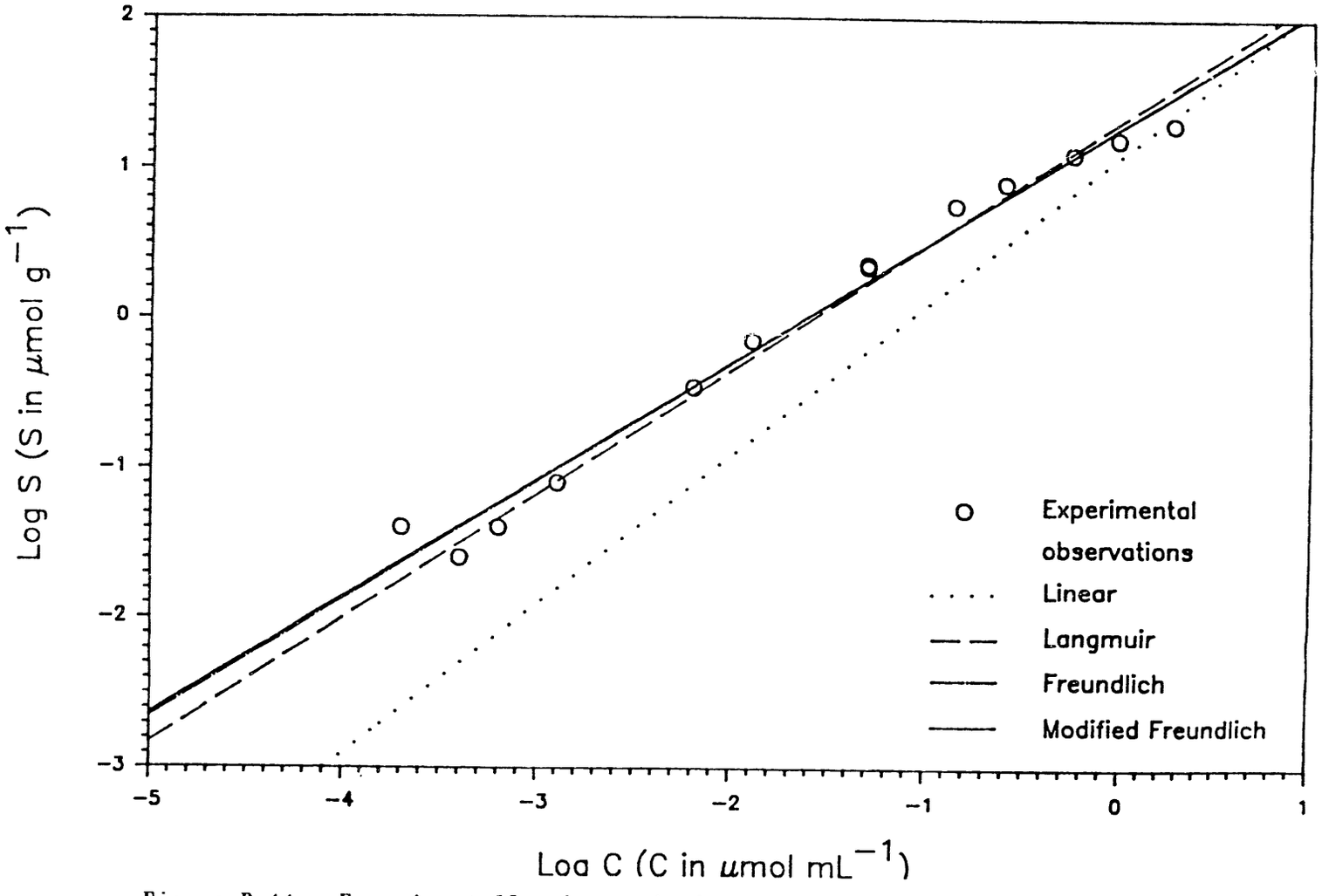

Figure B.11. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1 2840 Sr 21 air 75-500 amb 430.0 Replicate 1.

TABLE B.XII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g1-2840 Sr 21 air 75-500 amb 430.0

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.8704	0.9958	0.9827	0.9836
C.V.	57.31	5.458	142.0	-5.451
SSE	1.03E+02	2.27E+03	2.42E+02	2.30E+02
SE Slope	1.376	0.0009600	0.03411	0.03335
SE Int.	n.a.	0.0006174	0.06445	0.06301
Isotherm Parameters				
Kd	11.83 +/- 1.38	n.a.	n.a.	n.a.
k	n.a.	2.596 +/- 0.124	n.a.	n.a.
b	n.a.	21.29 +/- 0.43	n.a.	n.a.
K	n.a.	n.a.	19.52 +/- 0.06	n.a.
N	n.a.	n.a.	0.8132 +/- 0.0341	n.a.
KD	n.a.	n.a.	n.a.	0.02362 +/- 0.02656
B	n.a.	n.a.	n.a.	0.8179 +/- 0.0334
Equivalent Isotherm Parameters				
Kd	11.83	55.24	9.596	10.16
KD	0.02751	2.596	0.02232	0.02362
B	1.0	1.0	0.8132	0.8179
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-1.07	-0.54	0.21	1.40
Keq	6.05E+00	2.48E+00	6.99E-01	9.46E-02

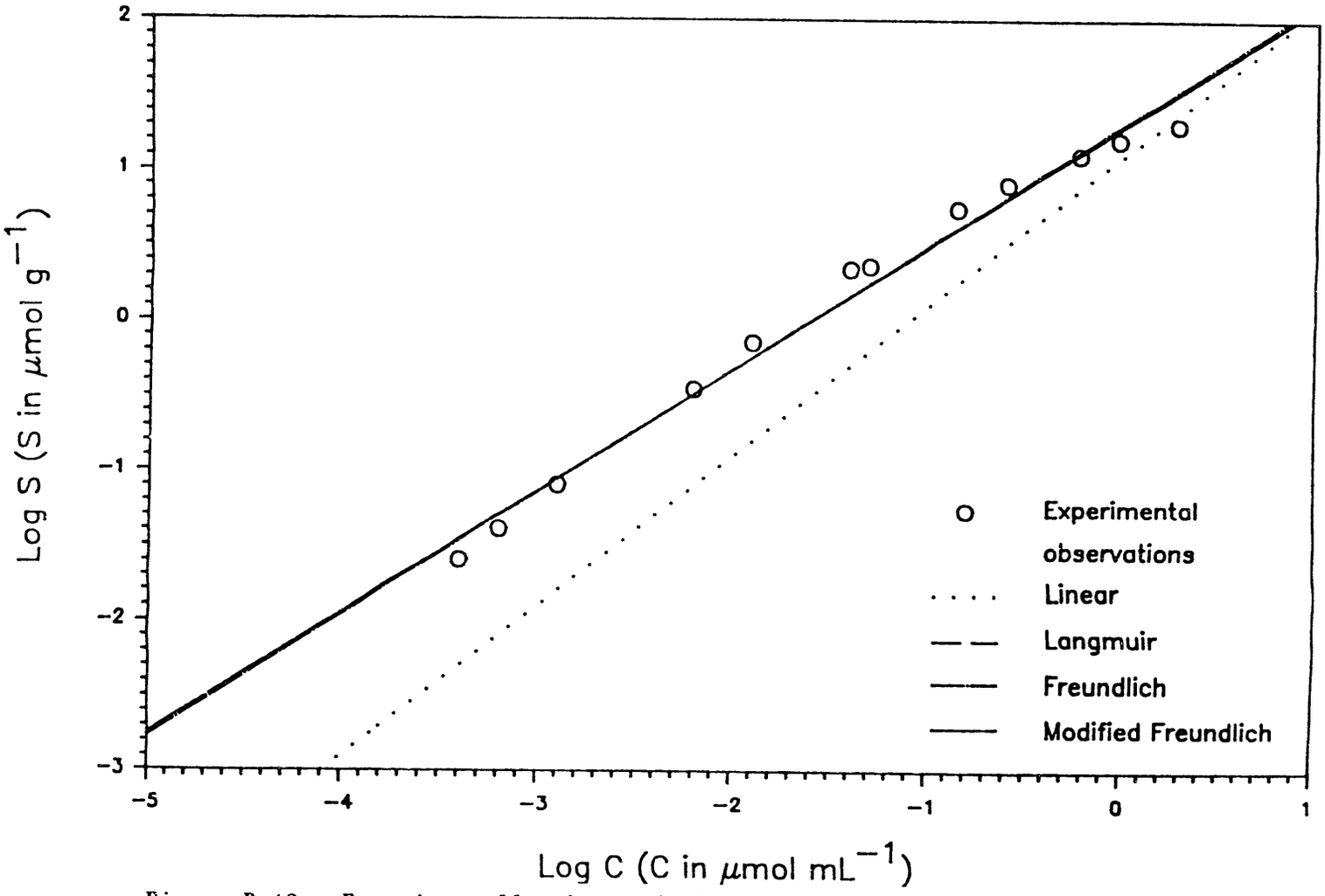

Figure B.12. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 2.

TABLE B.XIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Sr 21 air - 75 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9999	0.9837	0.9983	n.a.
C.V.	2.300	10.50	-10.43	n.a.
SSE	3.14E-01	1.53E+04	4.07E+01	n.a.
SE Slope	0.09340	0.0008659	0.02045	n.a.
SE Int.	n.a.	0.001162	0.05963	n.a.
Isotherm Parameters				
Kd	20.00 +/- 0.09	n.a.	n.a.	n.a.
k	n.a.	0.7737 +/- 0.0998	n.a.	n.a.
b	n.a.	85.82 +/- 6.38	n.a.	n.a.
K	n.a.	n.a.	25.50 +/- 0.06	n.a.
N	n.a.	n.a.	0.8709 +/- 0.0205	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

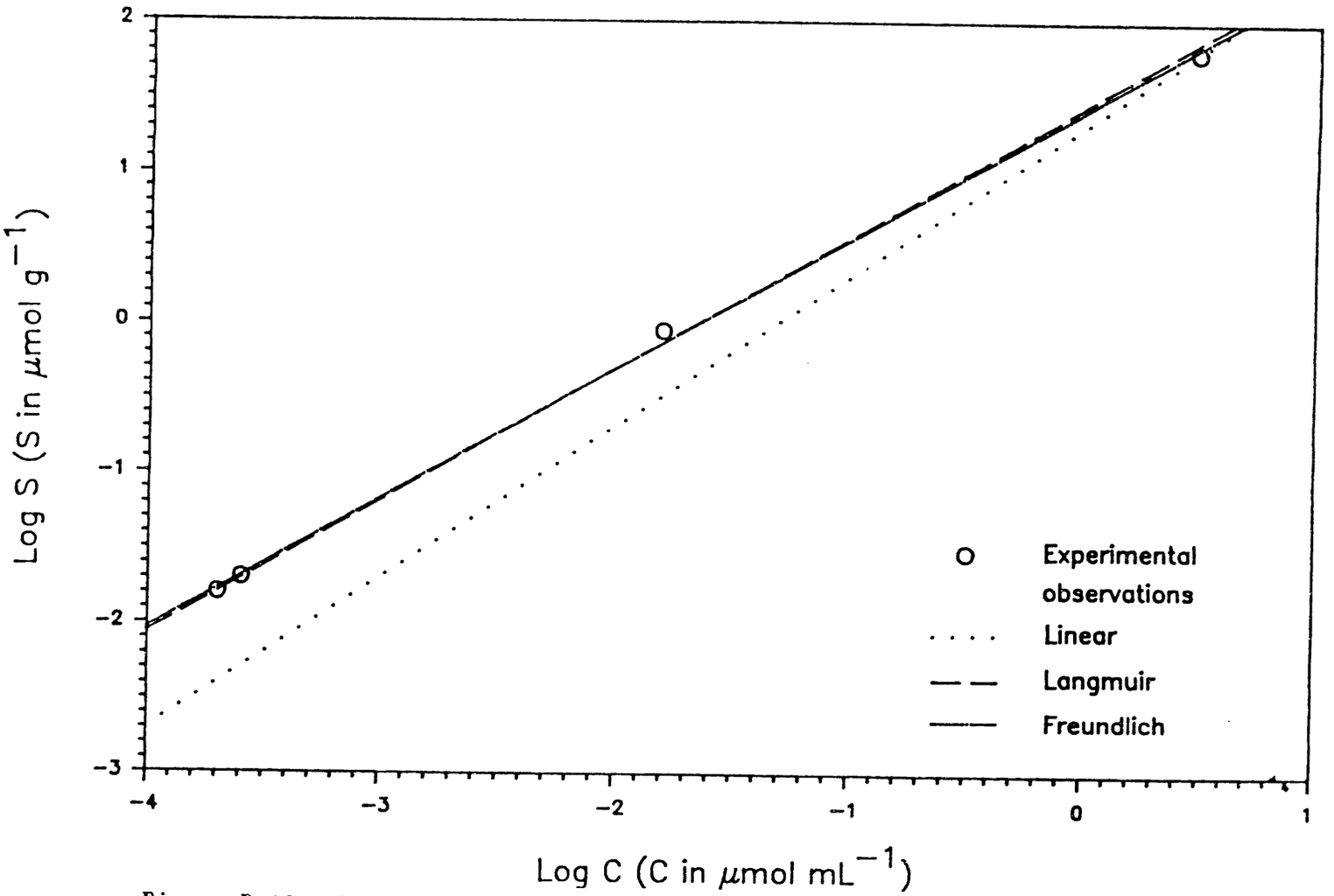

Figure B.13. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Sr 21 air -75 amb 44.0.

TABLE B.XIV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Sr 21 air 75-500 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9996	0.9959	0.9931	n.a.
C.V.	4.702	9.318	-19.22	n.a.
SSE	5.36E-01	2.81E+03	6.40E+01	n.a.
SE Slope	0.08929	0.0008439	0.03820	n.a.
SE Int.	n.a.	0.001547	0.1122	n.a.
Isotherm Parameters				
Kd	9.269 +/- 0.089	n.a.	n.a.	n.a.
k	n.a.	1.584 +/- 0.203	n.a.	n.a.
b	n.a.	43.85 +/- 1.62	n.a.	n.a.
K	n.a.	n.a.	14.9[illegible] - 0.11	n.a.
N	n.a.	n.a.	0.7947 +/- 0.0382	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

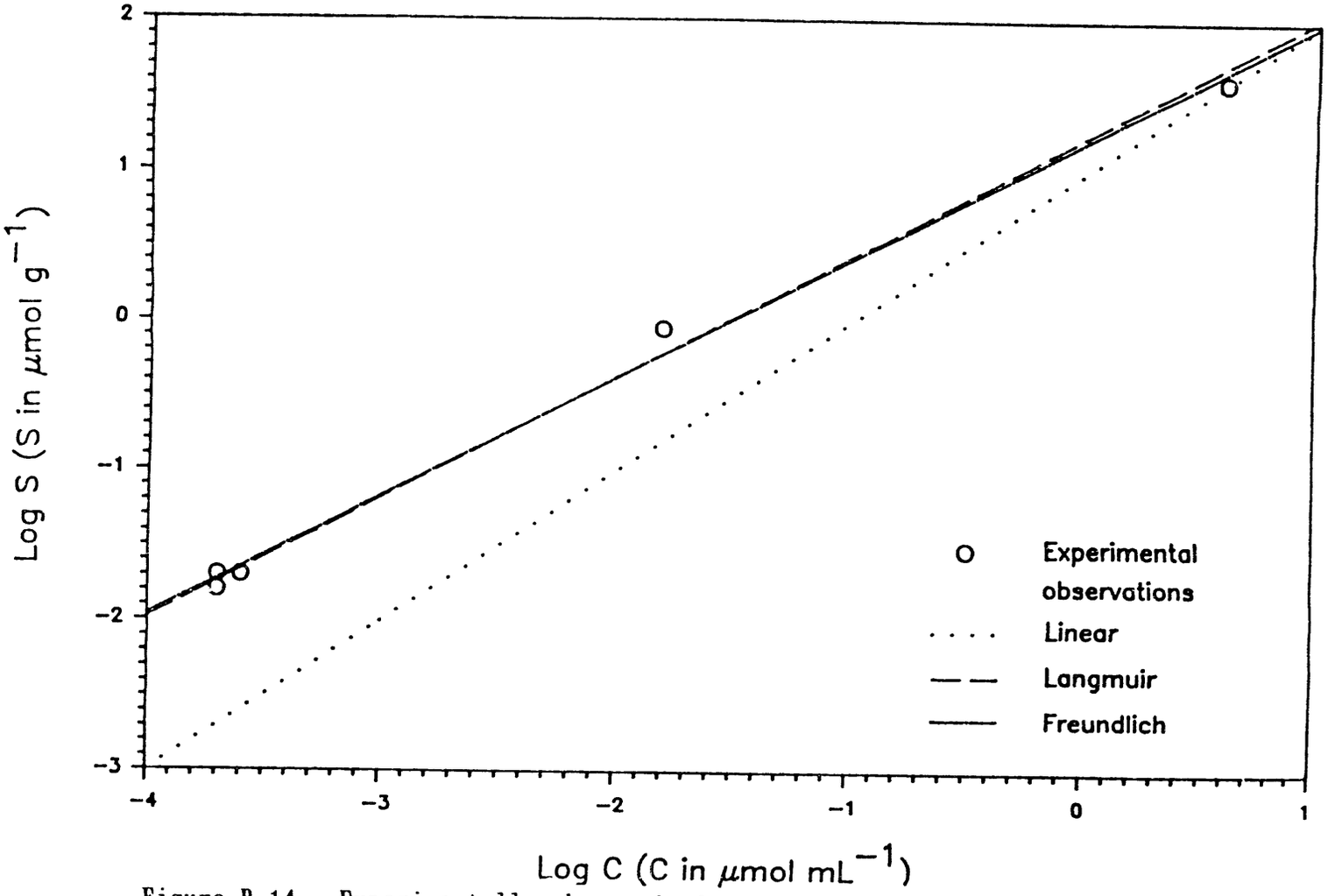

Figure B.14. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Sr 21 air 75-500 amb 58.0.

TABLE B.XV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g4-1608 Np 42 CO2 75-500 amb n.a.

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9714	0.5502	0.9947	n.a.
C.V.	39.96	39.22	-6.279	n.a.
SSE	9.70E+04	2.30E+04	1.16E+05	n.a.
SE Slope	0.09725	0.2124	0.02195	n.a.
SE Int.	n.a.	0.03806	0.08199	n.a.
Isotherm Parameters				
Kd	1.879 +/- 0.097	n.a.	n.a.	n.a.
k	n.a.	0.1827 +/- 1.1450	n.a.	n.a.
b	n.a.	1.346 +/- 0.385	n.a.	n.a.
K	n.a.	n.a.	2.514 +/- 0.082	n.a.
N	n.a.	n.a.	0.9746 +/- 0.0220	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
C	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

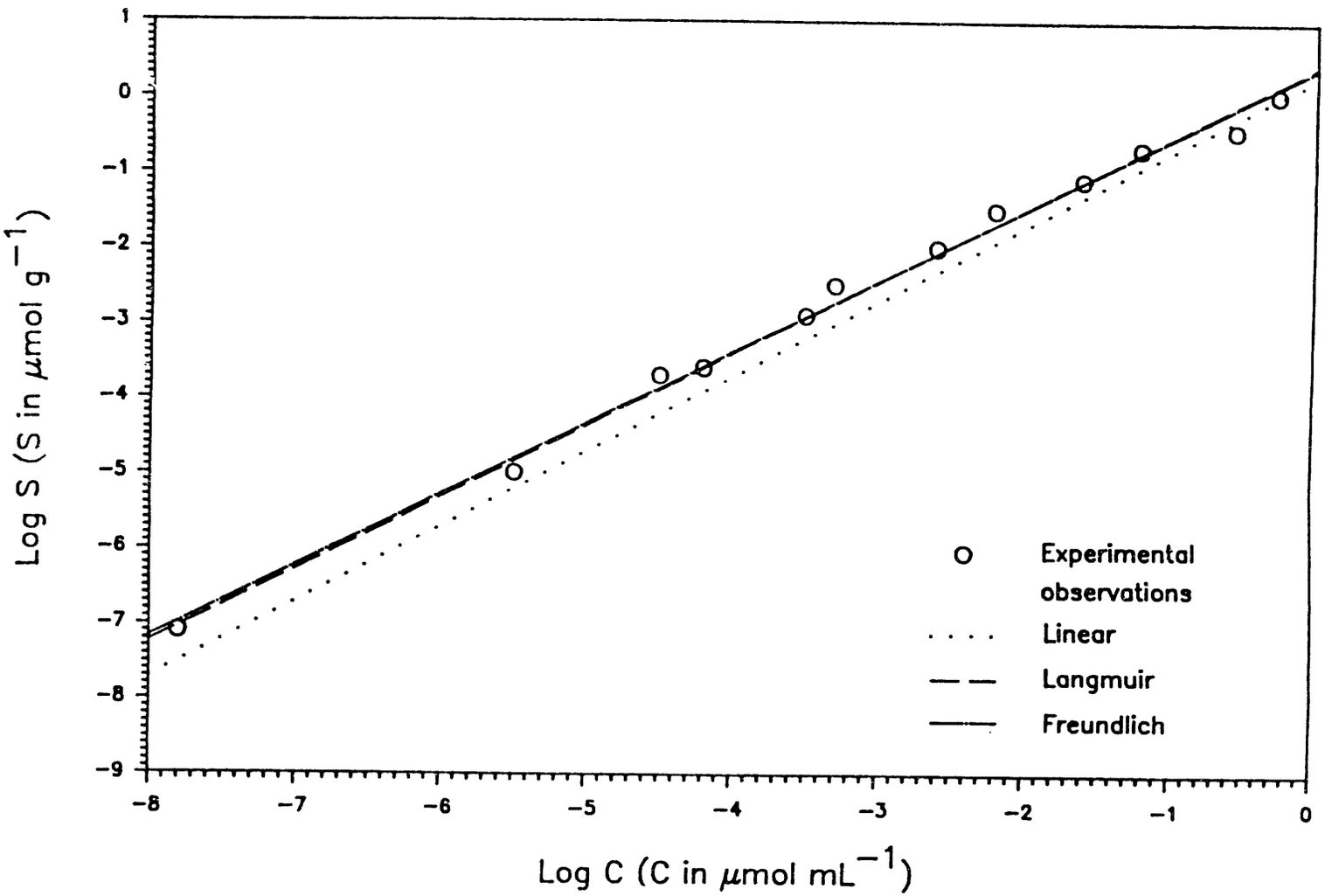

Figure B.15. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlisotherm models are plotted as log S versus log C for Data Set G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 1.

TABLE B.XVI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g4-1608 Np 42 CO2 75-500 amb n.a.

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.8633	0.2550	0.9876	n.a.
C.V.	97.04	112.2	-10.11	n.a.
SSE	1.25E+05	2.09E+04	4.49E+04	n.a.
SE Slope	0.2743	0.7577	0.03420	n.a.
SE Int.	n.a.	0.1388	0.1265	n.a.
Isotherm Parameters				
Kd	2.180 +/- 0.274	n.a.	n.a.	n.a.
k	n.a.	0.3391 +/- 4.9580	n.a.	n.a.
b	n.a.	0.7519 +/- 0.4284	n.a.	n.a.
K	n.a.	n.a.	2.113 +/- 0.127	n.a.
N	n.a.	n.a.	0.9163 +/- 0.0342	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

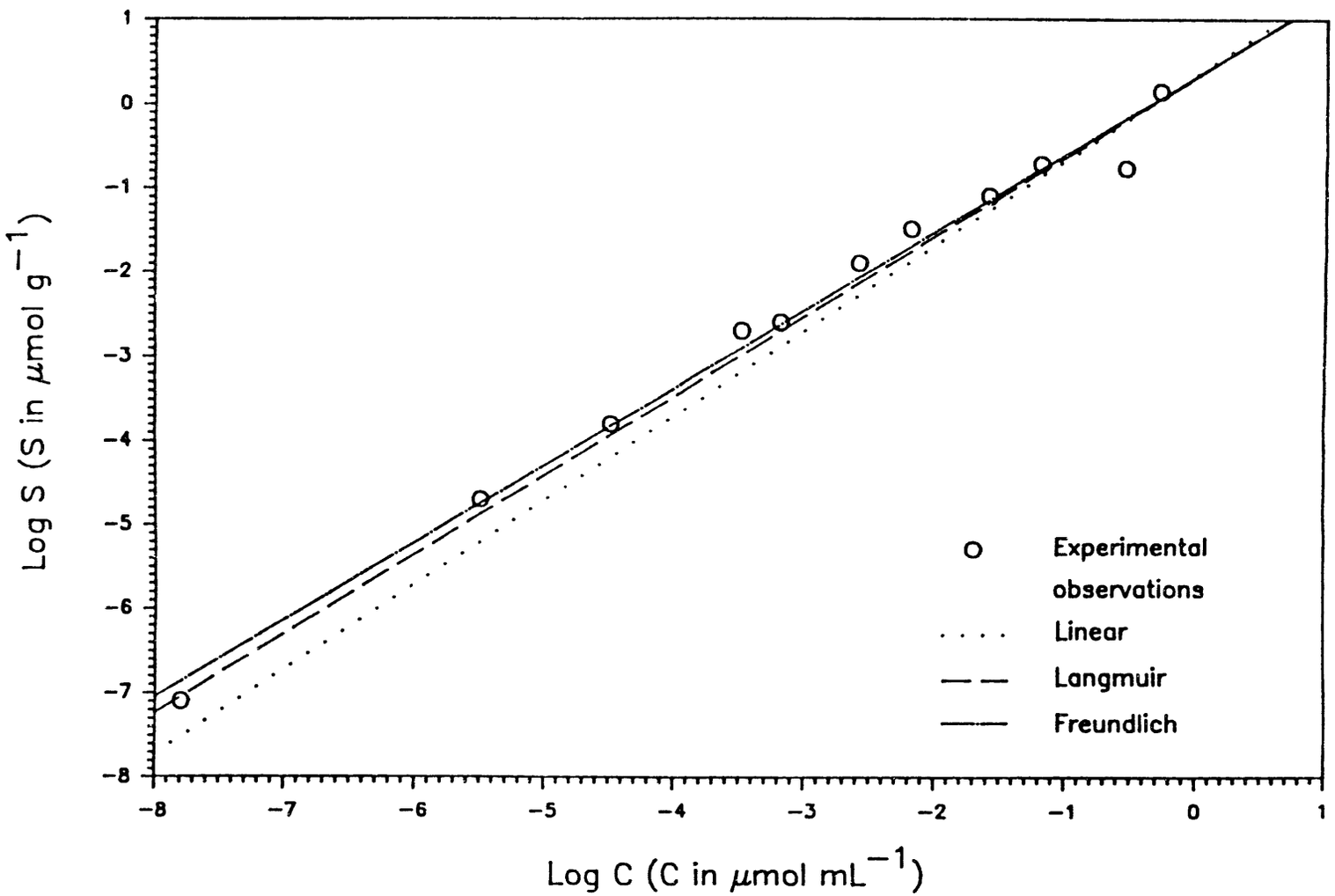

Figure B.16. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlisotherm models are plotted as log S versus log C for Data Set G1 1608 Np 42 C02 75-500 amb n.a. Replicate 2.

TABLE B.XVII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

gu3-433 Np 42 CO2 75-500 amb 26.0

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9704	0.0038	0.9401	0.9402
C.V.	86.38	139.1	-14.36	-10.38
SSE	1.99E+05	3.65E+04	4.33+05	1.49E+06
SE Slope	0.2318	18.81	0.07969	0.07968
SE Int.	n.a.	0.2610	0.3688	0.3688
Isotherm Parameters				
Kd	2.[illegible]6 +/- 0.232	n.a.	n.a.	n.a.
k	n.a.	6.400 +/- 34.230	n.a.	n.a.
b	n.a.	0.2736 +/- 1.4070	n.a.	n.a.
K	n.a.	n.a.	3.271 +/- 0.369	n.a.
N	n.a.	n.a.	0.9985 +/- 0.0797	n.a.
KD	n.a.	n.a.	n.a.	0.1257 +/- 0.1770
B	n.a.	n.a.	n.a.	0.9986 +/- 0.0797
Equivalent Isotherm Parameters				
Kd	2.406	1.751	3.261	3.268
KD	0.09255	6.340	0.1254	0.1257
B	1.0	1.0	0.9985	0.9986
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	0.73	1.01	1.43	2.12
Keq	2.93E-01	1.82E-01	8.98E-02	2.79E-02

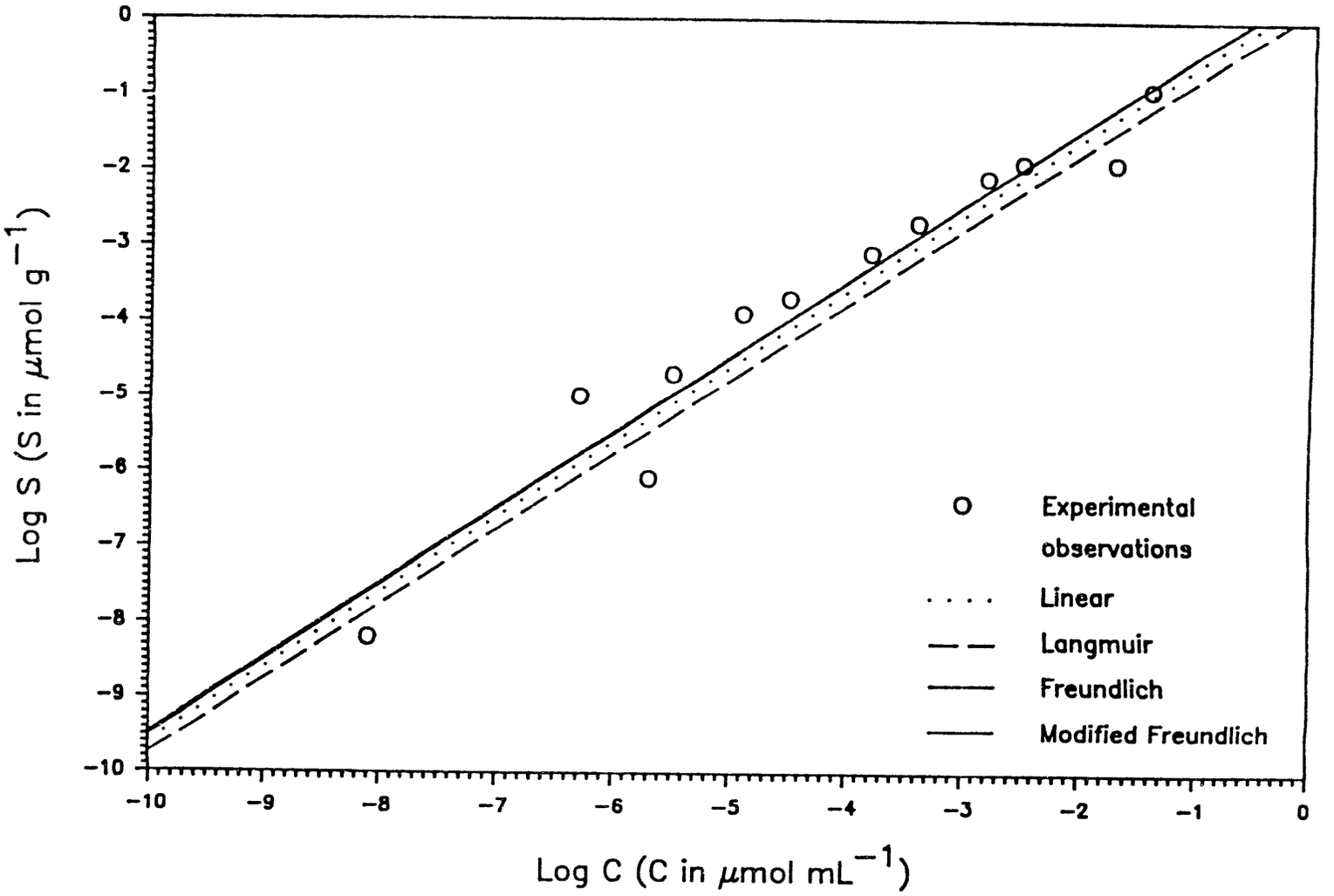

Figure B.17. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set GU3 433 Np 42 CO2 75-500 amb 26.0 Replicate 1.

TABLE B.XVIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

gu3-433 Np 42 CO2 75-500 amb 26.0

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.8562	0.1282	0.9481	0.9481
C.V.	99.68	177.5	-12.63	-9.172
SSE	4.05E+04	3.64E+04	8.18E+04	5.28E+05
SE Slope	0.1734	35.77	0.07163	0.07163
SE Int.	n.a.	0.5492	0.3297	0.3300
Isotherm Parameters				
Kd	1.403 +/- 0.173	n.a.	n.a.	n.a.
k	n.a.	65.13 +/- 87.74	n.a.	n.a.
b	n.a.	0.02796 +/- 0.02305	n.a.	n.a.
K	n.a.	n.a	2.017 +/- 0.330	n.a.
N	n.a.	n.a.	0.9683 +/- 0.0716	n.a.
KD	n.a.	n.a.	n.a.	0.07148 +/- 0.13320
B	n.a.	n.a.	n.a.	0.9684 +/- 0.0716
Equivalent Isotherm Parameters				
Kd	1.403	1.821	1.855	1.858
KD	0.05397	65.13	0.07136	0.07148
B	1.0	1.0	0.9683	0.9684
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	1.06	1.41	1.93	2.79
Keq	1.67E-01	9.24E-02	3.85E-02	9.01E-03

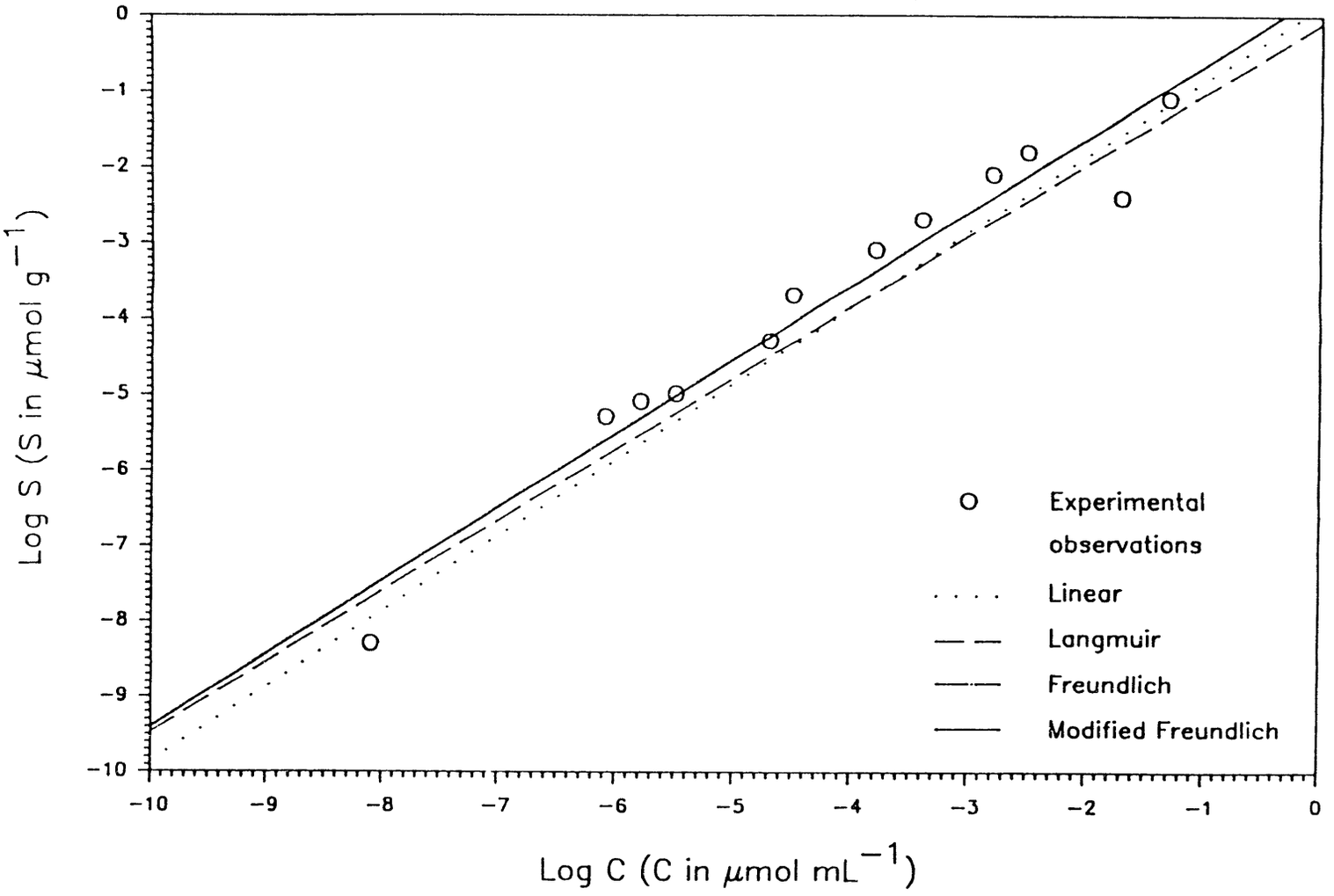

Figure B.18. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich. and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set GU3-433 Np 42 CO2 75-500 amb 26.0 Replicate 2.

TABLE B.XIX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ja-37 U 7 air 355-500 amb n.a.

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.6347	0.1954	0.5960	n.a.
C.V.	92.80	141.0	-28.68	n.a.
SSE	1.44E+05	5.81E+03	7.83E+03	n.a.
SE Slope	1.452	169.7	0.5386	n.a.
SE Int.	n.a.	1.001	1.376	n.a.
Isotherm Parameters				
Kd	3.315 +/- 1.452	n.a.	n.a.	n.a.
k	n.a.	1558.0 +/- 22540.0	n.a.	n.a.
b	n.a.	0.008457 +/- 0.012140	n.a.	n.a.
K	n.a.	n.a.	1.635 +/- 1.376	n.a.
N	n.a.	n.a.	0.9252 +/- 0.5386	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

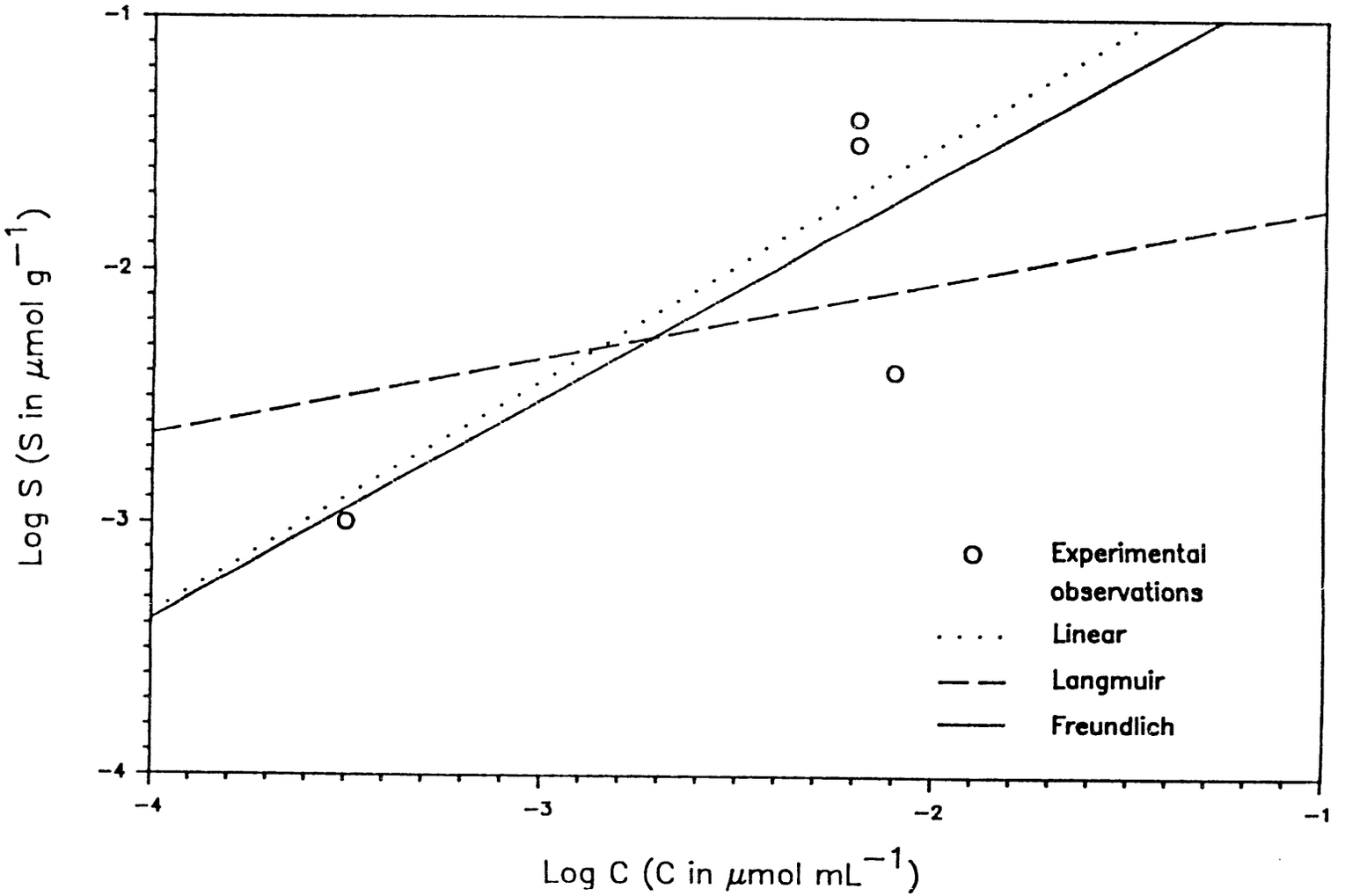

Figure B.1[illegible]. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set JA-37 U 7 air 355-500 amb n.a. Replicate 1.

TABLE B.XX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF DESORPTION DATA FOR ISOTHERM MODELS

ja-37 U 7 air 355-500 amb n.a.

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	1.0000	1.0000	1.0000	n.a.
C.V.	0.2576	n.a.	n.a.	n.a.
SSE	2.70E+06	6.06E+03	4.28E+06	n.a.
SE Slope	0.01456	n.a.	n.a.	n.a.
SE Int.	n.a.	n.a.	n.a.	n.a.
Isotherm Parameters				
Kd	12.86 +/- 0.01	n.a.	n.a.	n.a.
k	n.a.	-14.29 +/- 0.00	n.a.	n.a.
b	n.a.	-0.8370 +/- 0.0000	n.a.	n.a.
K	n.a.	n.a.	14.54 +/- 0.00	n.a.
N	n.a.	n.a.	1.023 +/- 0.000	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Equivalent Isotherm Parameters				
Kd	n.a.	n.a.	n.a.	n.a.
KD	n.a.	n.a.	n.a.	n.a.
B	n.a.	n.a.	n.a.	n.a.
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

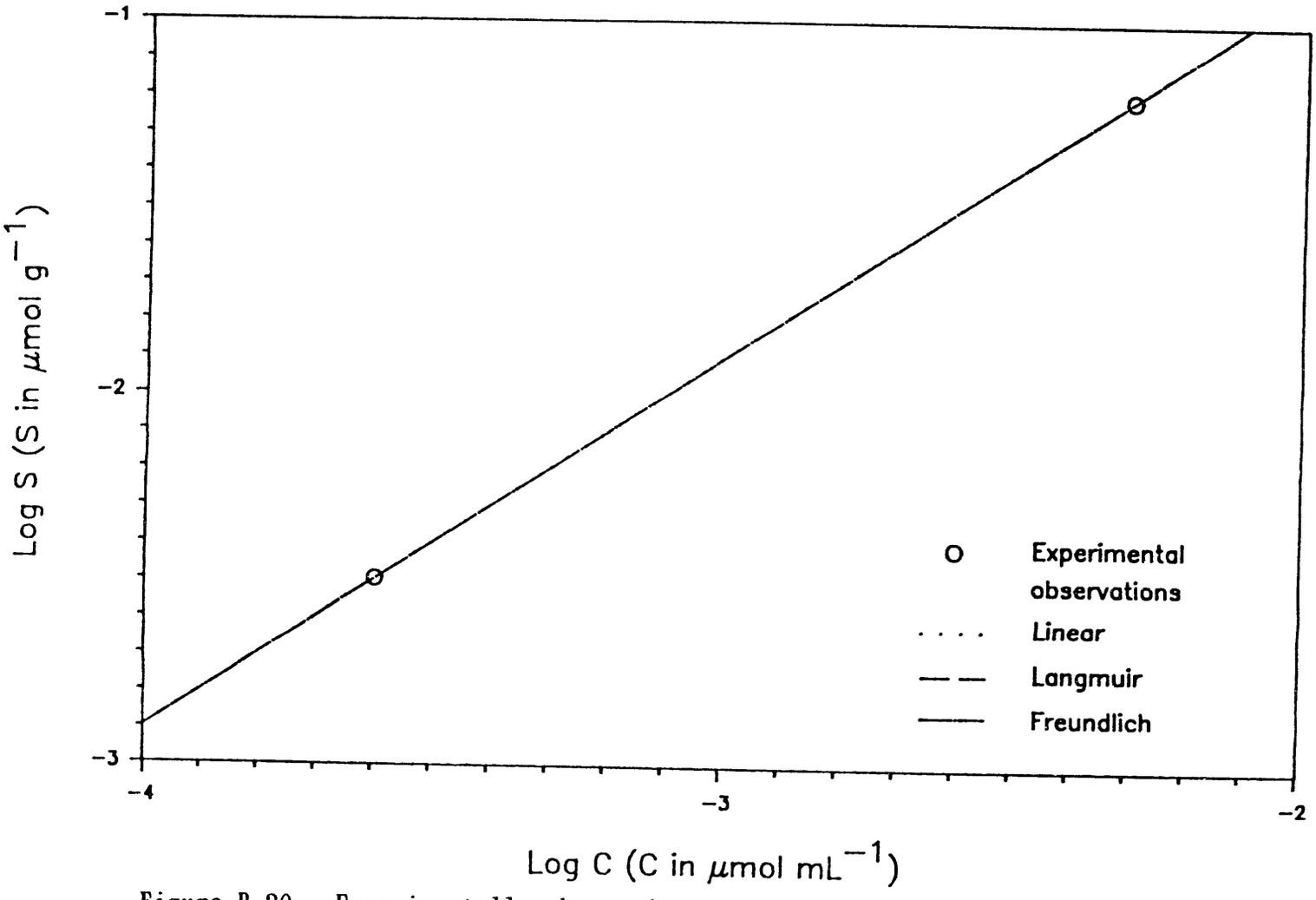

Figure B.20. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set JA-37 U 7 air 355-500 amb n.a. Replicate 2.

TABLE B.XXI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-48 Tc 42 air 106-500 amb 484.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	1.0000	0.3328	0.9979	0.9979
C.V.	0.1177	39.28	-4.065	-2.708
SSE	1.04E-08	3.59E-02	3.54E-03	3.54E-03
SE Slope	0.00005950	3.437	0.03242	0.03242
SE Int.	n.a.	1.702	0.1820	0.1821
Isotherm Parameters				
Kd	0.2020 +/- 0.0001	n.a.	n.a.	n.a.
k	n.a.	-0.4112 +/- 0.3767	n.a.	n.a.
b	n.a.	-0.2912 +/- 0.2916	n.a.	n.a.
K	n.a.	n.a.	0.1419 +/- 0.1820	n.a.
N	n.a.	n.a.	1.000 +/- 0.0324	n.a.
KD	n.a.	n.a.	n.a.	0.0002937 +/- 0.00825
B	n.a.	n.a.	n.a.	1.000 +/- 0.032
Equivalent Isotherm Parameters				
Kd	0.2020	0.1197	0.1421	0.1421
KD	0.0004174	-0.4112	0.0002936	0.0002937
B	1.0	1.0	1.000	1.000
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

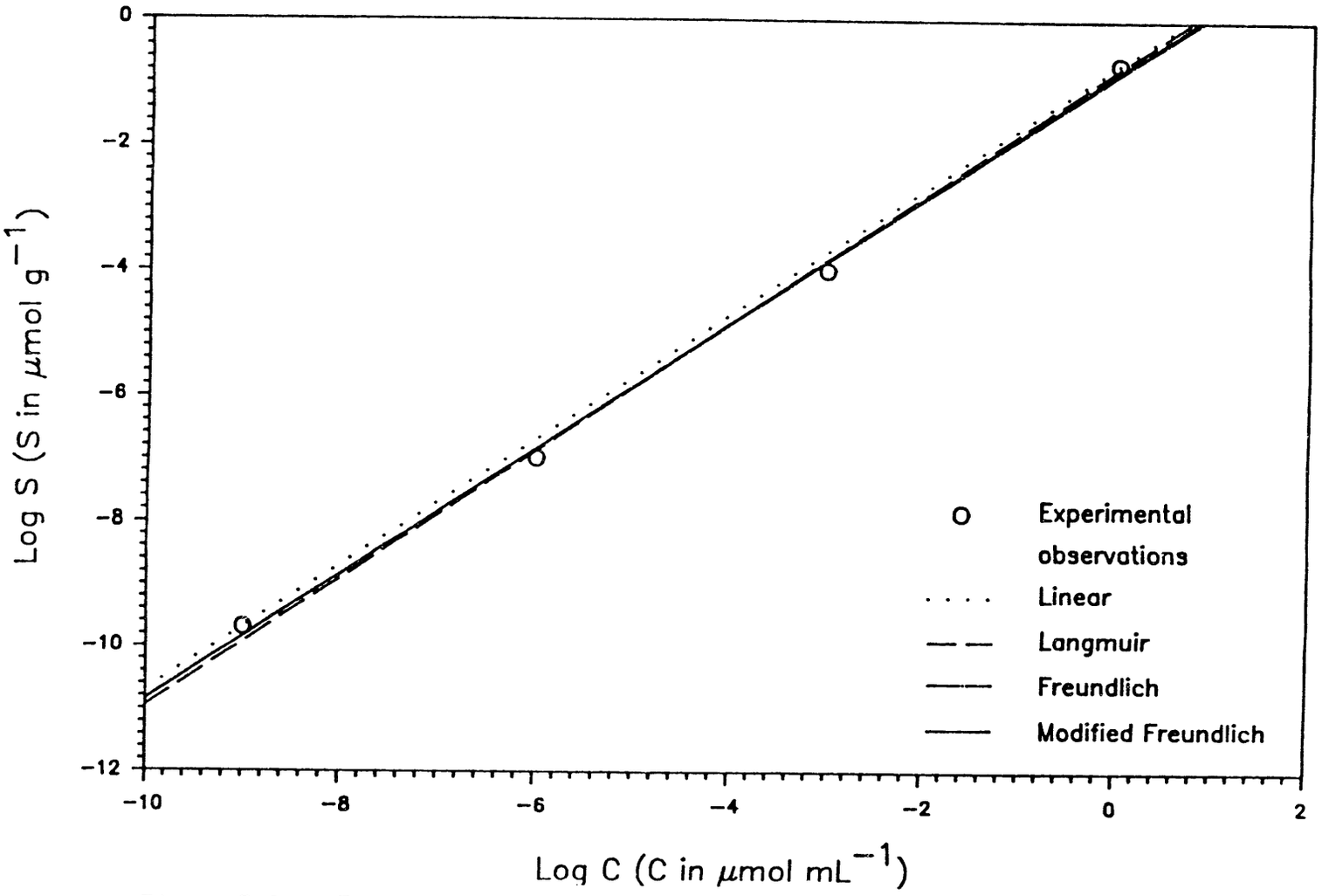

Figure B.21. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-48 Tc 42 air 106-500 amb 484.0.

TABLE B.XXII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-49 Tc 42 air 106-500 amb 1170.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	1.0000	0.1114	0.9995	0.9995
C.V.	0.0001154	20.99	-2.021	-1.267
SSE	1.00E-14	1.01E-01	6.85E-05	6.83E-05
SE Slope	0.00000005832	1.111	0.01553	0.01553
SE Int.	n.a.	0.5501	0.08722	0.08721
Isotherm Parameters				
Kd	0.2020 +/- 0.0000	n.a.	n.a.	n.a.
k	n.a.	0.1265 +/- 0.2609	n.a.	n.a.
b	n.a.	1.797 +/- 3.589	n.a.	n.a.
K	n.a.	n.a.	0.2104 +/- 0.0872	n.a.
N	n.a.	n.a.	0.9941 +/- 0.0155	n.a.
KD	n.a.	n.a.	n.a.	0.0001709 +/- 0.00322
B	n.a.	n.a.	n.a.	0.9941 +/- 0.0155
Equivalent Isotherm Parameters				
Kd	0.2020	0.2273	0.2000	0.2000
KD	0.0001727	0.1265	0.0001709	0.0001709
B	1.0	1.0	0.9941	0.9941
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

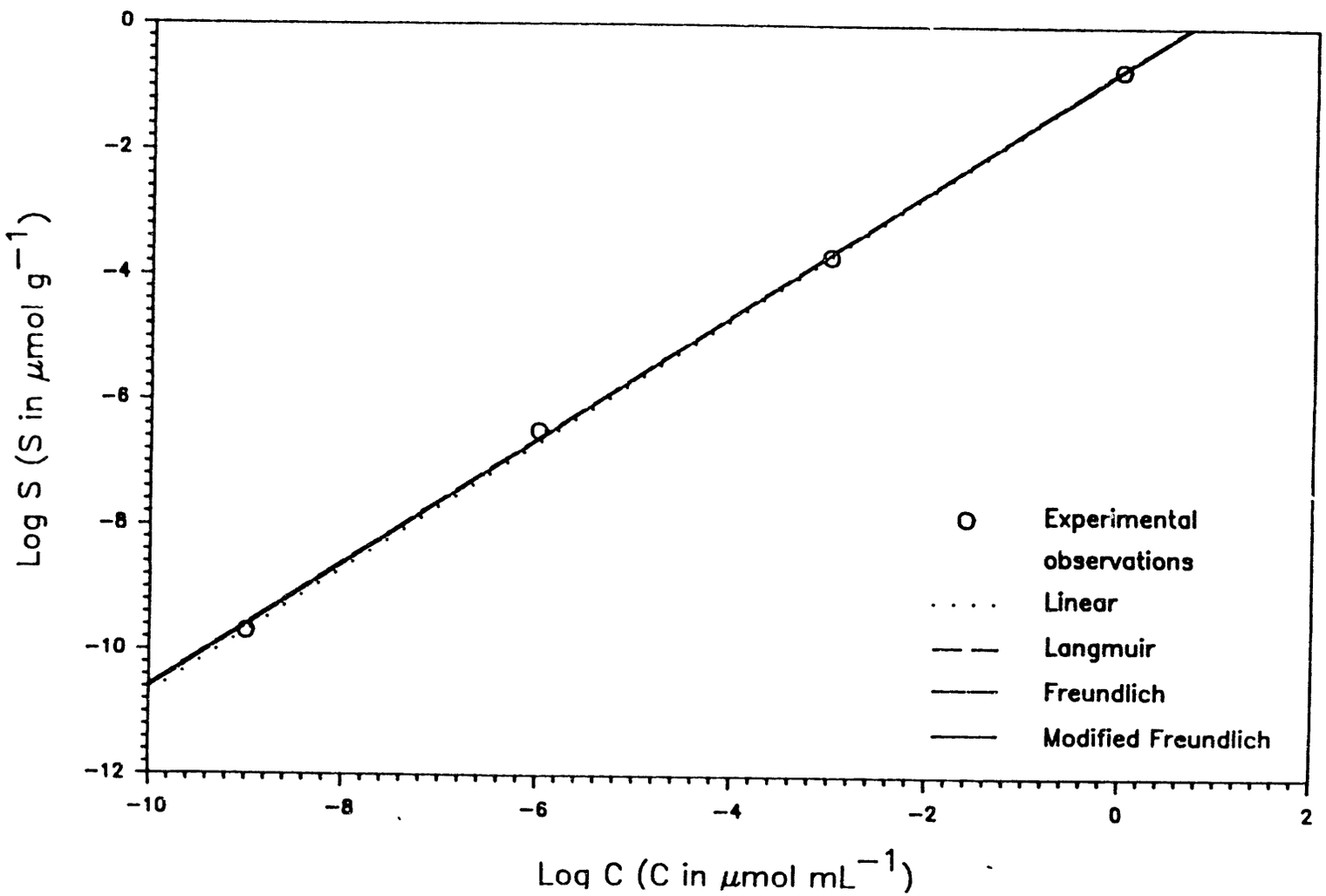

Figure B.22. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM 49 Tc 42 air 106 500 amb 1170.0.

TABLE B.XXIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF DESORPTION DATA FOR ISOTHERM MODELS

ym-48 Tc 63 air 106-500 amb 484.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	1.0000	0.0075	0.9991	0.9991
C.V.	0.05193	33.24	-3.199	-1.977
SSE	9.93E-08	8.26E+02	9.28E-03	9.50E-03
SE Slope	0.0001956	0.2650	0.02063	0.02065
SE Int.	n.a.	0.1232	0.1164	0.1165
Isotherm Parameters				
Kd	1.505 +/- 0.000	n.a.	n.a.	n.a.
k	n.a.	0.05123 +/- 0.42280	n.a.	n.a.
b	n.a.	30.77 +/- 250.90	n.a.	n.a.
K	n.a.	n.a.	1.400 +/- 0.116	n.a.
N	n.a.	n.a.	0.9870 +/- 0.0206	n.a.
KD	n.a.	n.a.	n.a.	0.002686 +/- 0.012570
B	n.a.	n.a.	n.a.	0.9871 +/- 0.0207
Equivalent Isotherm Parameters				
Kd	1.505	1.577	1.296	1.300
KD	0.003110	0.05123	0.002679	0.002686
B	1.0	1.0	0.9870	0.9871
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

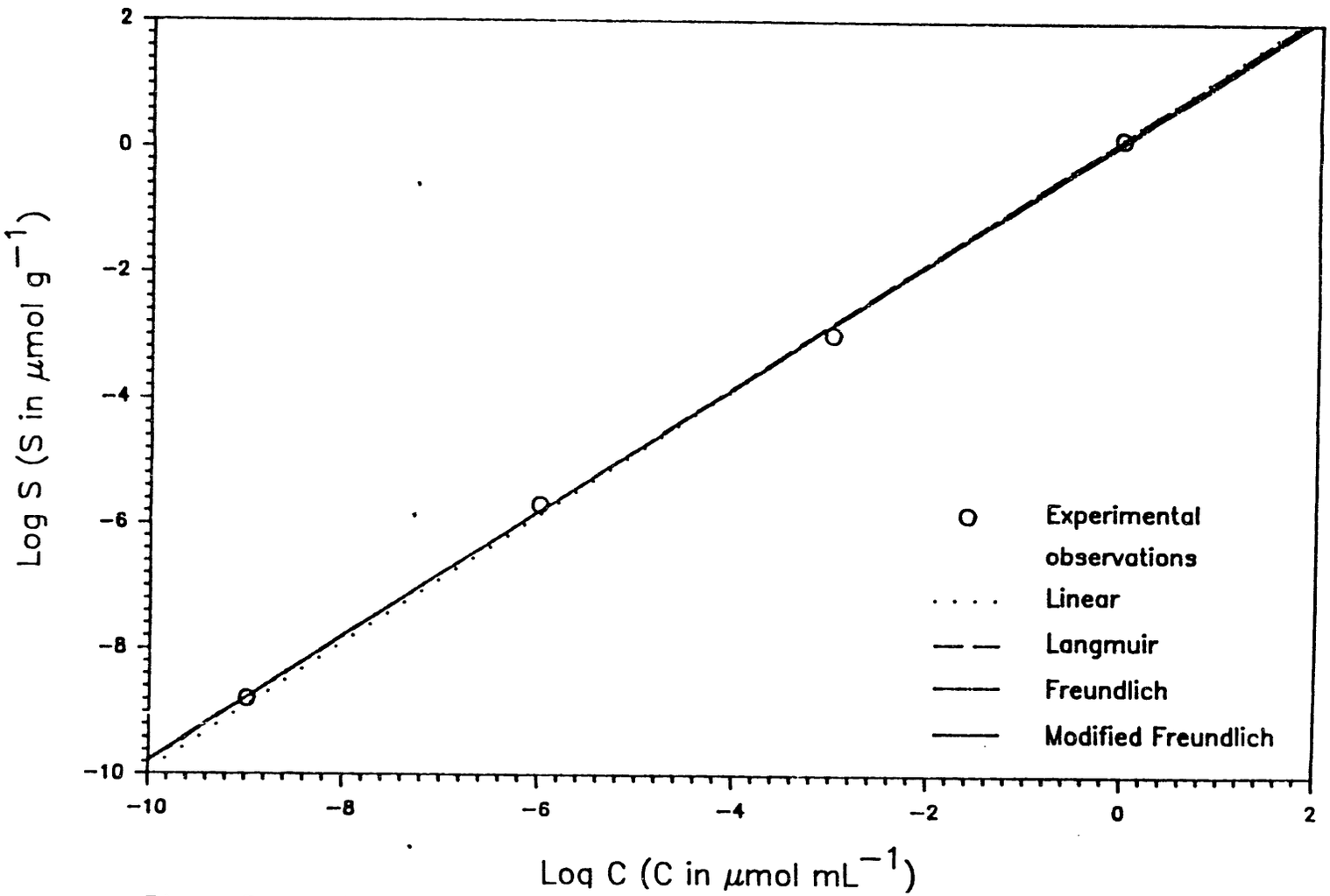

Figure B.23. Experimentally observed desorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-48 Tc 63 air 106-500 amb 484.0.

TABLE B.XXIV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF DESORPTION DATA FOR ISOTHERM MODELS

ym-49 Tc 63 air 106-500 amb 1170.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	1.0000	0.5735	0.9996	0.9996
C.V.	0.04090	27.98	-2.213	-1.287
SSE	4.53E-08	2.31E+00	6.32E-04	6.13E-04
SE Slope	0.0001308	0.1928	0.01404	0.01404
SE Int.	n.a.	0.09060	0.07935	0.07933
Isotherm Parameters				
Kd	1.277 +/- 0.000	n.a.	n.a.	n.a.
k	n.a.	0.6500 +/- 0.4688	n.a.	n.a.
b	n.a.	3.163 +/- 1.929	n.a.	n.a.
K	n.a.	n.a.	1.301 +/- 0.079	n.a.
N	n.a.	n.a.	0.9653 +/- 0.0140	n.a.
KD	n.a.	n.a.	n.a.	0.0008711 +/- 0.00566
B	n.a.	n.a.	n.a.	0.9653 +/- 0.0140
Equivalent Isotherm Parameters				
Kd	1.277	2.056	1.018	1.019
KD	0.001091	0.650	0.0008702	0.0008711
B	1.0	1.0	0.9653	0.9653
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	n.a.	n.a.	n.a.	n.a.
Keq	n.a.	n.a.	n.a.	n.a.

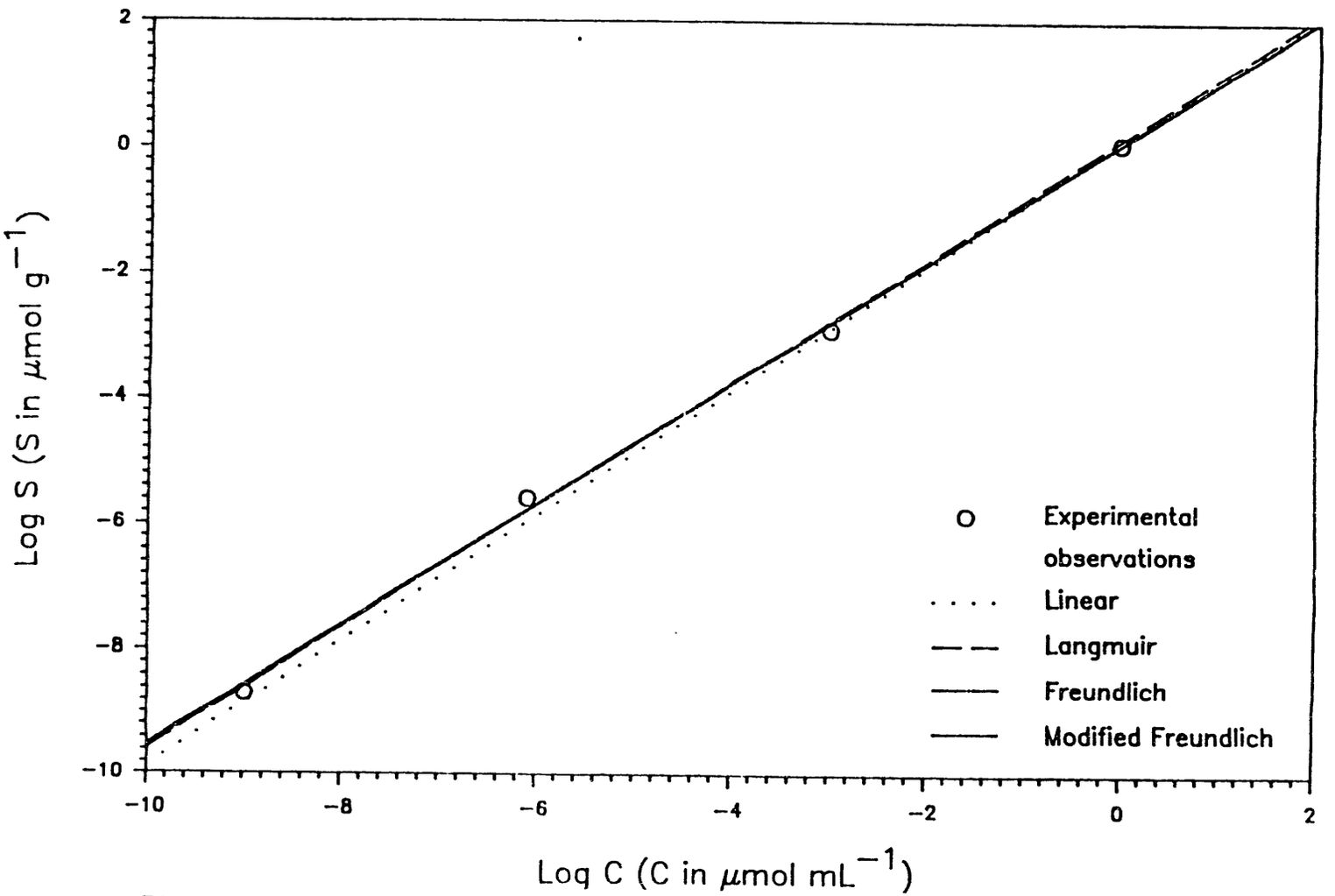

Figure B.24. Experimentally observed desorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-49 Tc 63 air 106-500 amb 1170.0.

TABLE B.XXV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Ba 21 air - 75 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9976	0.9349	0.9979	0.9982
C.V.	11.01	16.57	-5.525	-1.983
SSE	3.47E-02	2.31E+01	8.20E-02	1.46E+01
SE Slope	9.795	0.02521	0.02263	0.02118
SE Int.	n.a.	0.0001073	0.09518	0.08906
Isotherm Parameters				
Kd	401.1 +/- [illegible] 8	n.a.	n.a.	n.a.
k	n.a	175.3 +/- 40.2	n.a.	n.a.
b	n.a.	6.046 +/- 0.921	n.a.	n.a.
K	n.a.	n.a.	211.5 +/- 0.1	n.a.
N	n.a.	n.a.	0.8478 +/- 0.0226	n.a.
KD	n.a.	n.a.	n.a.	5.060 +/- 0.177
B	n.a.	n.a.	n.a.	0.8564 +/- 0.0212
Equivalent Isotherm Parameters				
Kd	401.1	1060.0	266.8	293.5
KD	6.9147	175.3	4.601	5.060
B	1.0	1.0	0.8478	0.8564
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-2.80	-2.99	-3.30	-3.84
Keq	1.13E+02	1.56E+02	2.63E+02	6.58E+02

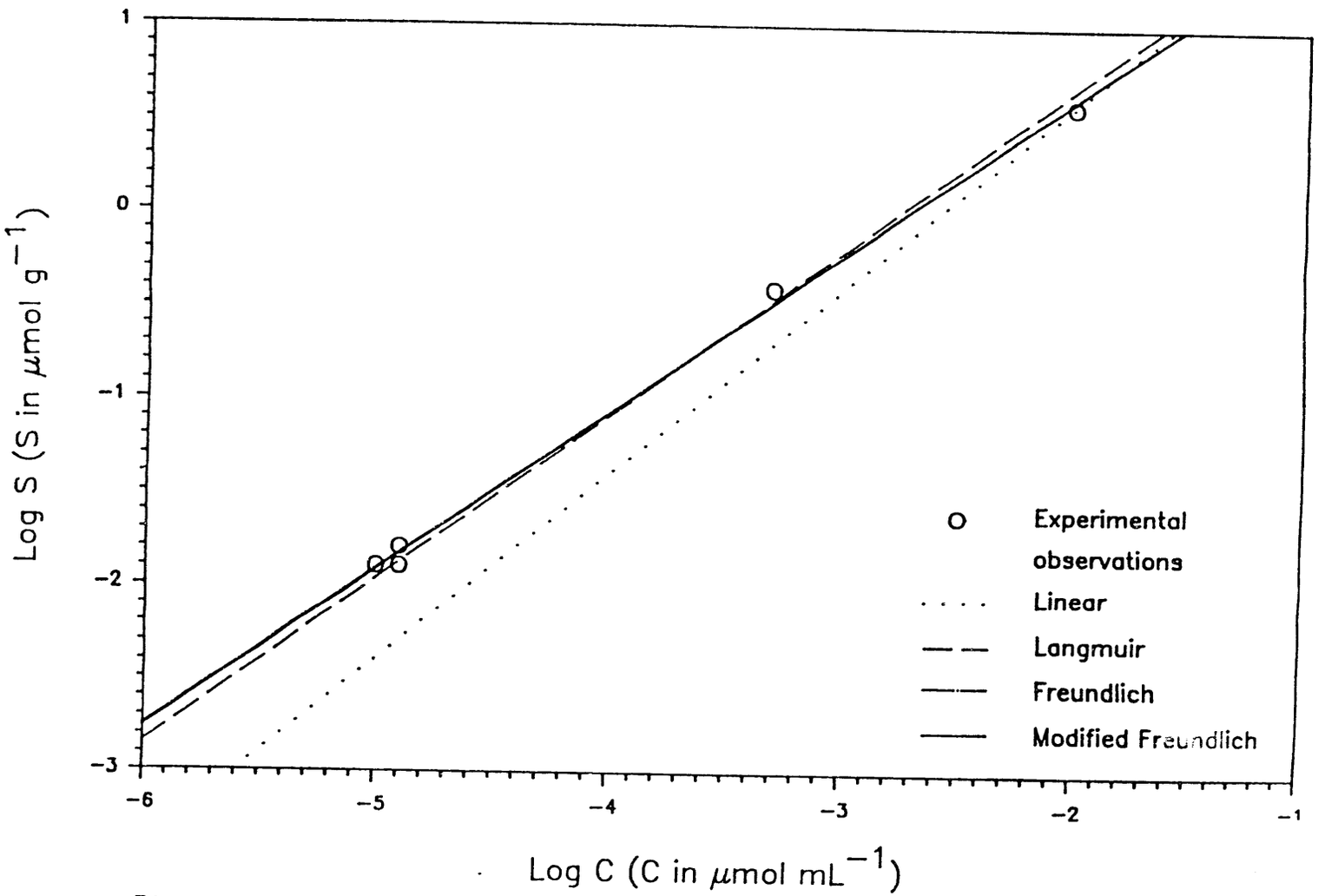

Figure B.25. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Mofidied Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Ba 21 air -75 amb 58.0.

TABLE B.XXVI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Ba 21 air 75-500 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9971	0.9576	0.9974	0.9979
C.V.	12.25	14.92	-6.006	-2.184
SSE	4.08E-02	1.76E+01	1.37E-01	1.38E+01
SE Slope	5.933	0.02186	0.02452	0.02220
SE Int.	n.a.	0.0001664	0.09796	0.08868
Isotherm Parameters				
Kd	218.2 +/- 5.9	n.a.	n.a.	n.a.
k	n.a.	115.5 +/- 22.6	n.a.	n.a.
b	n.a.	5.558 +/- 0.022	n.a.	n.a.
K	n.a.	n.a.	123.1 +/- 0.1	n.a.
N	n.a.	n.a.	0.8370 +/- 0.0245	n.a.
KD	n.a.	n.a.	n.a.	3.859 +/- 0.162
B	n.a.	n.a.	n.a.	0.8480 +/- 0.0222
Equivalent Isotherm Parameters				
Kd	218.3	642.2	150.4	169.8
KD	4.960	115.5	3.418	3.859
B	1.0	1.0	0.8370	0.8480
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-2.52	-2.69	-2.96	-3.44
Keq	7.00E+01	9.34E+01	1.49E+02	1.35E+02

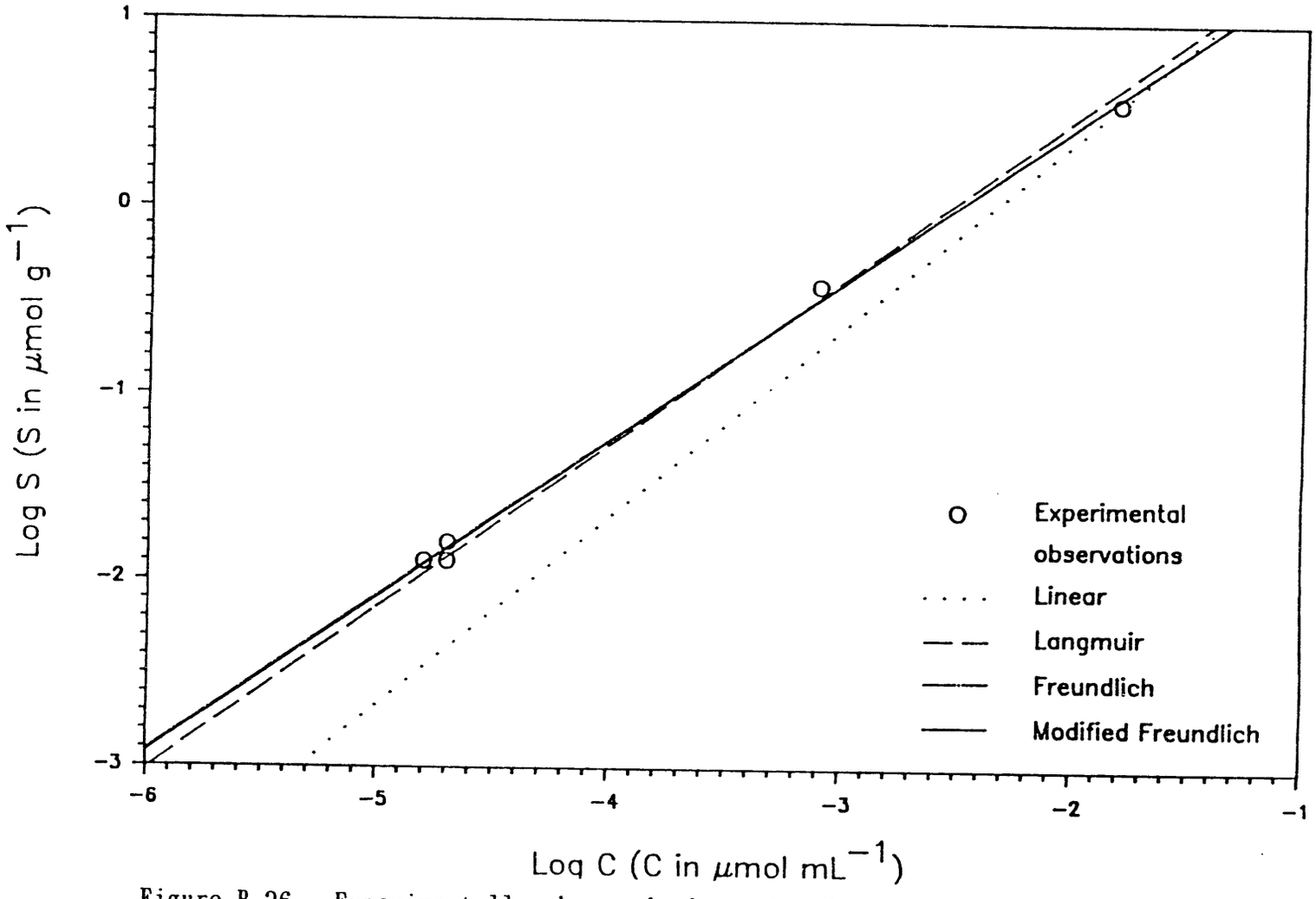

Figure B.26. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Ba 21 air 75-500 amb 44.0.

TABLE B.XXVII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g1-2840 Cs 21 air 75-500 amb 43.0

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9900	0.7146	0.9975	0.9968
C.V.	23.22	64.37	-6.809	-3.747
SSE	2.21E+00	5.31E+02	1.74E+00	1.31E+01
SE Slope	0.6120	0.07412	0.01146	0.01304
SE Int.	n.a.	0.003134	0.05234	0.05960
Isotherm Parameters				
Kd	20.20 +/- 0.61	n.a.	n.a.	n.a.
k	n.a.	8.323 +/- 3.920	n.a.	n.a.
b	n.a.	13.49 +/- 2.70	n.a.	n.a.
K	n.a.	n.a.	15.68 +/- 0.05	n.a.
N	n.a.	n.a.	0.7174 +/- 0.0115	n.a.
KD	n.a.	n.a.	n.a.	0.3062 +/- 0.0536
B	n.a.	n.a.	n.a.	0.7284 +/- 0.0130
Equivalent Isotherm Parameters				
Kd	20.20	112.3	10.54	13.17
KD	0.4698	8.323	0.2451	0.3062
B	1.0	1.0	0.7174	0.7284
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	0.11	0.30	0.57	1.01
Keq	8.28E-01	6.04E-01	3.82E-01	1.81E-01

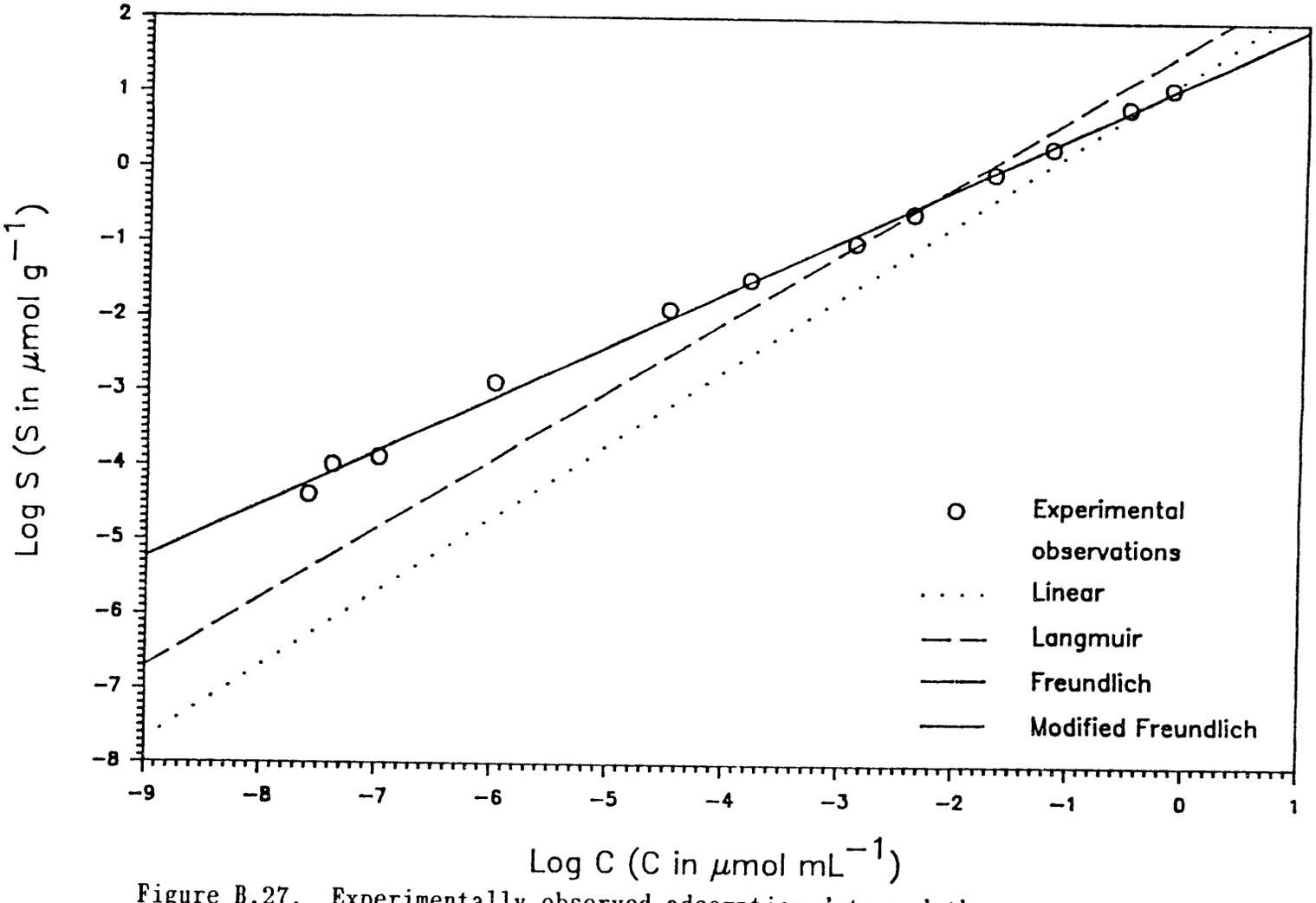

Figure B.27. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1 2840 Cs 21 air 75-500 amb 43.0 Replicate 1.

TABLE B.XXVIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

gl-2840 Cs 21 air 75-500 amb 43.0

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9912	0.6974	0.9969	0.9963
C.V.	20.88	60.67	-8.519	-4.226
SSE	1.95E+00	5.57E+02	1.27E+00	1.17E+01
SE Slope	0.6378	0.01578	0.01353	0.01514
SE Int.	n.a.	0.003294	0.05697	0.06377
Isotherm Parameters				
Kd	21.46 +/- 0.64	n.a.	n.a.	n.a.
k	n.a.	7.393 +/- 3.527	n.a.	n.a.
b	n.a.	13.92 +/- 3.06	n.a.	n.a.
K	n.a.	n.a.	16.75 +/- 0.06	n.a.
N	n.a.	n.a.	0.7287 +/- 0.0135	n.a.
KD	n.a.	n.a.	n.a.	0.3440 +/- 0.0591
B	n.a.	n.a.	n.a.	0.7409 +/- 0.0151
Equivalent Isotherm Parameters				
Kd	21.46	102.9	11.79	14.79
KD	0.4991	7.393	0.2742	0.3440
B	1.0	1.0	0.7287	0.7409
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	0.04	0.22	0.47	0.87
Keq	9.30E-01	6.94E-01	4.55E-01	2.29E-01

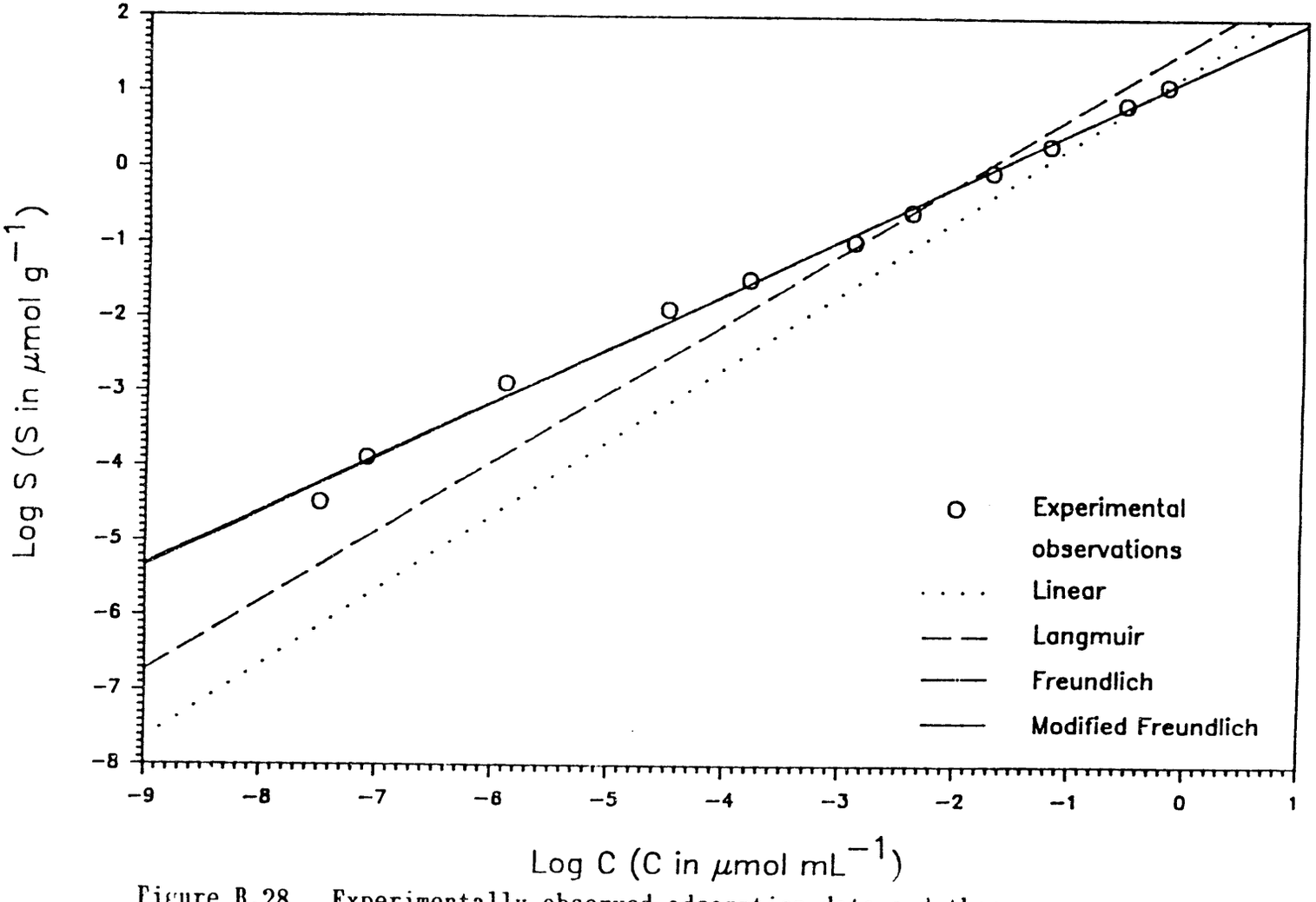

Figure B.28. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 2.

TABLE B.XXIX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Cs 21 air - 75 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9995	0.9957	0.9880	0.9906
C.V.	5.19	14.08	-14.95	-7.566
SSE	1.02E-01	1.99E+02	1.65E+02	1.09E+02
SE Slope	0.1226	0.002431	0.05074	0.04565
SE Int.	n.a.	0.001413	0.2728	0.2454
Isotherm Parameters				
Kd	11.54 +/- 0.12	n.a.	n.a.	n.a.
k	n.a.	19.70 +/- 8.37	n.a.	n.a.
b	n.a.	15.60 +/- 0.59	n.a.	n.a.
K	n.a.	n.a.	22.59 +/- 0.27	n.a.
N	n.a.	n.a.	0.7975 +/- 0.0507	n.a.
KD	n.a.	n.a.	n.a.	0.4031 +/- 0.2165
B	n.a.	n.a.	n.a.	0.8114 +/- 0.0457
Equivalent Isotherm Parameters				
Kd	11.54	307.4	17.78	23.38
KD	0.1989	19.70	0.3066	0.4031
B	1.0	1.0	0.7975	0.8114
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-0.12	0.04	0.27	0.64
Keq	1.22E+00	9.28E-01	6.30E-01	3.37E-01

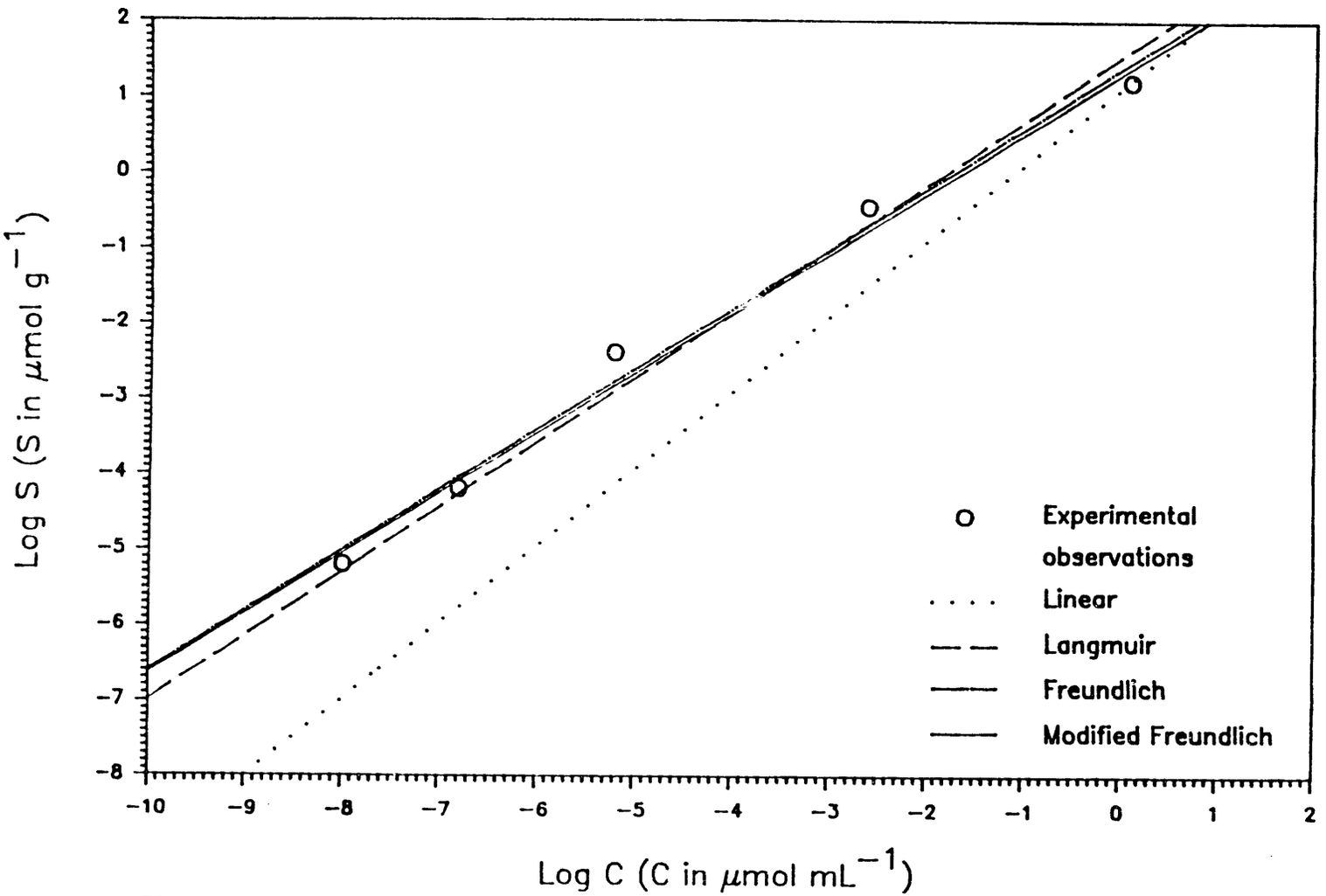

Figure B.29. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Cs 21 air -75 amb 58.0.

TABLE B.XXX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Cs 21 air 75-500 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9994	0.9952	0.9936	0.9959
C.V.	5.790	14.76	-10.74	-5.084
SSE	9.55E-02	1.45E+02	7.85E+01	4.31E+01
SE Slope	0.1189	0.002951	0.03641	0.02957
SE Int.	n.a.	0.001716	0.1952	0.1585
Isotherm Parameters				
Kd	10.00 +/- 0.12	n.a.	n.a.	n.a.
k	n.a.	18.58 +/- 8.38	n.a.	n.a.
b	n.a.	13.54 +/- 0.54	n.a.	n.a.
K	n.a.	n.a.	17.79 +/- 0.20	n.a.
N	n.a.	n.a.	0.7851 +/- 0.0364	n.a.
KD	n.a.	n.a.	n.a.	0.4330 +/- 0.1454
B	n.a.	n.a.	n.a.	0.8010 +/- 0.0296
Equivalent Isotherm Parameters				
Kd	10.00	251.6	13.88	19.05
KD	0.2273	18.58	0.3156	0.4330
B	1.0	1.0	0.7851	0.8010
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-0.10	0.05	0.26	0.60
Keq	1.18E+00	9.21E-01	6.46E-01	3.64E-01

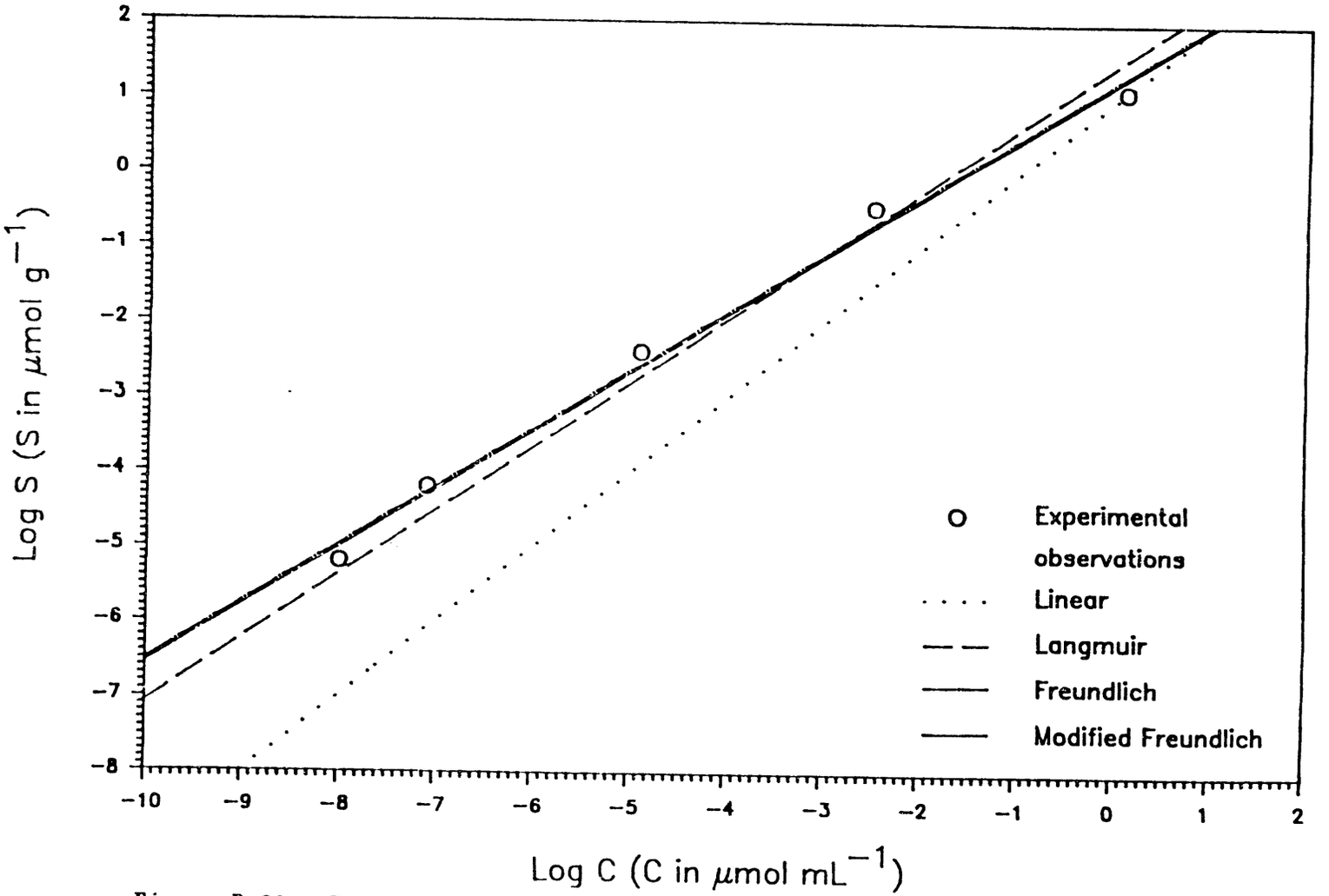

Figure B.30. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Cs 21 air 75-500 amb 44.0.

TABLE B.XXXI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Eu 21 air - 75 amb 58.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.3770	0.6141	0.9297	0.9294
C.V.	144.7	63.79	-26.90	-13.34
SSE	2.00E-01	2.88E-01	2.13E-01	2.14E-01
SE Slope	967.2	2.089	0.1888	0.1895
SE Int.	n.a.	0.0002787	0.9750	0.9784
Isotherm Parameters				
Kd	1303.0 +/- 967.2	n.a.	n.a.	n.a.
k	n.a.	10770.0 +/- 13390.0	n.a.	n.a.
b	n.a.	0.2683 +/- 0.1504	n.a.	n.a.
K	n.a.	n.a.	1408.0 +/- 1.0	n.a.
N	n.a.	n.a.	0.9710 +/- 0.1888	n.a.
KD	n.a.	n.a.	n.a.	27.01 +/- 3.09
B	n.a.	n.a.	n.a.	0.9719 +/- 0.1895
Equivalent Isotherm Parameters				
Kd	1303.0	2890.0	1549.0	1567.0
KD	22.47	10770.0	26.71	27.01
B	1.0	1.0	0.9710	0.9719
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-4.82	-5.23	-5.88	-7.00
Keq	3.40E+03	6.78E+03	2.03E+04	1.35E+05

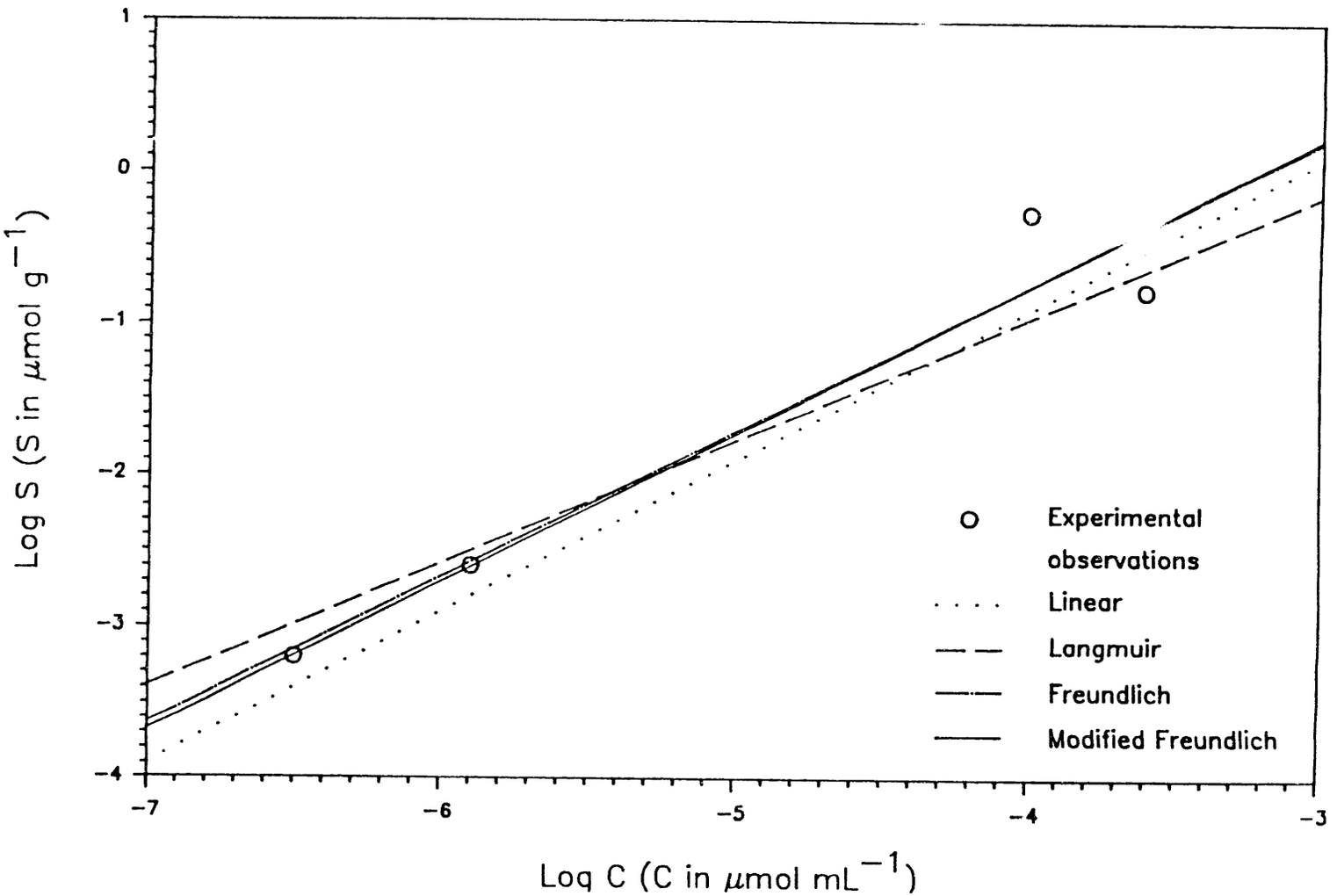

Figure B.31. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Eu 21 air -75 amb 58.0.

TABLE B.XXXII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Eu 21 air 75-500 amb 44.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9994	0.7883	0.9997	0.9997
C.V.	4.825	16.85	-1.517	-0.8450
SSE	1.89E-04	1.14E-02	4.81E-05	3.46E-05
SE Slope	13.69	0.2621	0.009673	0.009557
SE Int.	n.a.	0.00005895	0.05351	0.05287
Isotherm Parameters				
Kd	1113.0 +/- 13.7	n.a.	n.a.	n.a.
k	n.a.	1633.0 +/- 607.5	n.a.	n.a.
b	n.a.	1.141 +/- 0.342	n.a.	n.a.
K	n.a.	n.a.	612.8 +/- 0.1	n.a.
N	n.a.	n.a.	0.9215 +/- 0.0097	n.a.
KD	n.a.	n.a.	n.a.	17.71 +/- 0.16
B	n.a.	n.a.	n.a.	0.9227 +/- 0.0096
Equivalent Isotherm Parameters				
Kd	1113.0	1863.0	767.0	779.1
KD	25.29	1633.0	17.43	17.71
B	1.0	1.0	0.9215	0.9227
Thermodynamic Parameters				
zB	1.0	1.[illegible]	1.5	2.0
G	-4.38	-4.76	-5.36	-6.38
Keq	1.63E+03	3.09E+03	8.45E+03	4.76E+04

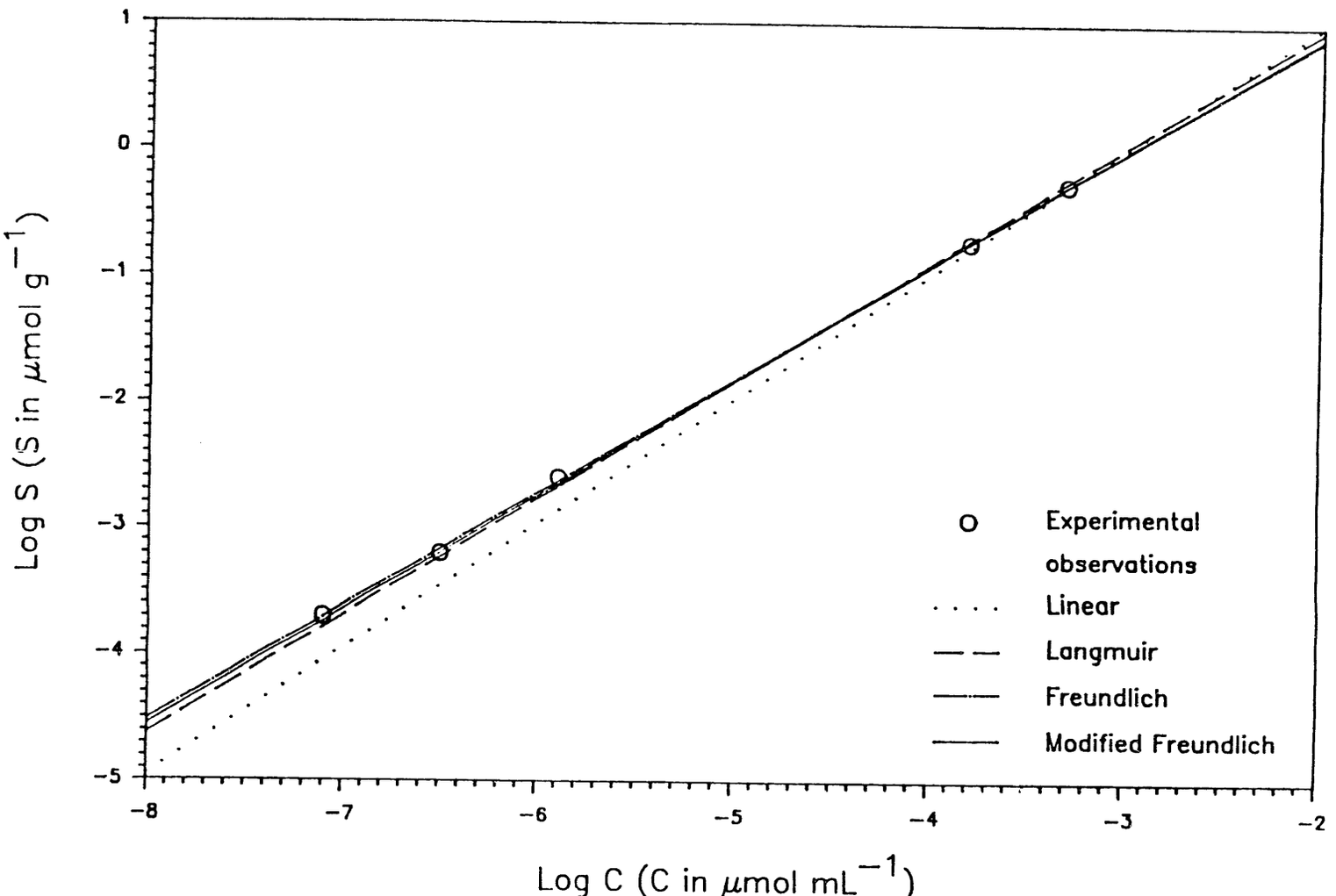

Figure B.32. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM 92 Eu 21 air 75-500 amb 44.0.

TABLE B.XXXIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

g1-2840 Sr 21 air 75-500 amb 43.0

REPLICATE 1

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.8585	0.9831	0.9827	0.9893
C.V.	62.02	11.65	-867.9	-7.736
SSE	1.17E+02	2.24E+03	2.04E+02	8.16E+01
SE Slope	1.396	0.001880	0.03181	0.02653
SE Int.	n.a.	0.001165	0.06605	0.05508
Isotherm Parameters				
Kd	11.91 +/- 1.40	n.a.	n.a.	n.a.
k	n.a.	2.820 +/- 0.268	n.a.	n.a.
b	n.a.	21.04 +/- 0.83	n.a.	n.a.
K	n.a.	n.a.	18.96 +/- 0.07	n.a.
N	n.a.	n.a.	0.7943 +/- 0.0318	n.a.
KD	n.a.	n.a.	n.a.	0.5642 +/- 0.0557
B	n.a.	n.a.	n.a.	0.8463 +/- 0.0265
Equivalent Isotherm Parameters				
Kd	11.91	59.32	13.27	24.26
KD	0.2770	2.820	0.3086	0.5462
B	1.0	1.0	0.7943	0.8463
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-1.37	-1.31	-1.25	-1.16
Keq	1.01E+01	9.17E+00	8.22E+00	7.09E+00

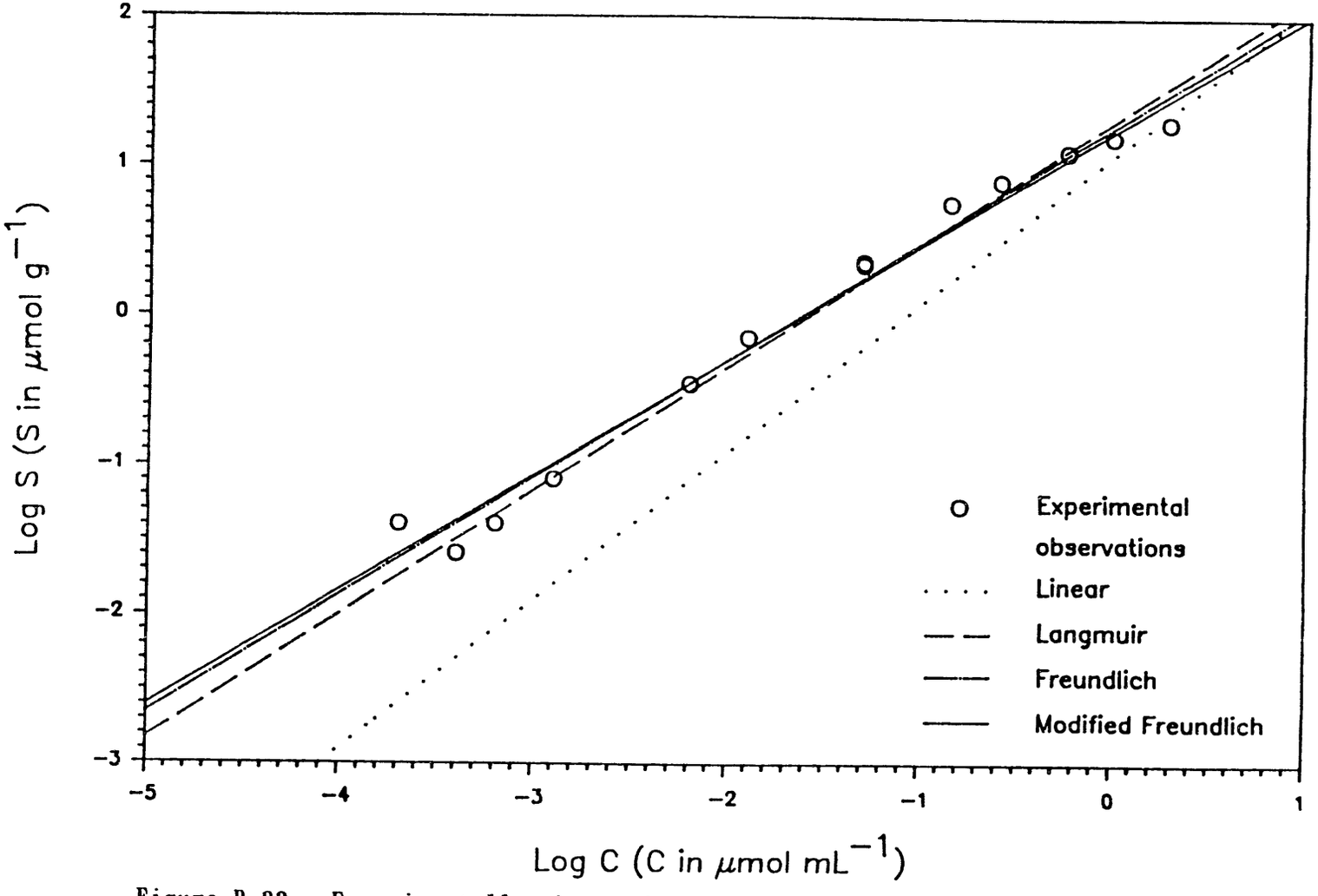

Figure B.33. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 1.

TABLE B.XXXIV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

gl-2840 Sr 21 air 75-500 amb 43.0

REPLICATE 2

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.8704	0.9958	0.9827	0.9925
C.V.	57.31	5.458	142.0	-6.719
SSE	1.03E+02	2.27E+03	2.42E+02	1.05E+02
SE Slope	1.376	0.0009600	0.03411	0.02389
SE Int.	n.a.	0.0006174	0.06445	0.04514
Isotherm Parameters				
Kd	11.83 +/- 1.38	n.a.	n.a.	n.a.
k	n.a.	2.596 +/- 0.124	n.a.	n.a.
b	n.a.	21.29 +/- 0.43	n.a.	n.a.
K	n.a.	n.a.	19.52 +/- 0.06	n.a.
N	n.a.	n.a.	0.8132 +/- 0.0341	n.a.
KD	n.a.	n.a.	n.a.	0.5960 +/- 0.0454
B	n.a.	n.a.	n.a.	0.8699 +/- 0.0239
Equivalent Isotherm Parameters				
Kd	11.83	55.24	16.29	25.63
KD	0.2751	2.596	0.3787	0.5960
B	1.0	1.0	0.8132	0.8699
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-1.40	-1.35	-1.30	-1.23
Keq	1.06E+01	9.79E+00	8.93E+00	7.91E+00

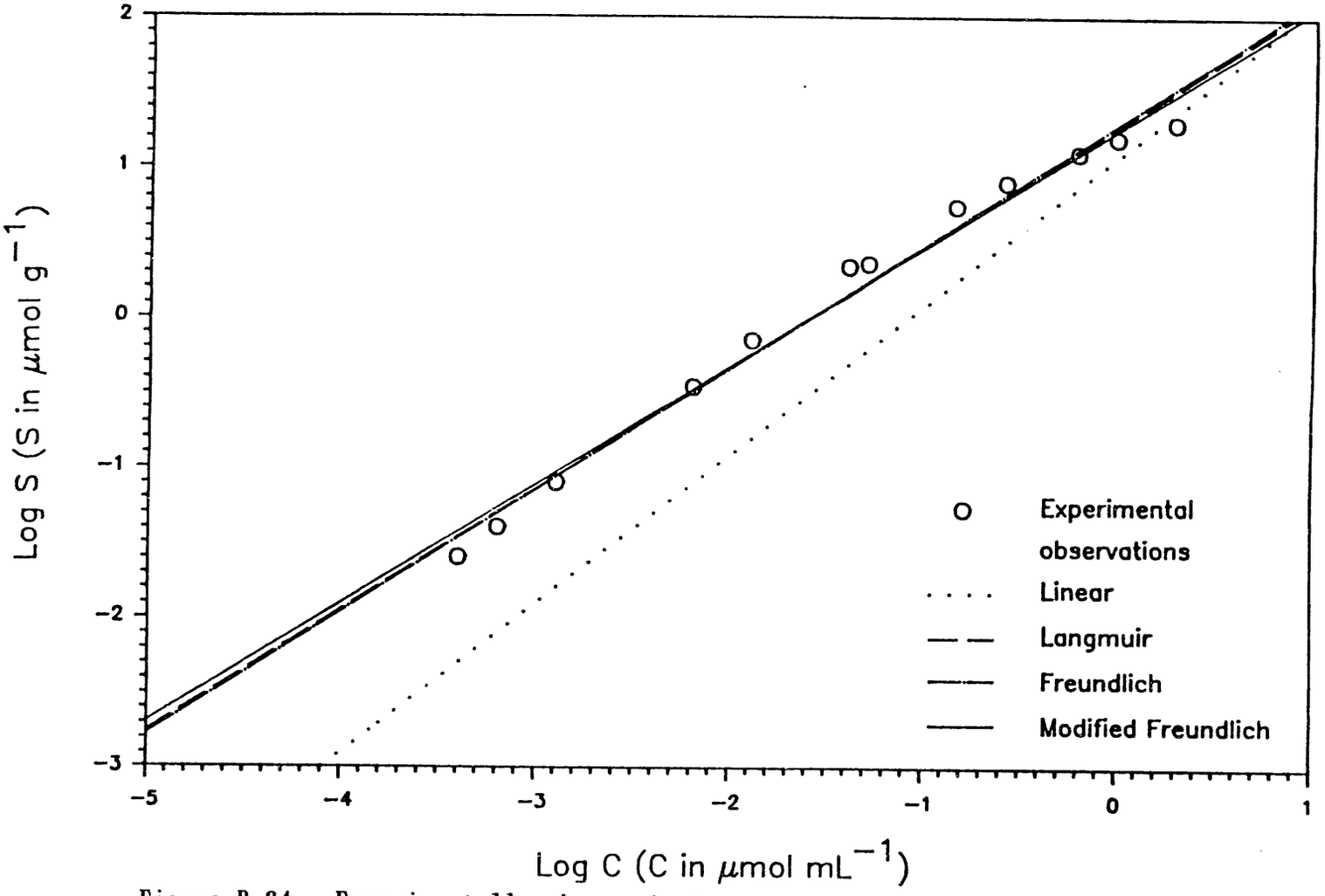

Figure B.34. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 2.

TABLE B.XXXV

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Ba 21 air - 75 amb 14.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9976	0.9349	0.9979	.9988
C.V.	11.01	16.57	-5.525	2.173
SSE	3.47E-02	2.31E+01	8.20E-02	2.26E+03
SE Slope	9.795	0.02521	0.02263	0.01799
SE Int.	n.a.	0.0001073	0.09518	0.07566
Isotherm Parameters				
Kd	401.1 +/- 9.8	n.a.	n.a.	n.a.
k	n.a.	175.3 +/- 40.2	n.a.	n.a.
b	n.a.	6.046 +/- 0.921	n.a.	n.a.
K	n.a.	n.a.	211.5 +/- 0.1	n.a.
N	n.a.	n.a.	0.8478 +/- 0.0226	n.a.
KD	n.a.	n.a.	n.a.	34.98 +/- 0.26
B	n.a.	n.a.	n.a.	0.8877 +/- 0.0180
Equivalent Isotherm Parameters				
Kd	401.1	1060.0	344.4	489.7
KD	28.65	175.3	24.60	34.98
B	1.0	1.0	0.8478	0.8877
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-4.47	-4.85	-5.45	-6.50
Keq	1.88E+03	3.57E+03	9.89E+03	5.86E+04

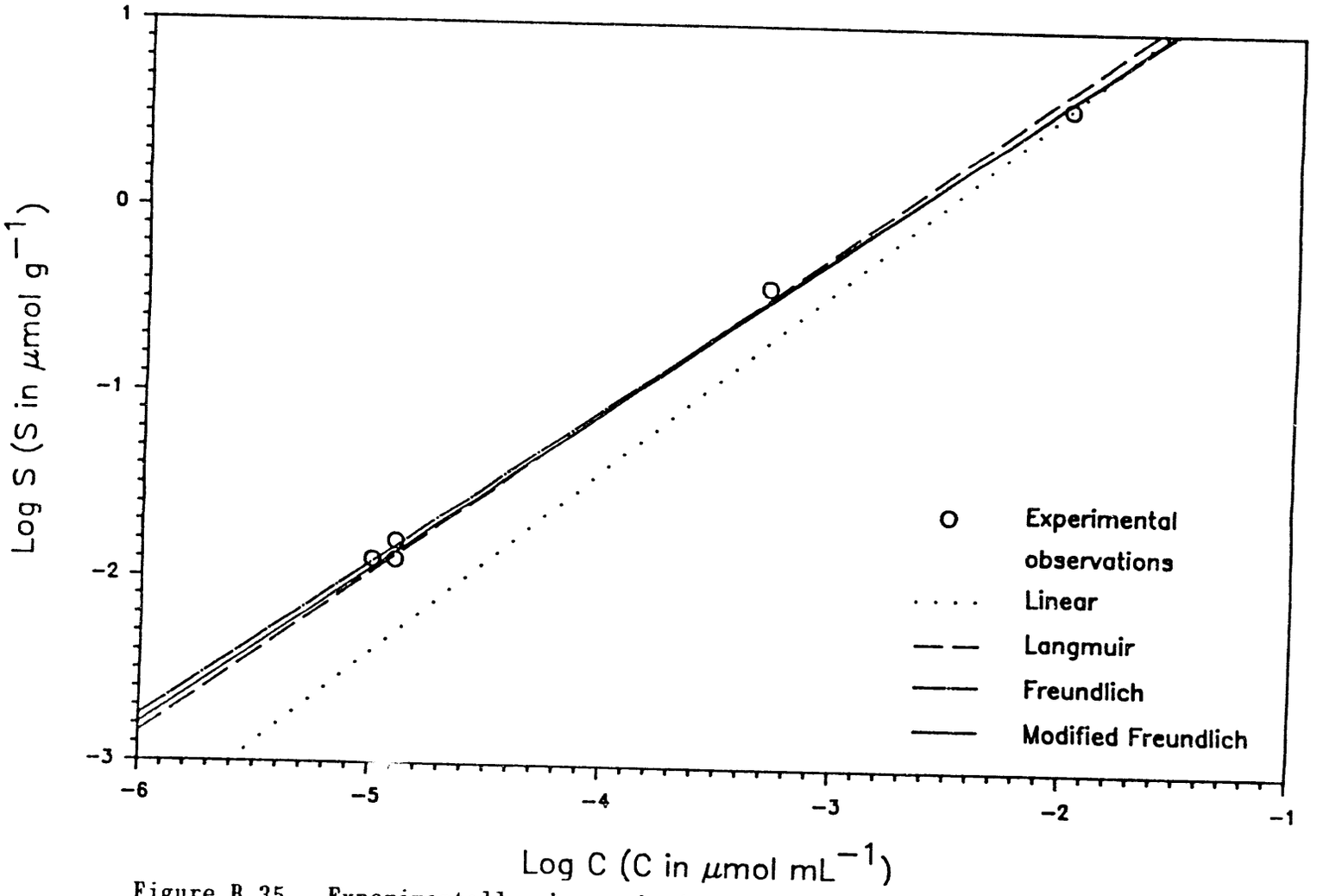

Figure B.35. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Ba 21 air -75 amb 14.0.

TABLE B.XXXVI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Ba 21 air 75-500 amb 8.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9971	0.9576	0.9974	0.9990
C.V.	12.25	14.92	-6.006	-2.329
SSE	4.08E-02	1.76E+01	1.37E-01	3.65E+03
SE Slope	5.933	0.02186	0.02452	0.01683
SE Int.	n.a.	0.0001664	0.09796	0.06721
Isotherm Parameters				
Kd	218.2 +/- 5.9	n.a.	n.a.	n.a.
k	n.a.	115.5 +/- 22.6	n.a.	n.a.
b	n.a.	5.558 +/- 0.675	n.a.	n.a.
K	n.a.	n.a.	123.1 +/- 0.1	n.a.
N	n.a.	n.a.	0.8370 +/- 0.0245	n.a.
KD	n.a.	n.a.	n.a.	48.52 +/- 0.24
B	n.a.	n.a.	n.a.	0.9149 +/- 0.0168
Equivalent Isotherm Parameters				
Kd	218.3	642.2	209.6	388.2
KD	27.28	115.5	26.20	48.52
B	1.0	1.0	0.8370	0.9149
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-4.31	-4.75	-5.44	-6.64
Keq	1.44E+03	3.04E+03	9.80E+03	7.33E+04

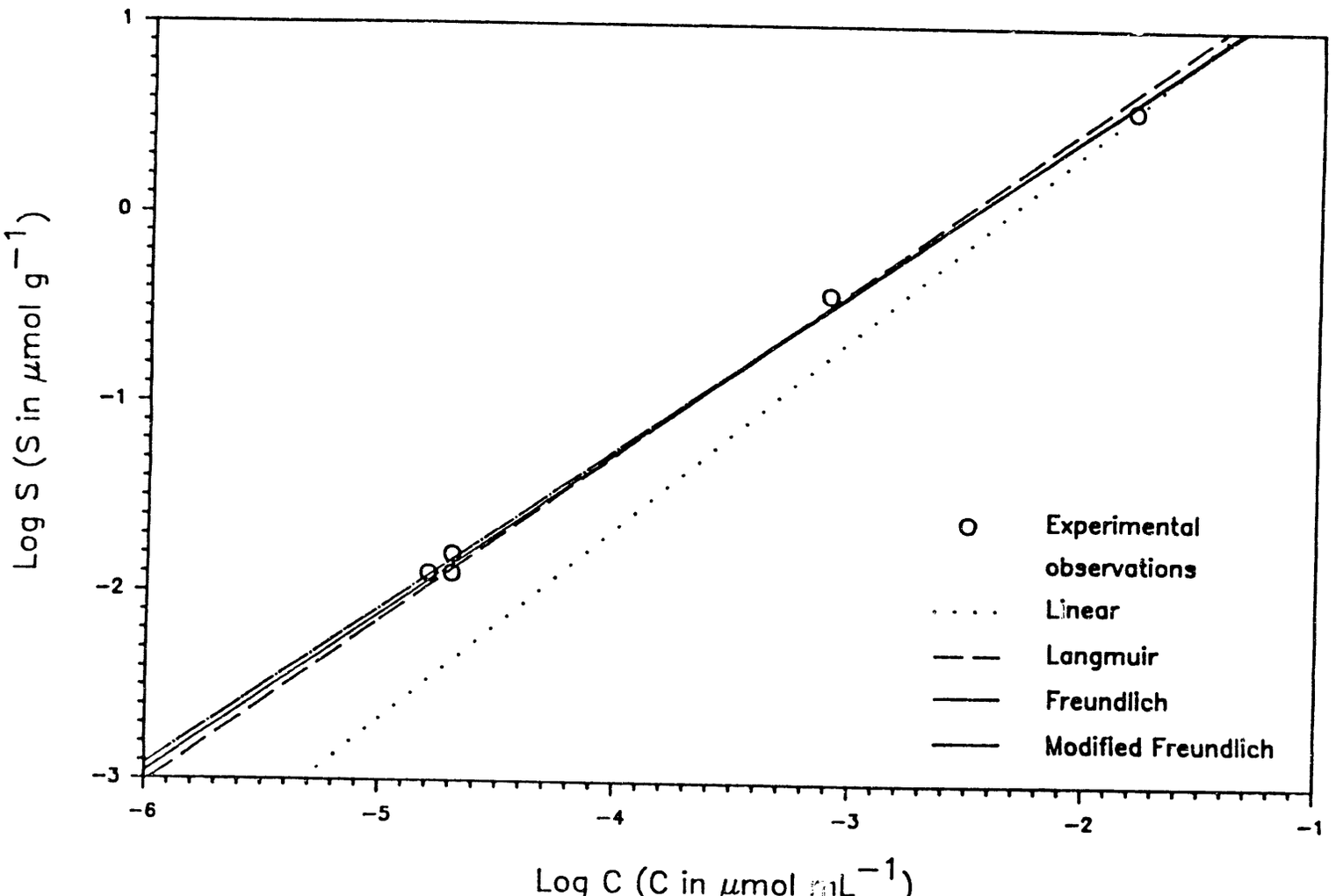

Figure B.36. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Ba 21 air 75-500 amb 8.0.

TABLE B.XXXVII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Cs 21 air - 75 amb 14.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9999	0.9738	0.9925	0.9927
C.V.	2.003	16.93	-7.262	-5.235
SSE	9.43E-06	2.75E-02	1.12E-02	1.84E+01
SE Slope	0.6566	0.2468	0.05483	0.05417
SE Int.	n.a.	0.0003332	0.3296	0.3256
Isotherm Parameters				
Kd	129.6 +/- 0.7	n.a.	n.a.	n.a.
k	n.a.	1083.0 +/- 269.3	n.a.	n.a.
b	n.a.	0.4697 +/- 0.0545	n.a.	n.a.
K	n.a.	n.a.	88.16 +/- 0.33	n.a.
N	n.a.	n.a.	0.8902 +/- 0.0548	n.a.
KD	n.a.	n.a.	n.a.	8.159 +/- 0.780
B	n.a.	n.a.	n.a.	0.8923 +/- 0.0542
Equivalent Isotherm Parameters				
Kd	129.6	508.7	110.6	114.2
KD	9.260	1083.0	7.901	8.159
B	1.0	1.0	0.8902	0.8923
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-2.16	-2.33	-2.61	-3.10
Keq	3.83E+01	5.14E+01	8.25E+01	1.89E+02

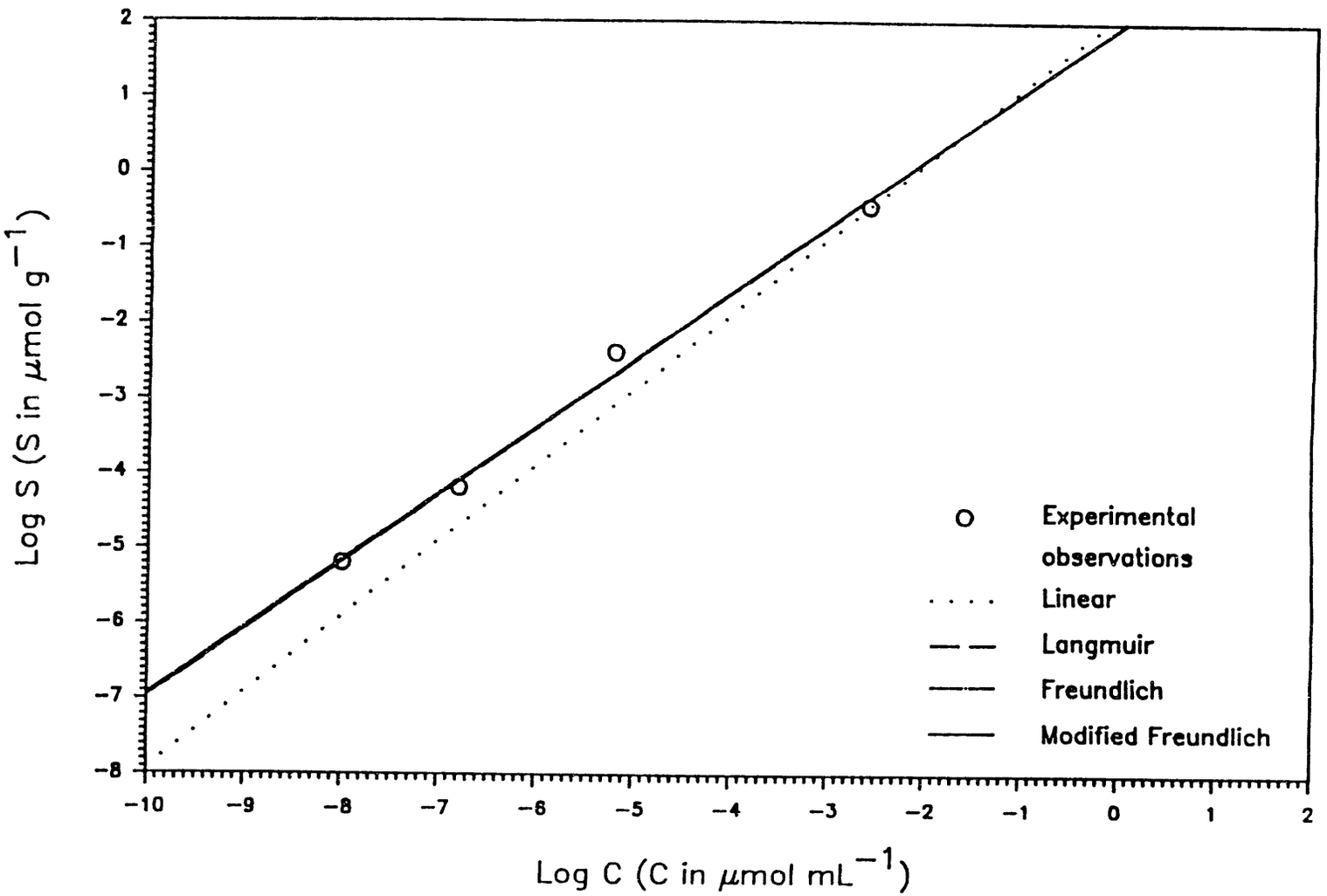

Figure B.37. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM 22 Cs 21 air -75 amb 14.0.

TABLE B.XXXVIII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Cs 21 air 75-500 amb 8.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	1.0000	0.9187	0.9985	0.9986
C.V.	1.454	30.62	-3.179	-2.402
SSE	4.69E-06	2.81E-02	5.03E-04	1.15E+01
SE Slope	0.4032	0.4609	0.02319	0.02260
SE Int.	n.a.	0.0007144	0.1389	0.1354
Isotherm Parameters				
Kd	109.7 +/- 0.4	n.a.	n.a.	n.a.
k	n.a.	941.0 +/- 424.1	n.a.	n.a.
b	n.a.	0.4562 +/- 0.0959	n.a.	n.a.
K	n.a.	n.a.	51.13 +/- 0.14	n.a.
N	n.a.	n.a.	0.8568 +/- 0.0232	n.a.
KD	n.a.	n.a.	n.a.	9.192 +/- 0.351
B	n.a.	n.a.	n.a.	0.8601 +/- 0.0226
Equivalent Isotherm Parameters				
Kd	109.7	429.3	69.71	73.53
KD	13.71	941.0	8.714	9.192
B	1.0	1.0	0.8568	0.8601
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-2.05	-2.26	-2.57	-3.12
Keq	3.20E+01	4.50E+01	7.68E+01	1.93E+02

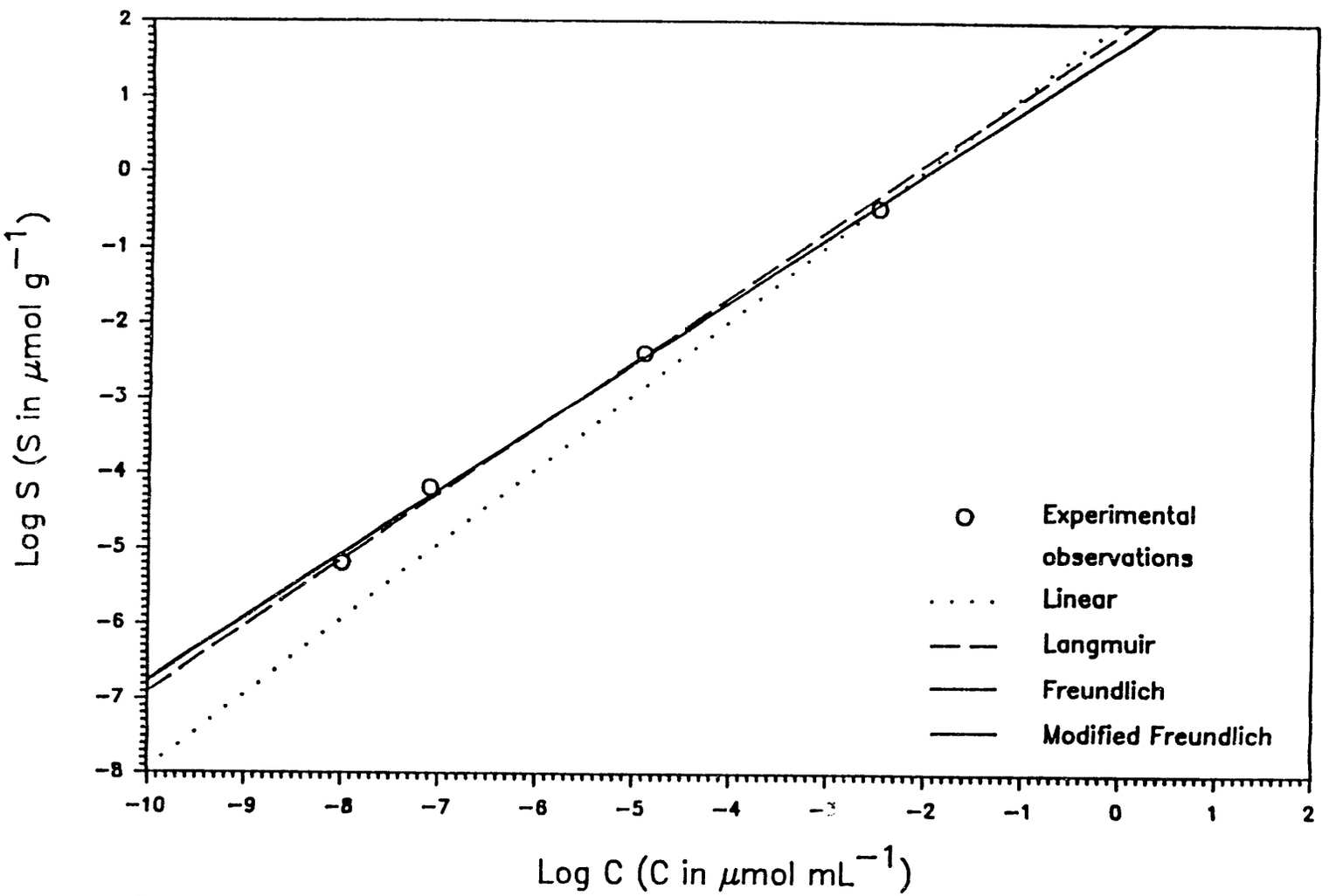

Figure B.38. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Cs 21 air 75-500 amb 8.0.

TABLE B.XXXIX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Eu 21 air - 75 amb 14.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.3770	0.6141	0.9297	0.9283
C.V.	144.7	63.79	-26.90	-16.42
SSE	2.00E-01	2.88E-01	2.13E-01	2.10E+01
SE Slope	967.2	2.089	0.1888	0.1916
SE Int.	n.a.	0.0002787	0.9750	0.9893
Isotherm Parameters				
Kd	1303.0 +/- 967.2	n.a.	n.a.	n.a.
k	n.a.	10770.0 +/- 13390.0	n.a.	n.a.
b	n.a.	0.2683 +/- 0.1504	n.a.	n.a.
K	n.a.	n.a.	1408.0 +/- 1.0	n.a.
N	n.a.	n.a.	0.9710 +/- 0.1888	n.a.
KD	n.a.	n.a.	n.a.	120.3 +/- 5.0
B	n.a.	n.a.	n.a.	0.9750 +/- 0.1916
Equivalent Isotherm Parameters				
Kd	1303.0	2890.0	1616.0	1684.0
KD	93.09	10770.0	115.4	120.3
B	1.0	1.0	0.9710	0.9750
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-6.48	-7.01	-7.85	-9.32
Keq	5.66E+04	1.37E+05	5.69E+05	6.83E+06

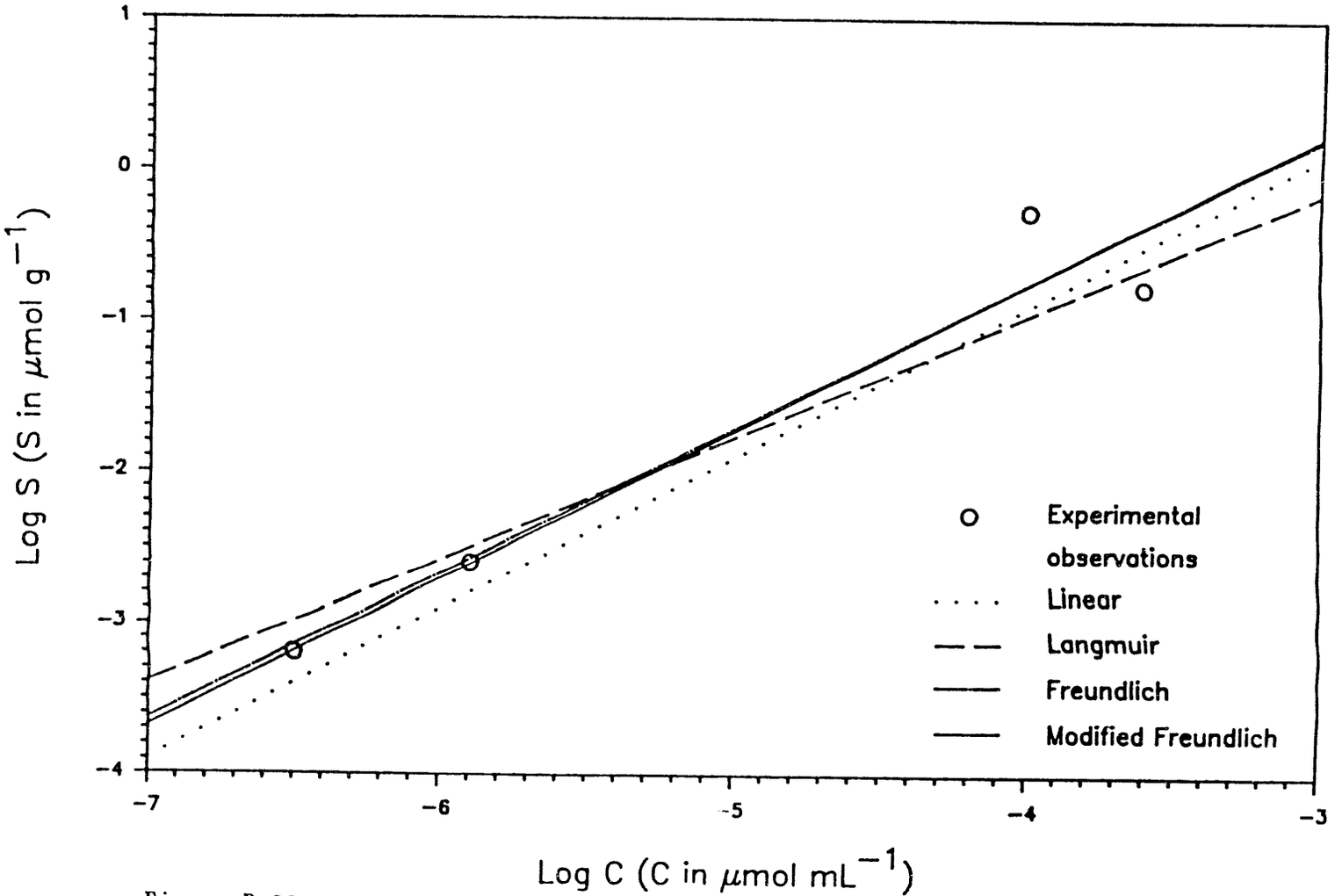

Figure B.39. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Eu 21 air -75 amb 14.0.

TABLE B.XXXX

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Eu 21 air 75-500 amb 8.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9994	0.7883	0.9997	0.9997
C.V.	4.825	16.85	-1.517	-1.018
SSE	1.89E-04	1.14E-02	4.81E-05	2.86E+01
SE Slope	13.69	0.2621	0.009673	0.009228
SE Int.	n.a.	0.00005895	0.05351	0.05105
Isotherm Parameters				
Kd	1113.0 +/- 13.7	n.a.	n.a.	n.a.
k	n.a.	1633.0 +/- 607.5	n.a.	n.a.
b	n.a.	1.141 +/- 0.342	n.a.	n.a.
K	n.a.	n.a.	612.8 +/- 0.1	n.a.
N	n.a.	n.a.	0.9215 +/- 0.0097	n.a.
KD	n.a.	n.a.	n.a.	119.4 +/- 0.3
B	n.a.	n.a.	n.a.	0.9282 +/- 0.0092
Equivalent Isotherm Parameters				
Kd	1113.0	1863.0	886.9	955.5
KD	139.1	1633.0	110.9	119.4
B	1.0	1.0	0.9215	0.9282
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-5.95	-6.51	-7.40	-8.93
Keq	2.30E+04	5.94E+04	3.52E+06	1.04E+10

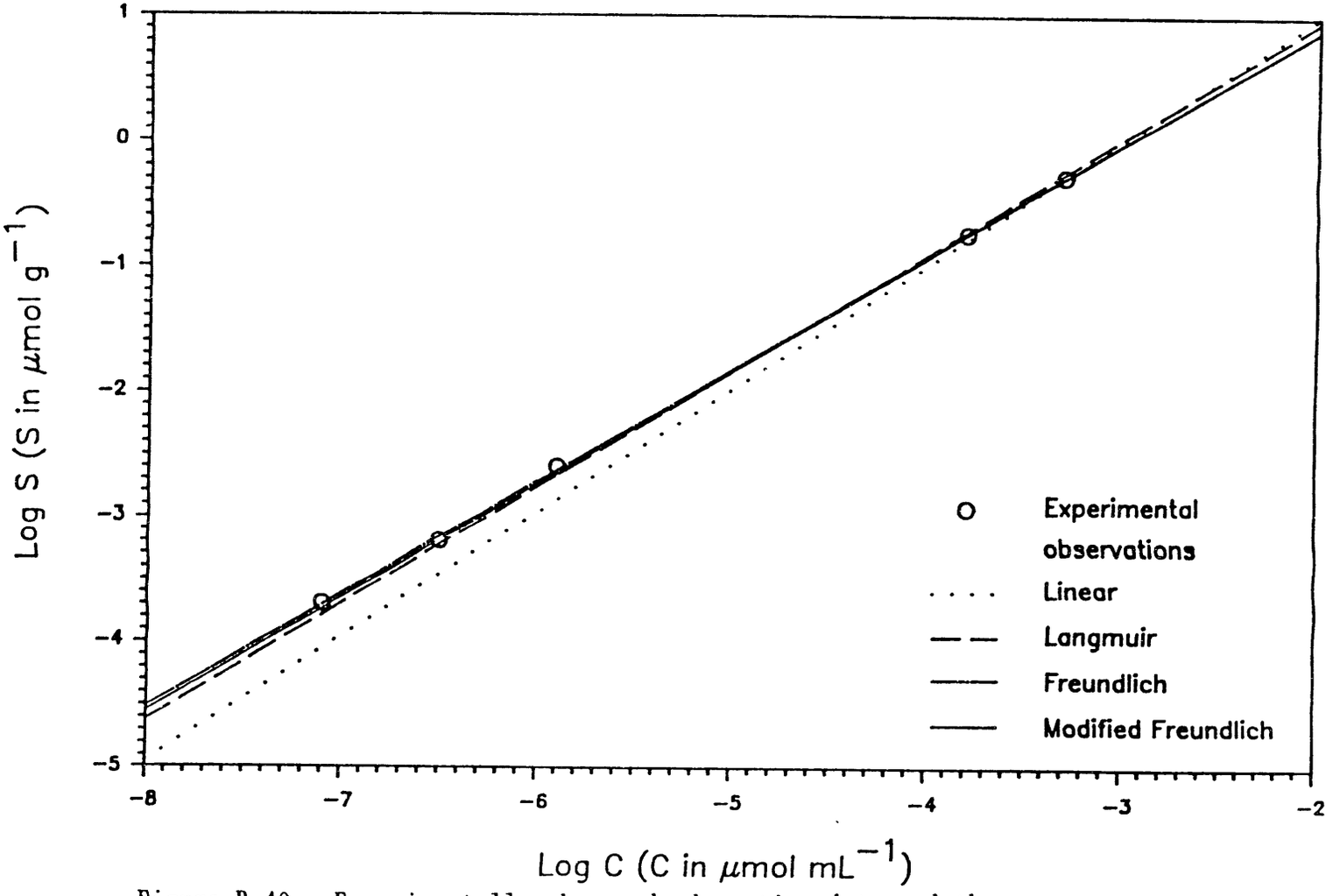

Figure B.40. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Eu 21 air 75-500 amb 8.0.

TABLE B.XXXXI

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Sr 21 air - 75 amb 14.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9999	0.7320	0.9983	0.9983
C.V.	1.732	10.06	-3.230	-1.785
SSE	4.90E-05	5.20E+00	5.69E-05	7.02E+01
SE Slope	0.2524	0.1115	0.02731	0.02801
SE Int.	n.a.	0.0008923	0.08876	0.09105
Isotherm Parameters				
Kd	55.01 +/- 0.25	n.a.	n.a.	n.a.
k	n.a.	18.58 +/- 8.63	n.a.	n.a.
b	n.a.	3.838 +/- 1.642	n.a.	n.a.
K	n.a.	n.a.	41.74 +/- 0.09	n.a.
N	n.a.	n.a.	0.9353 +/- 0.0273	n.a.
KD	n.a.	n.a.	n.a.	3.609 +/- 0.140
B	n.a.	n.a.	n.a.	0.9505 +/- 0.0280
Equivalent Isotherm Parameters				
Kd	55.01	71.32	45.02	50.53
KD	3.929	18.58	3.216	3.609
B	1.0	1.0	0.9353	0.9505
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-3.12	-3.23	-3.43	-3.81
Keq	1.94E+02	2.34E+02	3.28E+02	6.24+02

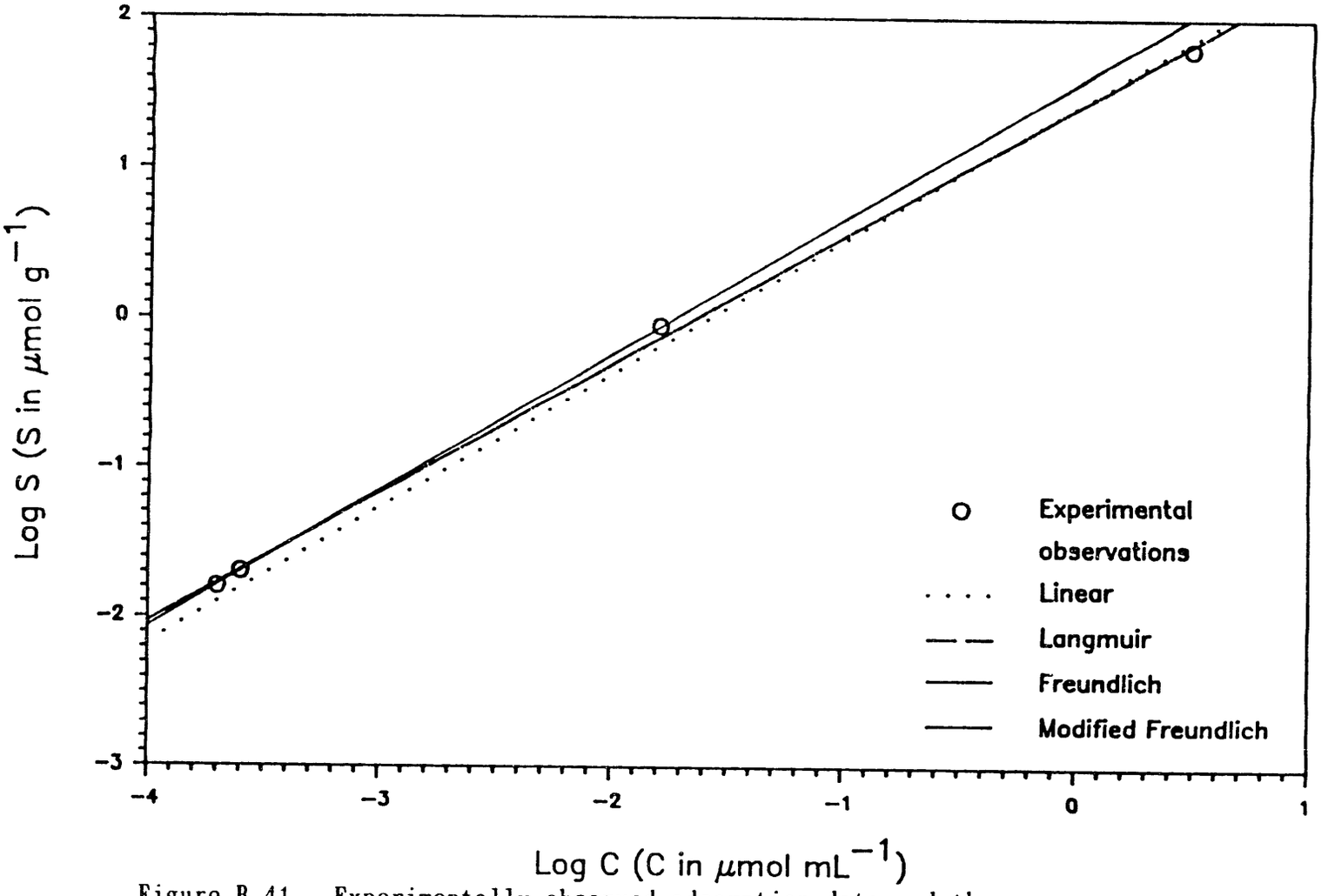

Figure B.41. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM-22 Sr 21 air -75 amb 14.0.

TABLE B.XXXXII

STATISTICAL, ISOTHERM, EQUIVALENT ISOTHERM, AND THERMODYNAMIC PARAMETERS ESTIMATED FROM THE REGRESSION OF ADSORPTION DATA FOR ISOTHERM MODELS

ym-22 Sr 21 air 75-500 amb 8.0

	Linear	Langmuir	Freundlich	Modified Freundlich
Statistical Parameters				
R2	0.9996	0.5830	0.9936	0.9937
C.V.	2.389	17.60	-6.262	-3.816
SSE	9.33E-05	2.84E+00	1.24E-04	7.73E+01
SE Slope	0.3485	0.0008439	0.05211	0.05309
SE Int.	n.a.	0.001547	0.1704	0.1736
Isotherm Parameters				
Kd	55 01 +/- 0.35	n.a.	n.a.	n.a.
k	n.a.	23.7 +/- 15.7	n.a.	n.a.
b	n.a.	3.199 +/- 1.913	n.a.	n.a.
K	n.a.	n.a.	38.85 +/- 0.17	n.a.
N	n.a.	n.a.	0.9187 +/- 0.0521	n.a.
KD	n.a.	n.a.	n.a.	6.766 +/- 0.318
B	n.a.	n.a.	n.a.	0.9457 +/- 0.0531
Equivalent Isotherm Parameters				
Kd	55.01	75.81	44.68	54.13
KD	6.877	23.70	5.586	6.766
B	1.0	1.0	0.9187	0.9457
Thermodynamic Parameters				
zB	1.0	1.2	1.5	2.0
G	-3.14	-3.35	-3.69	-4.30
Keq	2.00E+02	2.86E+02	5.11E+02	1.42E+03

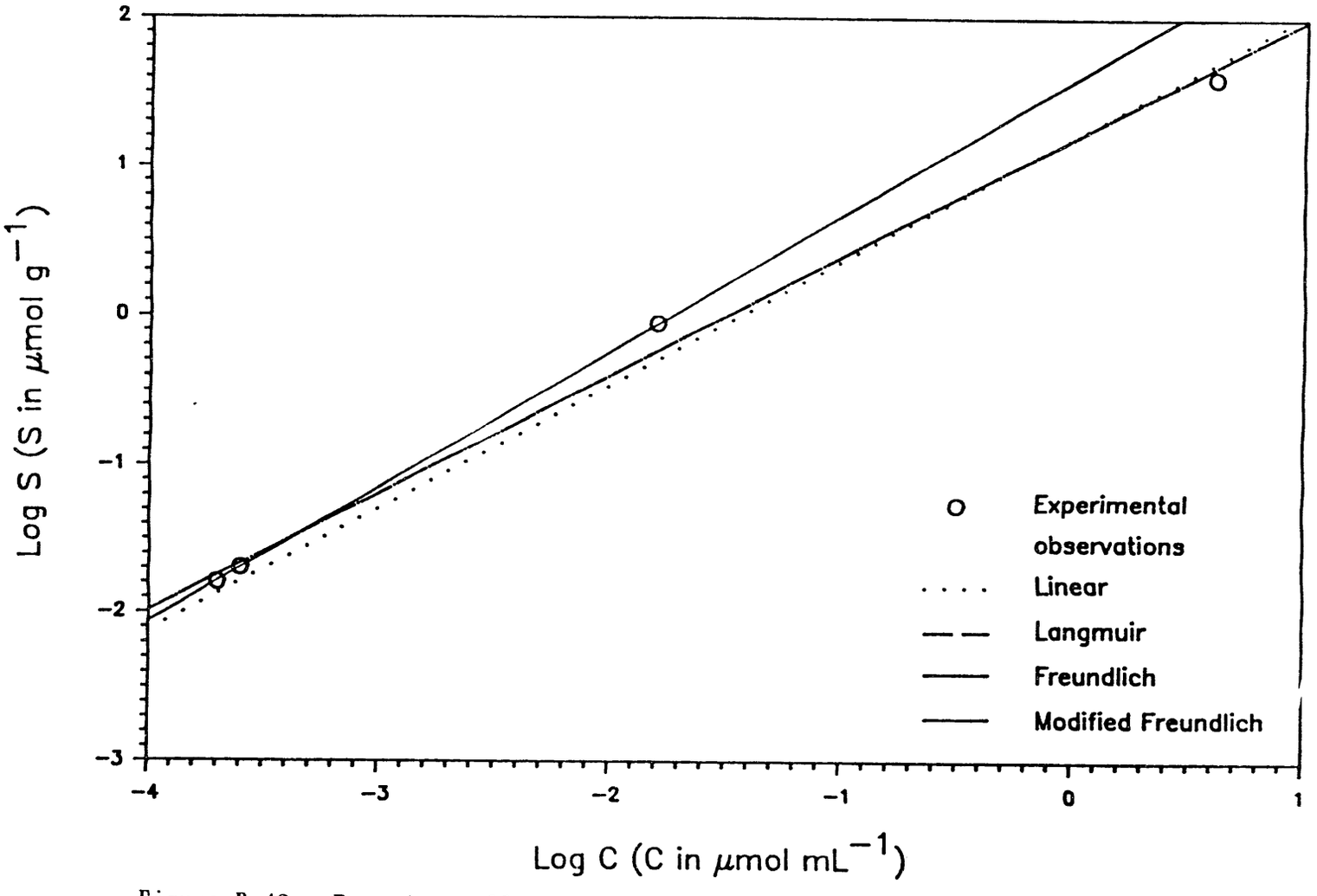

Figure B.42. Experimentally observed adsorption data and those predicted by regression according to the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models are plotted as log S versus log C for Data Set YM 22 Sr 21 air 75-500 amb 8.0.

Appendix C

Effect of Variables on the Modeling of Isotherms

Appendix C is a compilation of F-test data in tables for the statistical evaluation of the effect of replication, particle size, mineralogy, and hysteresis on the regression line, intercept, and slope of the Linear, Langmuir, Freundlich, and Modified Freundlich isotherm models. Plots are also presented which show the two data sets used to test the statistical significance of the variable at the 95% confidence level (CL), the regression line for each of the two data sets, and the regression line of the combined data sets. If the calculated F (F_c) is less than the tabulated F (F_t), then the parameter tested (regression line, slope or intercept) is the same for the two data sets (i.e., the variable has no effect on the parameter). If F_c is greater than F_t, then the parameter tested is different for the two data sets (i.e., the variable has a significant effect on the parameter).

A description of the data sets is given in a manner similar to that given in Appendix A. The sequence of the description is sample, element, reaction time, atmosphere, particle size, temperature, and CEC (e.g., gu 3-433 Np 42 CO_2 75-500 and 26.0). The abbreviation n.a. indicates not applicable. The conclusion as to whether the parameter for two data sets is the same or different is presented within parentheses. In all the figures, circles and triangles correspond to experimental data and the lines are the model predictions.

TABLE C.I

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS; ADSORPTION

g4-1608 Np 42 CO2 75-500 amb n.a. VERSUS g4-1608 Np CO2 75-500 amb n.a.

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.51<Ft=3.52 (Same)	Fc=0.40<Ft=3.52 (Same)	Fc=0.33<Ft=3.52 (Same)	n.a. n.a.
Intercept	n.a. n.a.	Fc=0.63<Ft=4.35 (Same)	Fc=0.64<Ft=4.35 (Same)	n.a. n.a.
Slope	Fc=0.00<Ft=4.35 (Same)	Fc=0.00<Ft=4.35 (Same)	Fc=0.27<Ft=4.35 (Same)	n.a. n.a.

gu3-433 Np 42 CO2 75-500 amb 26.0 VERSUS gu3-433 Np 42 CO2 75-500 amb 26.0

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=5.52>Ft=3.49 (Different)	Fc=0.48<Ft=3.49 (Same)	Fc=0.12<Ft=3.49 (Same)	Fc=0.12<Ft=3.49 (Same)
Intercept	n.a. n.a.	Fc=0.87<Ft=4.32 (Same)	Fc=-12.39<Ft=4.32 (Same)	Fc=0.08<Ft=4.32 (Same)
Slope	Fc=0.00<Ft=4.32 (Same)	Fc=0.00<Ft=4.32 (Same)	Fc=0.19<Ft=4.32 (Same)	Fc=0.19<Ft=4.32 (Same)

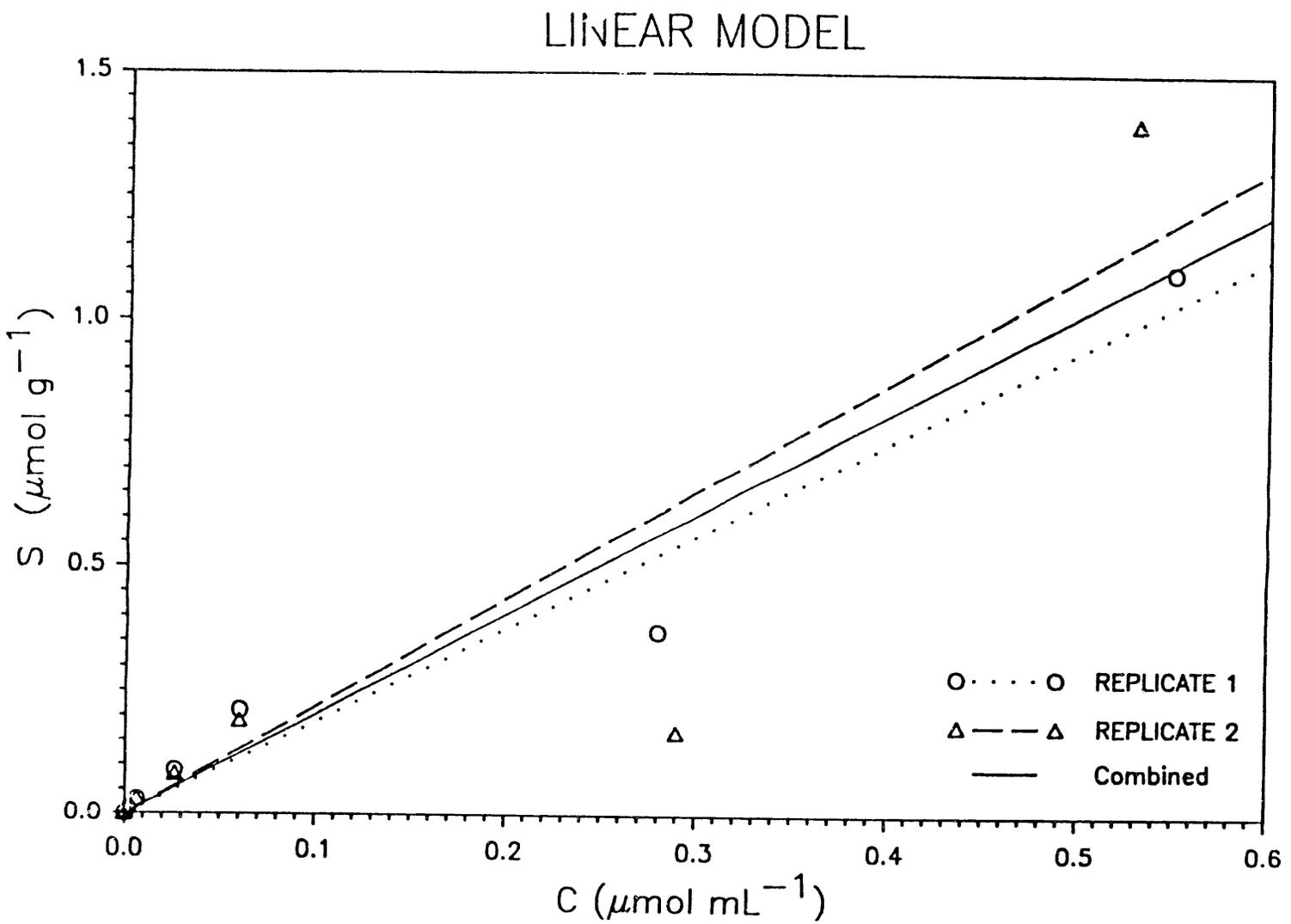

Figure C.1. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm models. The two data sets are G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 1 and G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 2; the variable being tested is replication.

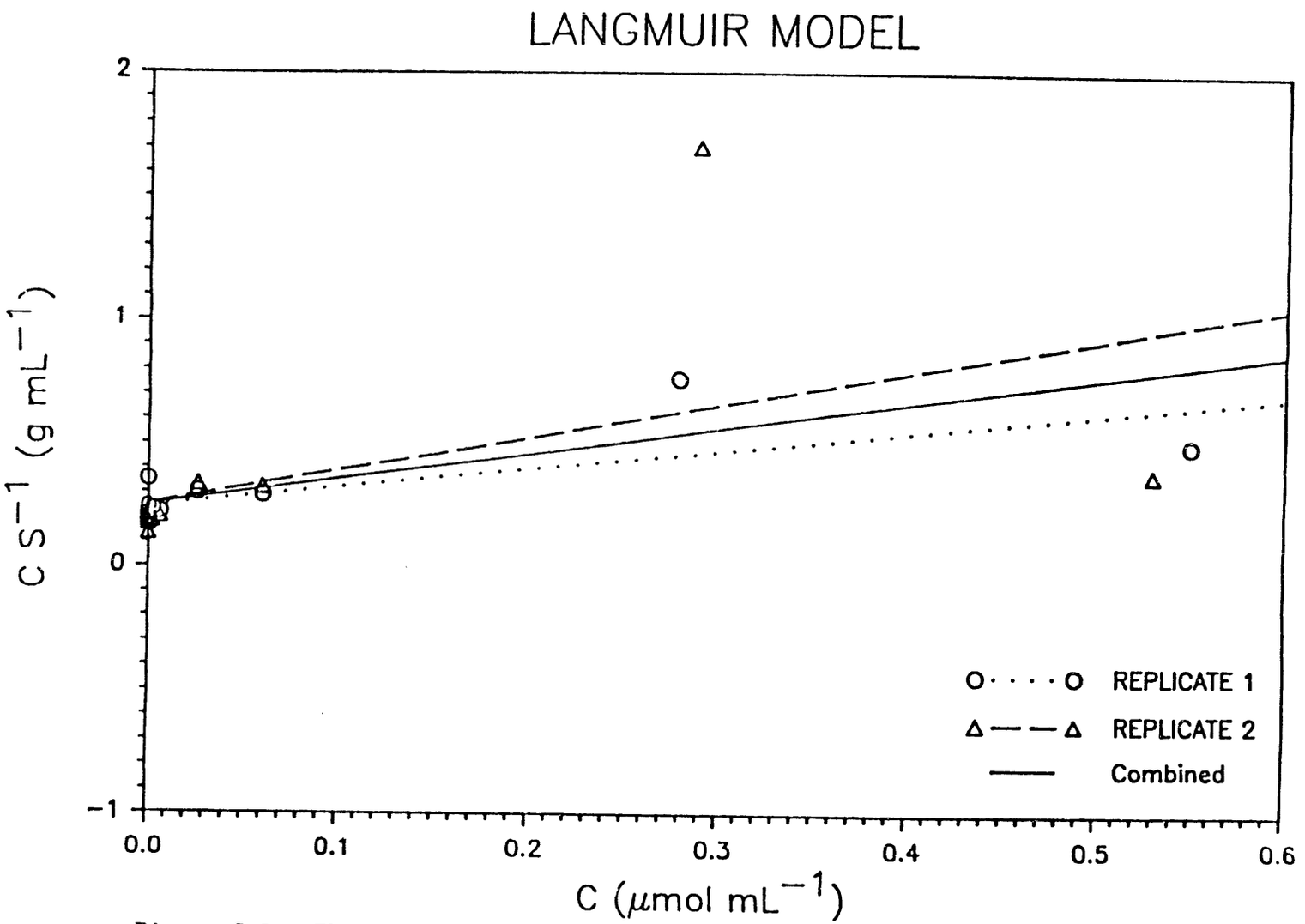

Figure C.2. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 1 and G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 2; the variable being tested is replication.

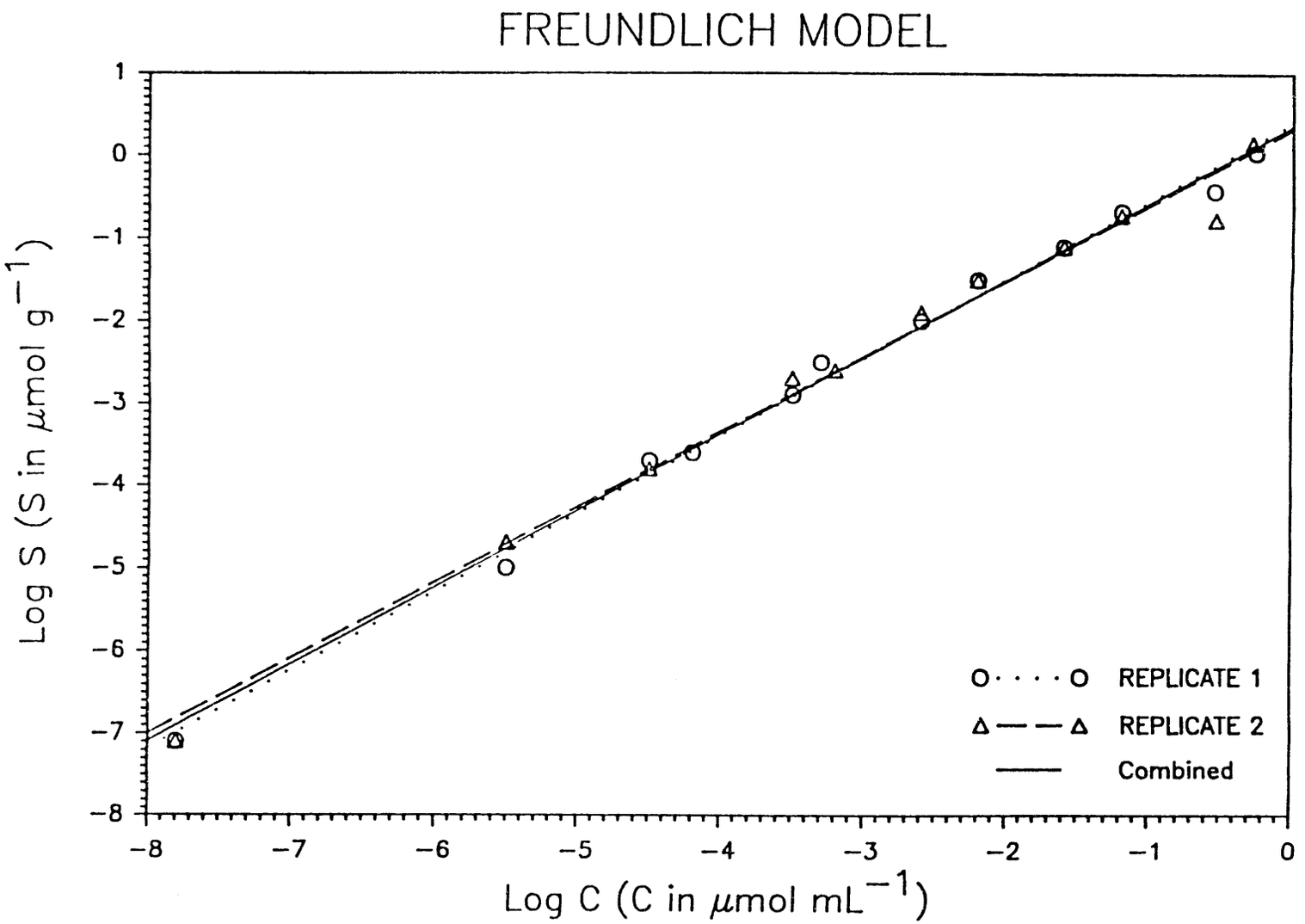

Figure C.3. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 1 and G4-1608 Np 42 CO2 75-500 amb n.a. Replicate 2; the variable being tested is replication.

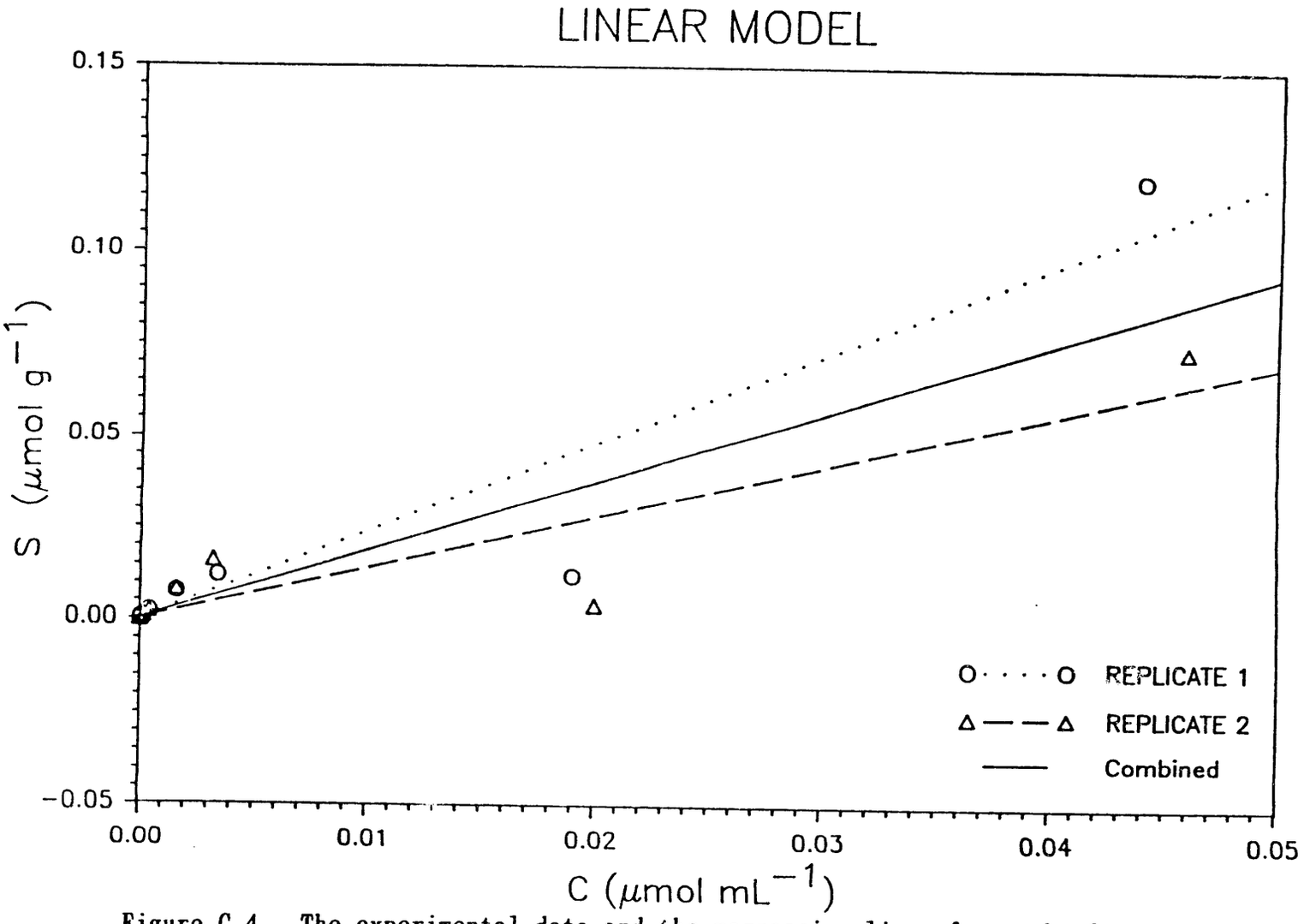

Figure C.4. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 1 and Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 2; the variable being tested is replication.

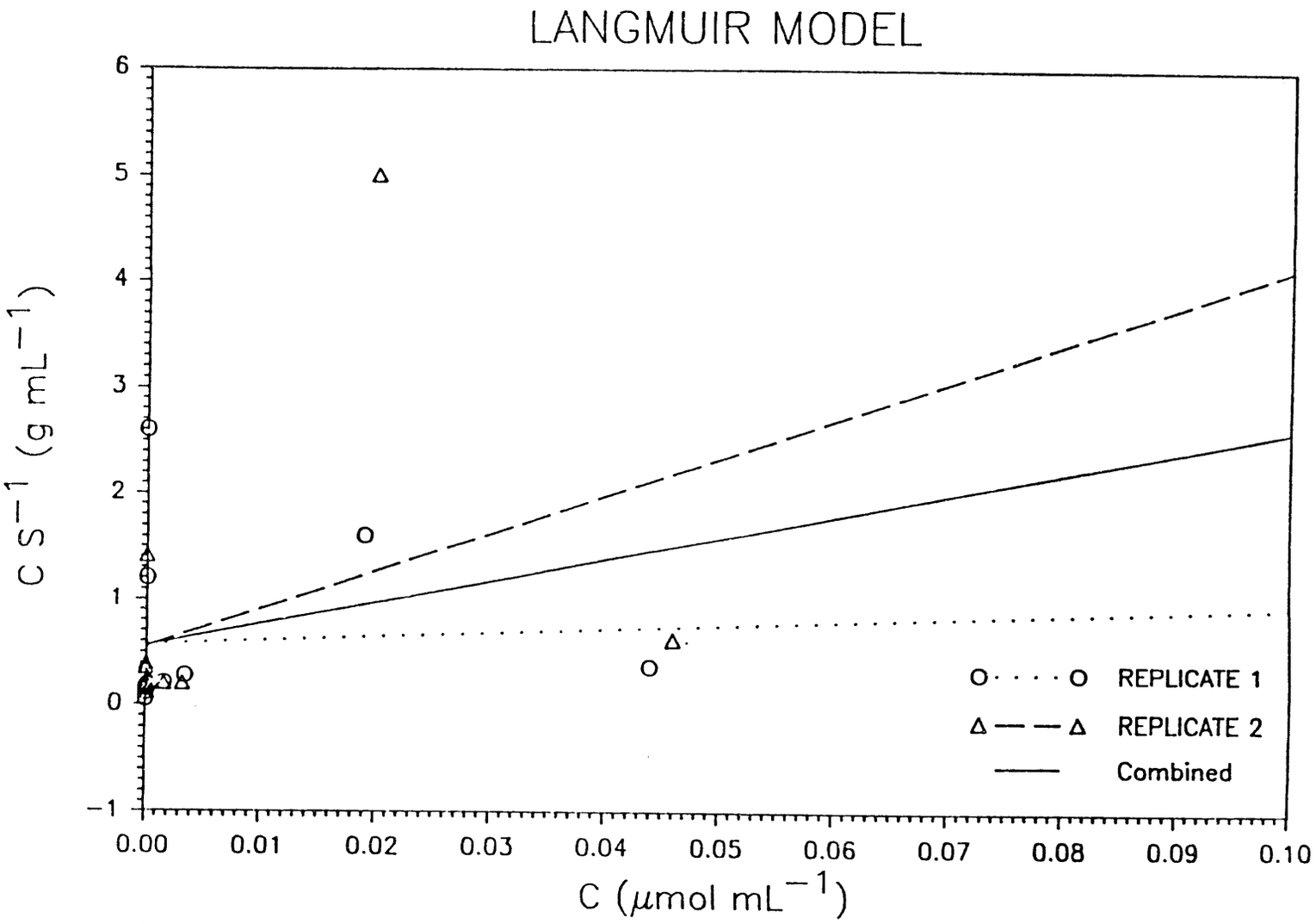

Figure C.5. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model The two data sets are Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 1 and Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 2; the variable being tested is replication.

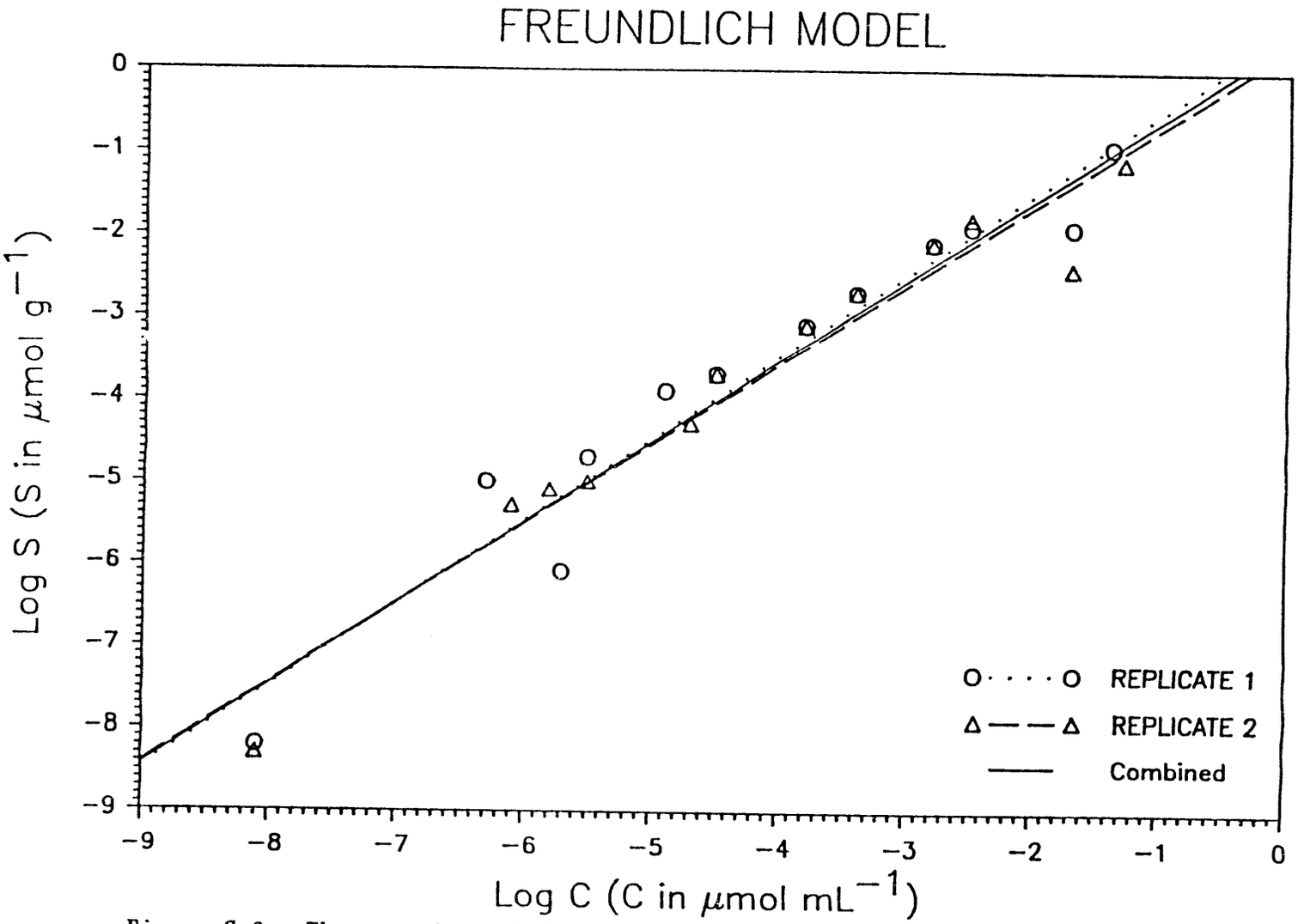

Figure C.6. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 1 and Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 2; the variable being tested is replication.

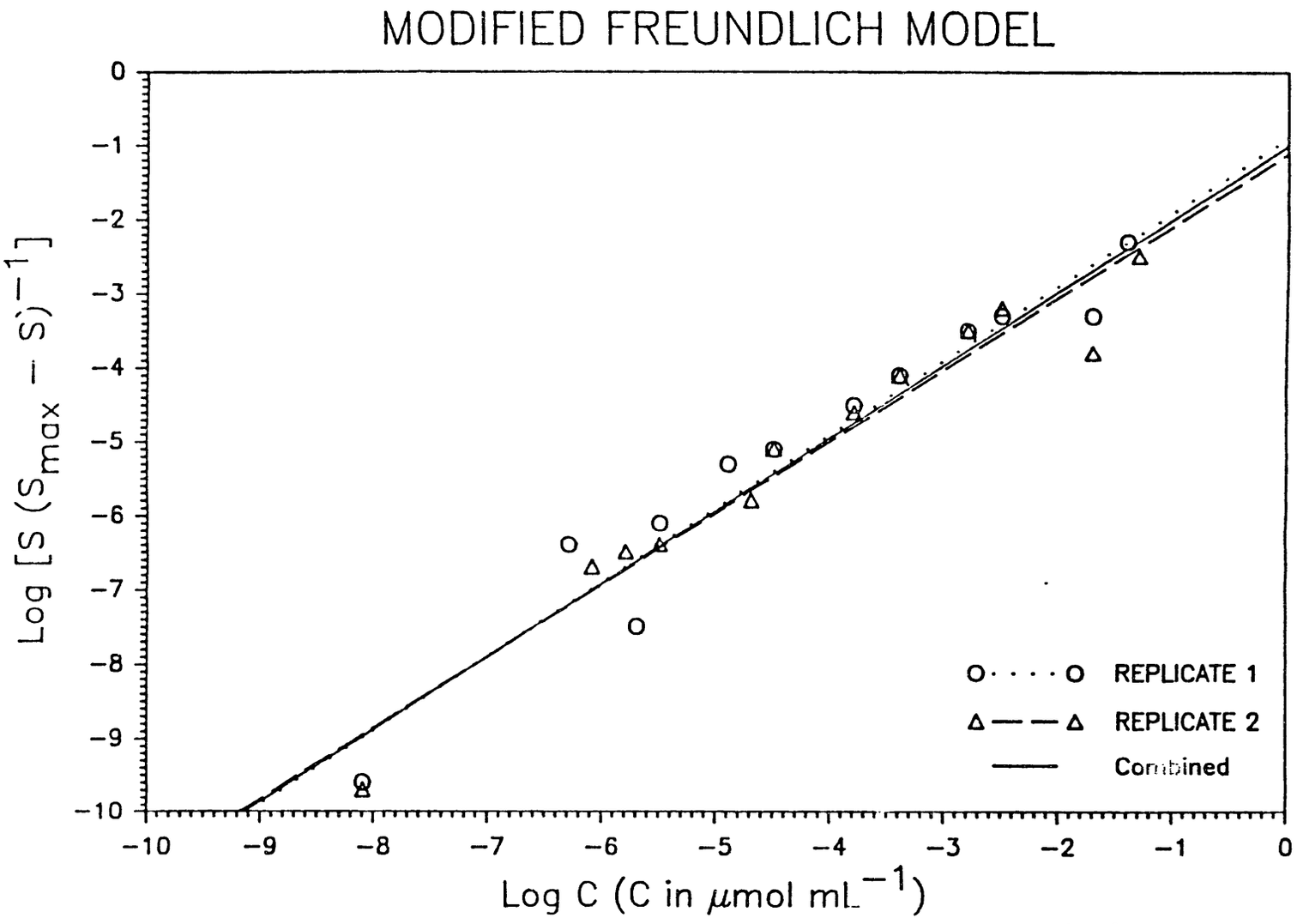

Figure C.7. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 1 and Gu3-433 Np 42 CO2 75-500 amb 26.0 Replicate 2; the variable being tested is replication.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS; ADSORPTION

ym-22 Ba 21 air - 75 amb 44.0 VERSUS ym-22 Ba 21 air 75-500 amb 58.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=91.58>Ft=5.14 (Different)	Fc=6.82>Ft=5.14 (Different)	Fc=11.57>Ft=5.14 (Different)	Fc=36.75>Fc=5.14 (Different)
Intercept	n.a. n.a.	Fc=0.31<Ft=5.59 (Same)	Fc=0.12<Ft=5.59 (Same)	Fc=0.24<Ft=5.59 (Same)
Slope	Fc=0.00<Ft=5.59 (Same)	Fc=11.51>Ft=5.59 (Different)	Fc=3.44<Ft=5.59 (Same)	Fc=10.11>Ft=5.59 (Different)

gl-2840 Cs 21 air 75-500 amb 430.0 VERSUS gl-2840 Cs 21 air 75-500 amb 430.0

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.92<Ft=3.52 (Same)	Fc=0.02<Ft=3.52 (Same)	Fc=0.24<Ft=3.52 (Same)	Fc=0.25<Ft=3.52 (Same)
Intercept	n.a. n.a.	Fc=0.01<Ft=4.35 (Same)	Fc=0.44<Ft=4.35 (Same)	Fc=0.44<Ft=4.35 (Same)
Slope	Fc=0.00<Ft=4.35 (Same)	Fc=0.03<Ft=4.35 (Same)	Fc=0.14<Ft=4.35 (Same)	Fc=0.14<Ft=4.35 (Same)

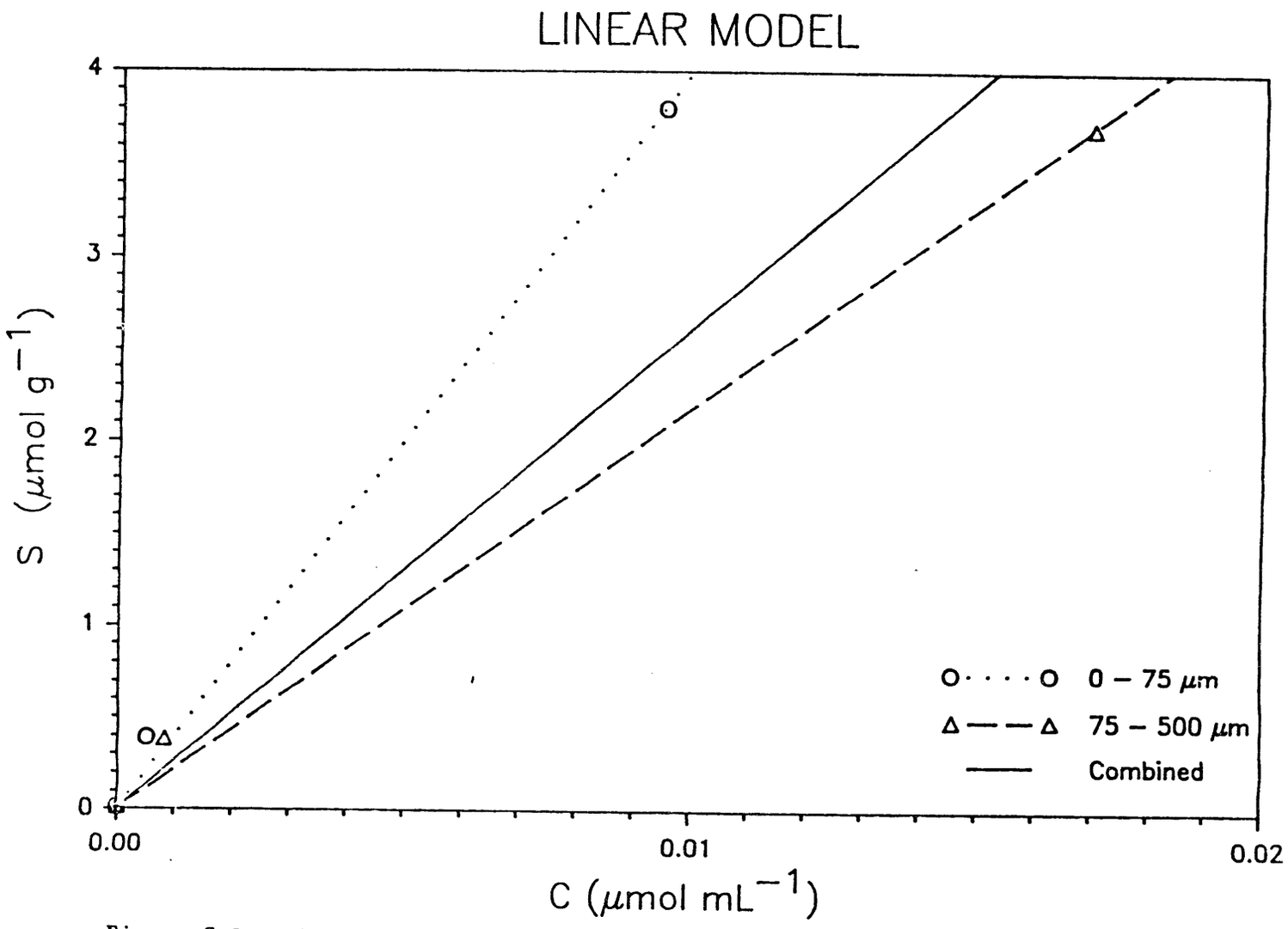

Figure C.8. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 44.0 and YM-22 Ba 21 air 75-500 amb 58.0; the variable being tested is particle size.

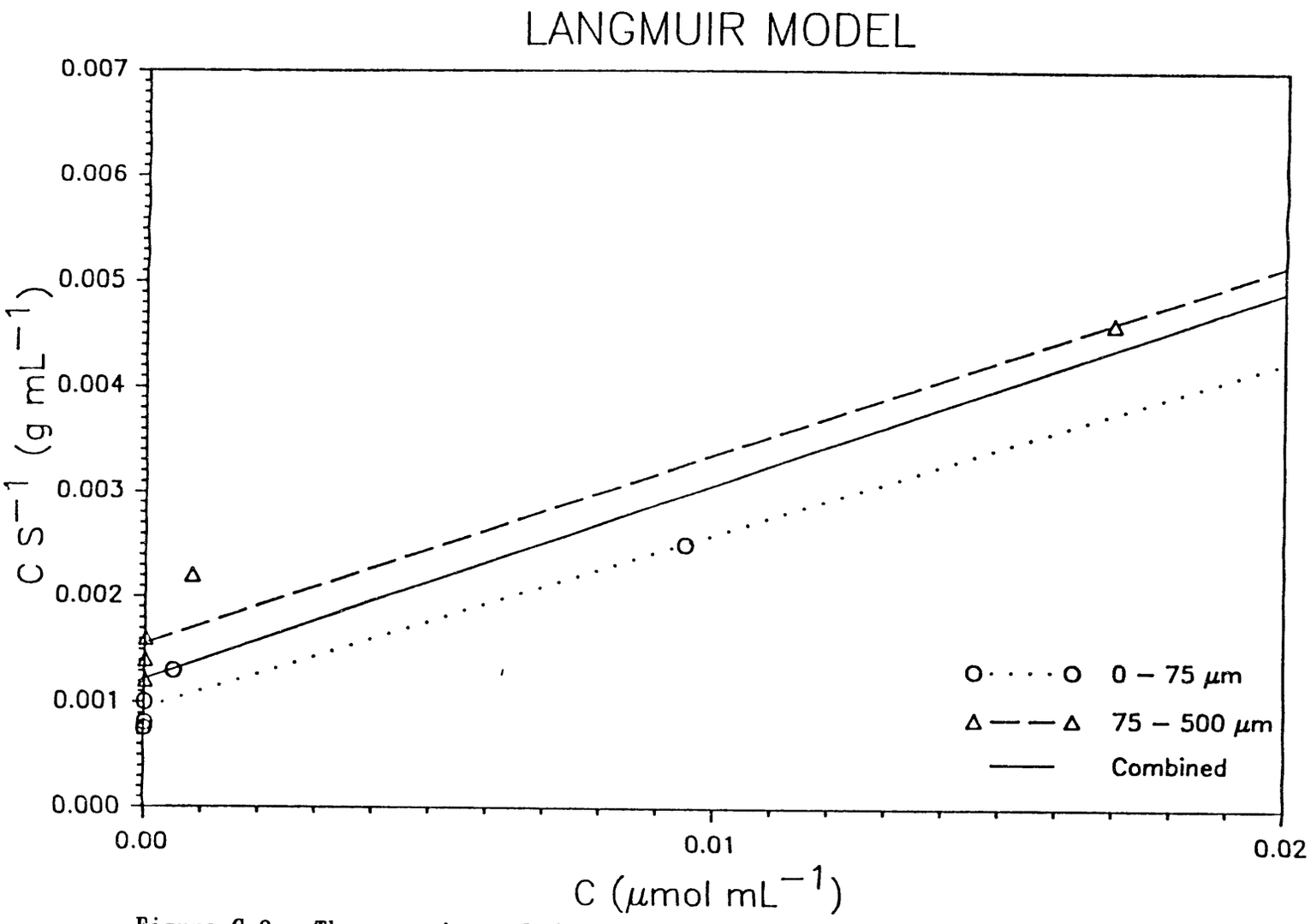

Figure C.9. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 44.0 and YM-22 Ba 21 air 75-500 amb 58.0; the variable being tested is particle size.

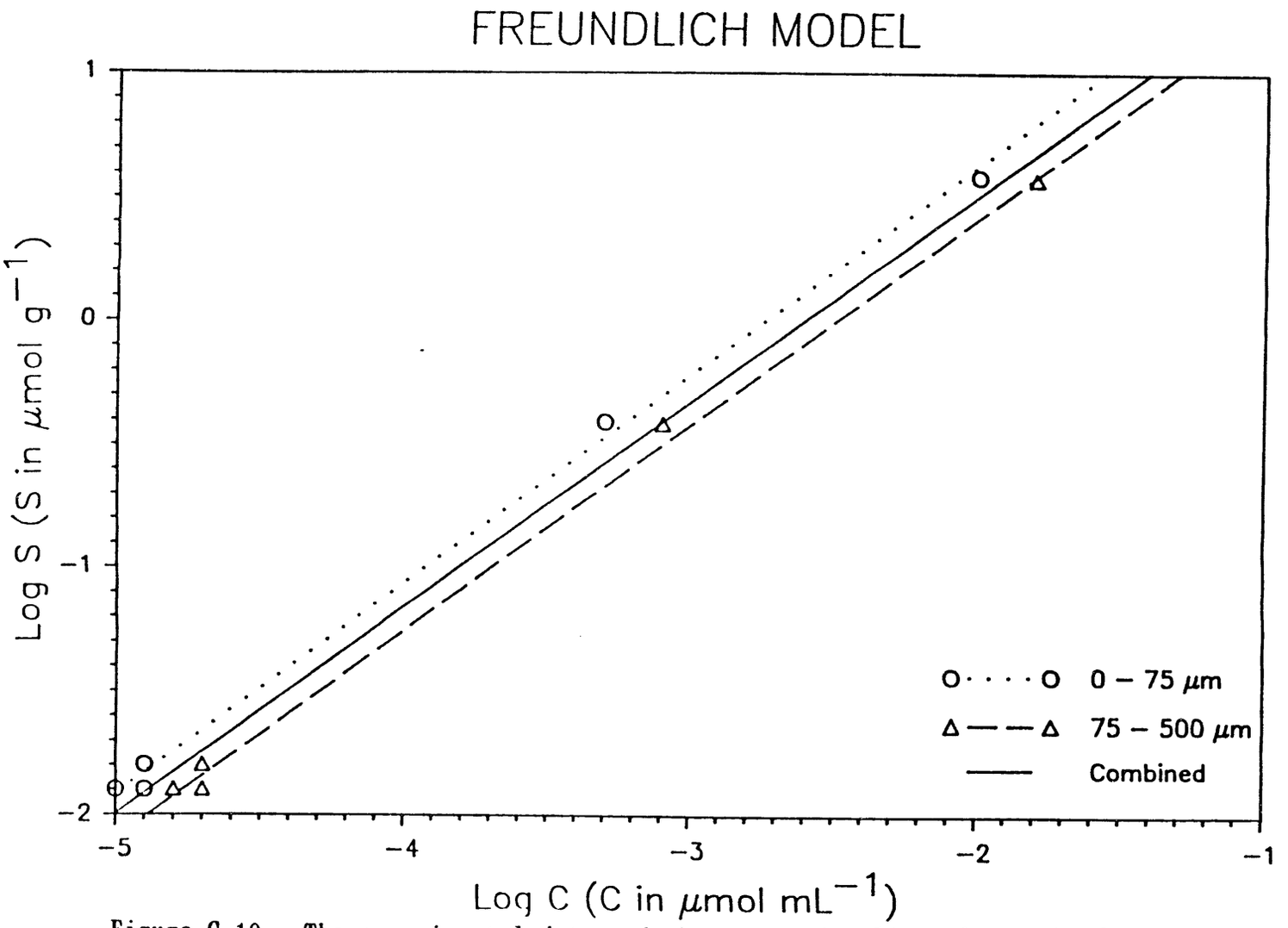

Figure C.10. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 44.0 and YM-22 Ba 21 air 75-500 amb 58.0; the variable being tested is particle size.

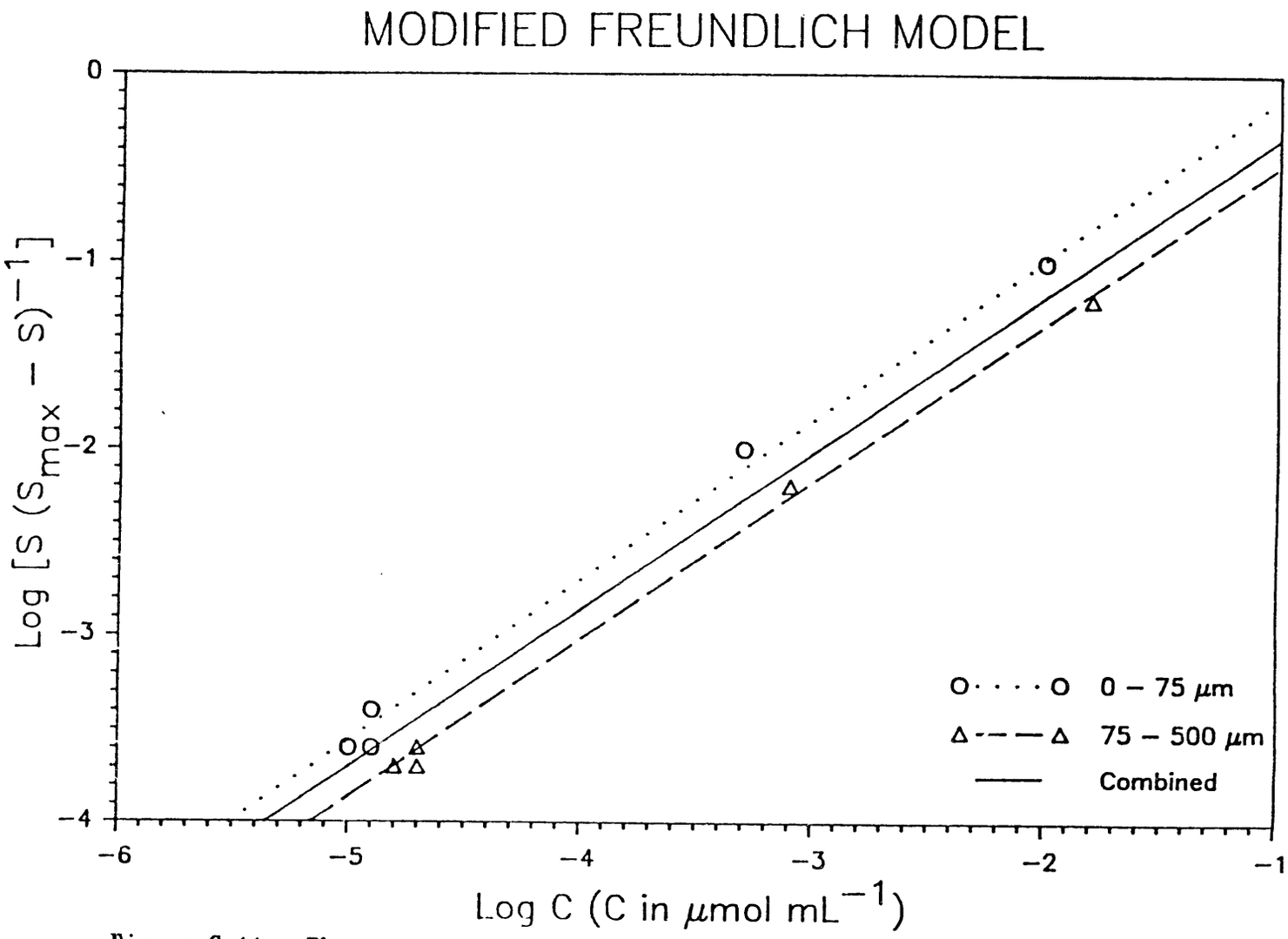

Figure C.11. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 44.0 and YM-22 Ba 21 air 75-500 amb 58.0; the variable being tested is particle size.

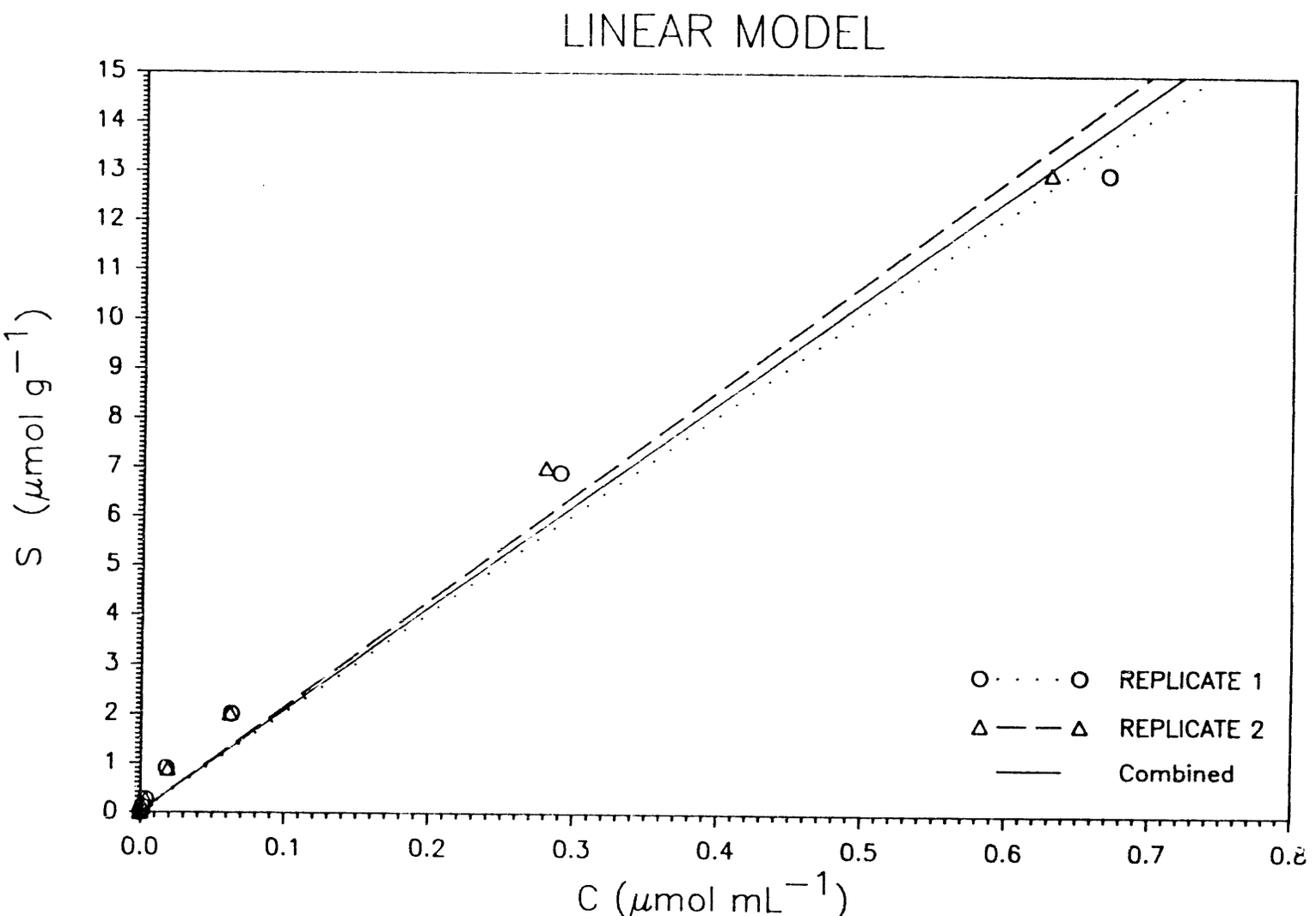

Figure C.12. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

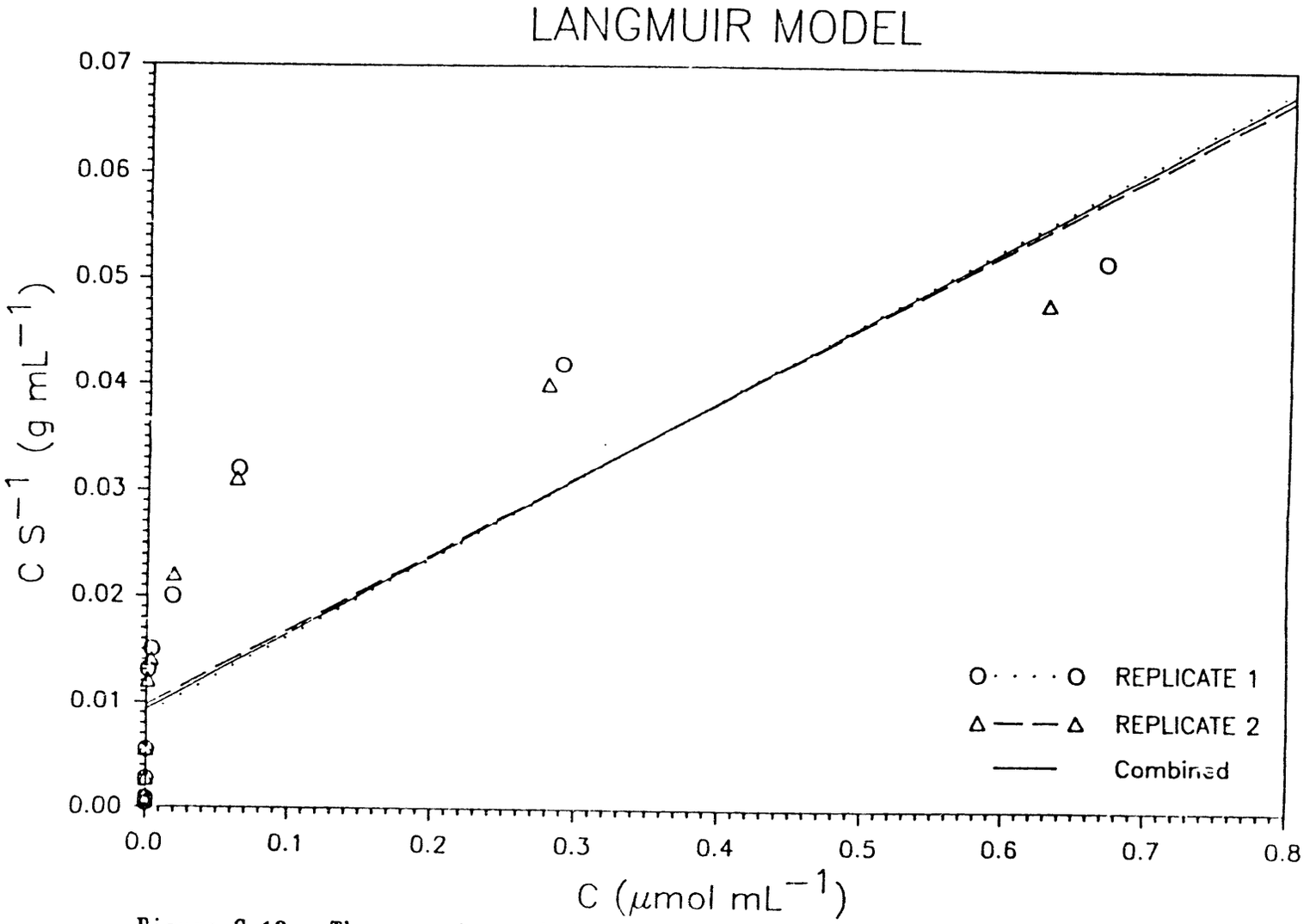

Figure C.13. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

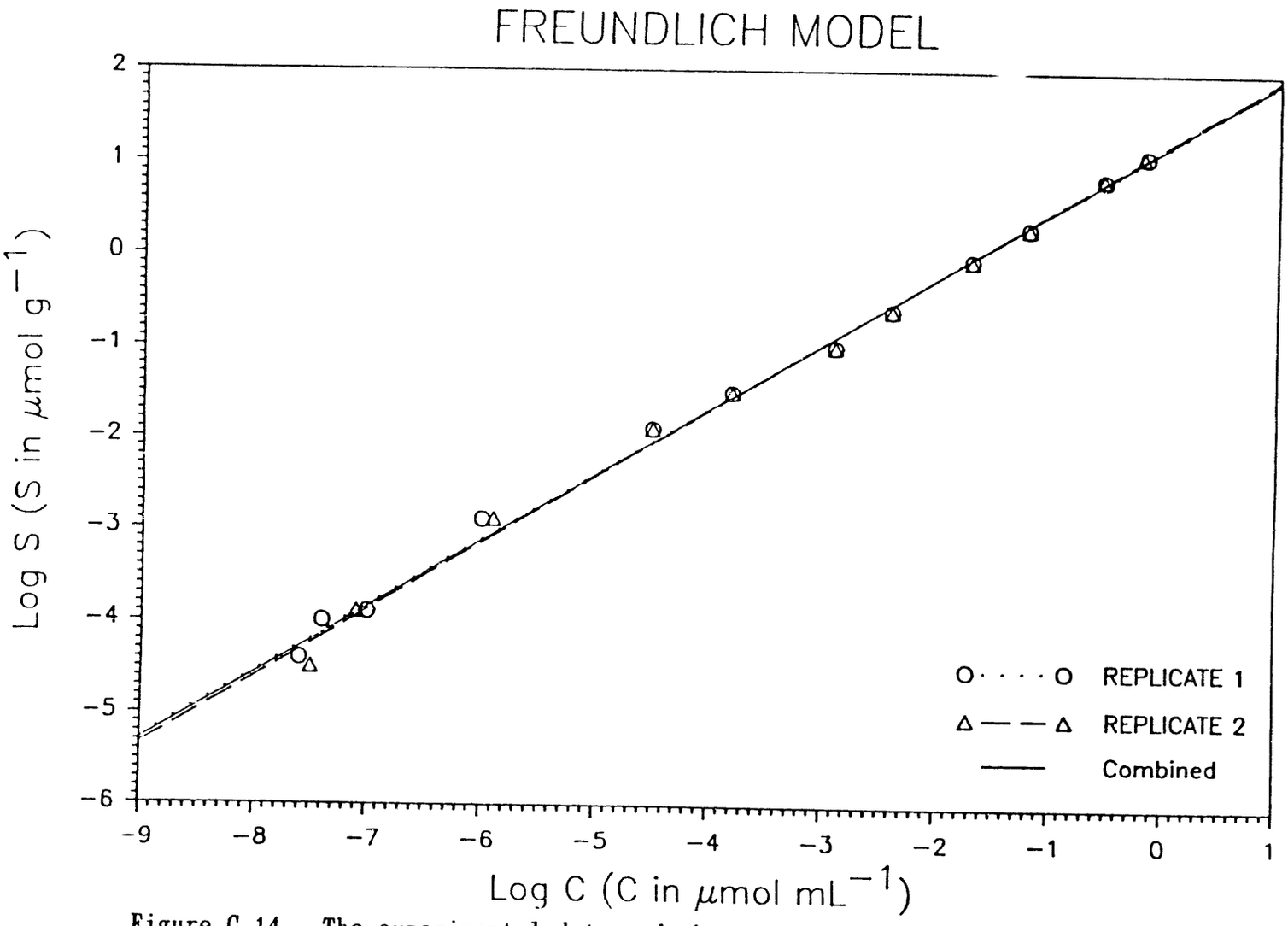

Figure C.14. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

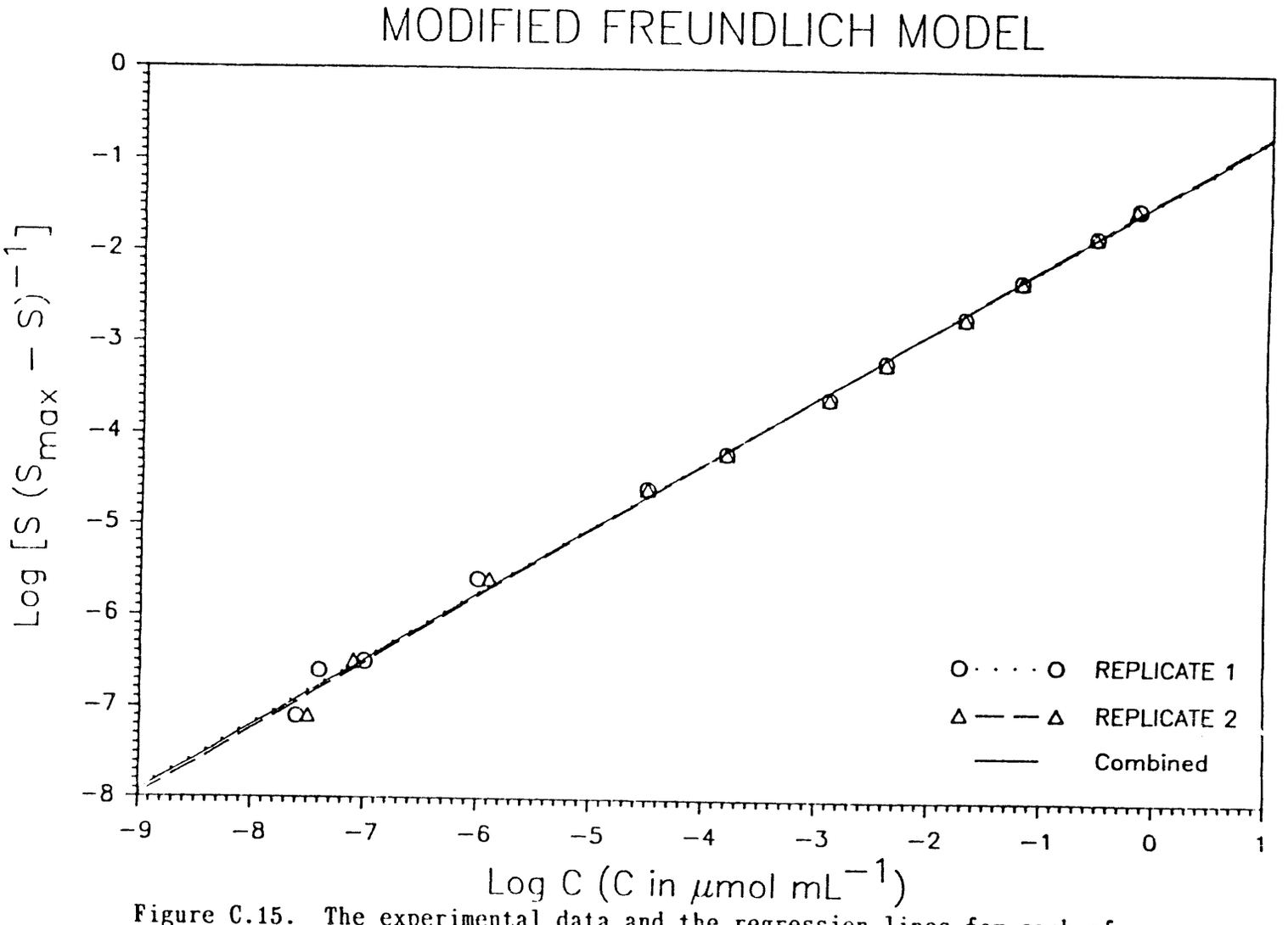

Figure C.15. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS; ADSORPTION

ym-22 Cs 21 air - 75 amb 44.0 VERSUS ym-22 Cs 21 air 75-500 amb 58.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=30.43>Ft=5.14 (Different)	Fc=4.54<Ft=5.14 (Same)	Fc=0.05<Ft=5.14 (Same)	Fc=0.73<Ft=5.14 (Same)
Intercept	n.a. n.a.	Fc=7.64>Ft=5.59 (Different)	Fc=0.05<Ft=5.59 (Same)	Fc=0.17<Ft=5.59 (Same)
Slope	Fc=0.00<Ft=5.59 (Same)	Fc=0.09<Ft=5.59 (Same)	Fc=0.11<Ft=5.59 (Same)	Fc=1.05<Ft=5.59 (Same)

ym-22 Eu 21 air - 75 amb 44.0 VERSUS ym-22 Eu 21 air 75-500 amb 58.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.03<Ft=5.79 (Same)	Fc=1.79<Ft=5.79 (Same)	Fc=0.20<Ft=5.79 (Same)	Fc=0.71<Ft=5.79 (Same)
Intercept	n.a. n.a.	Fc=4.05<Ft=5.99 (Same)	Fc=0.13<Ft=5.99 (Same)	Fc=0.13<Ft=5.99 (Same)
Slope	Fc=0.00<Ft=5.99 (Same)	Fc=0.75<Ft=5.99 (Same)	Fc=0.25<Ft=5.99 (Same)	Fc=0.45<Ft=5.99 (Same)

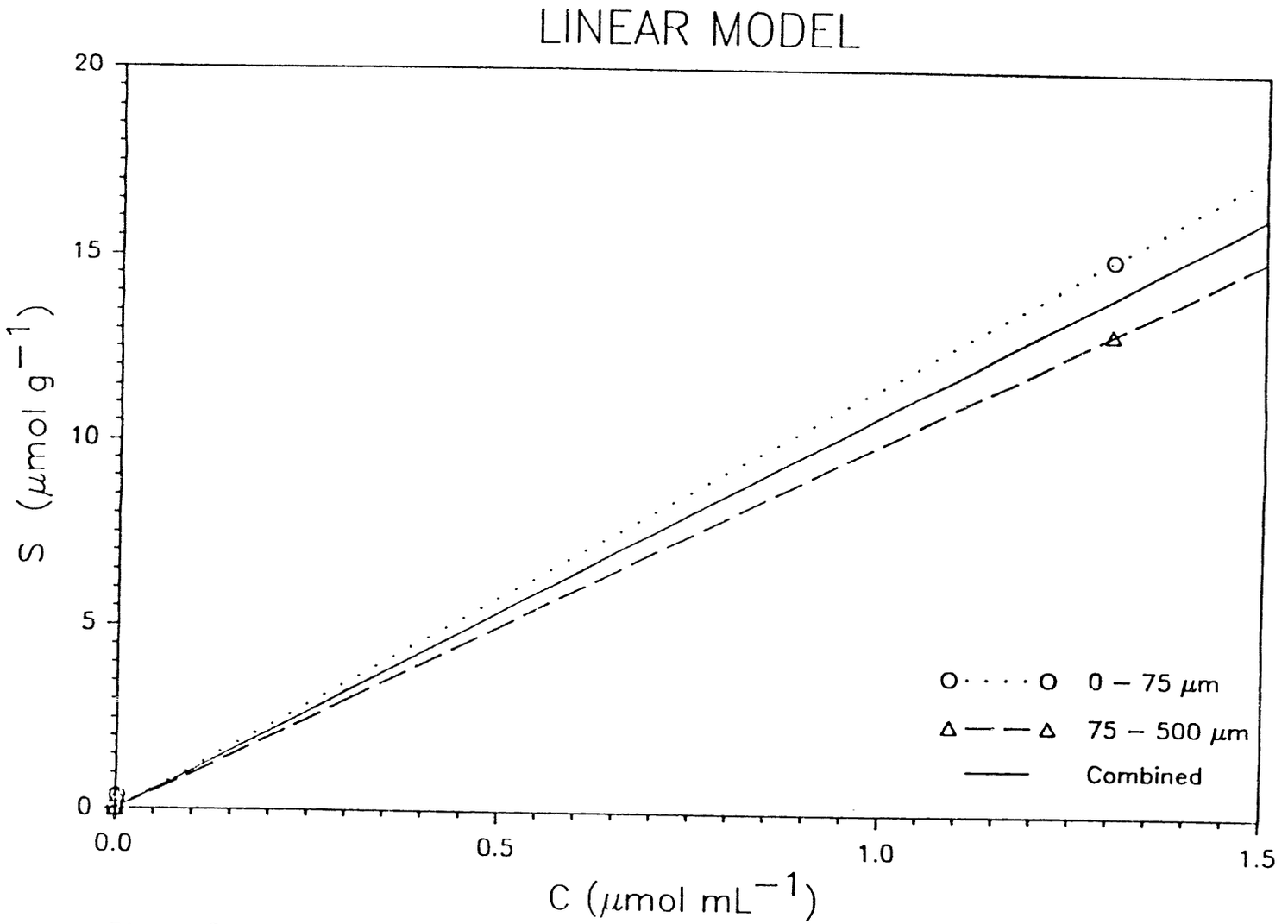

Figure C.16. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Cs 21 air 0-75 amb 44.0 and YM-22 Cs 21 air 75-500 amb 58.0; the variable being tested is particle size.

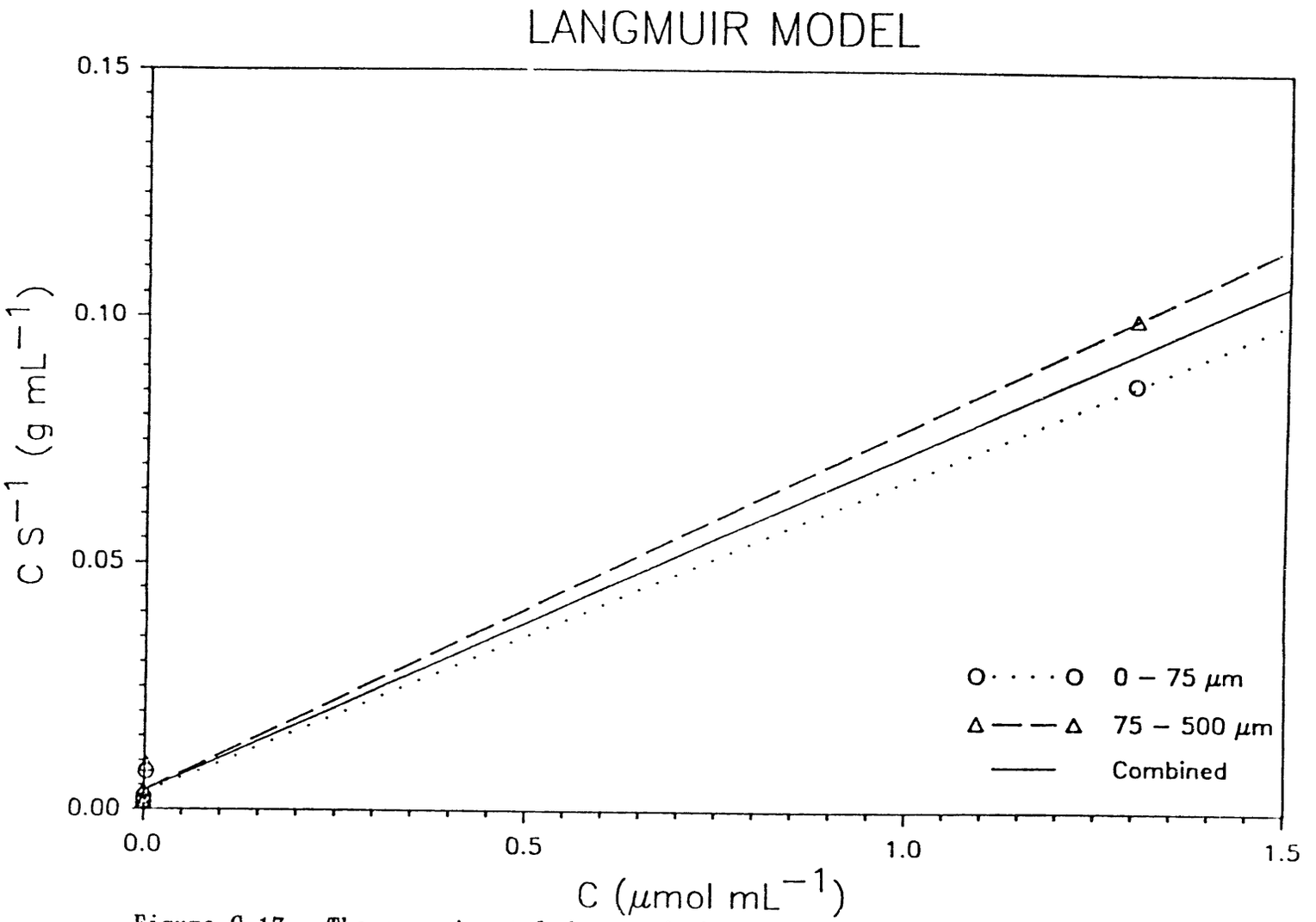

Figure C.17. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 44.0 and YM-22 Cs 21 air 75-500 amb 58.0; the variable being tested is particle size.

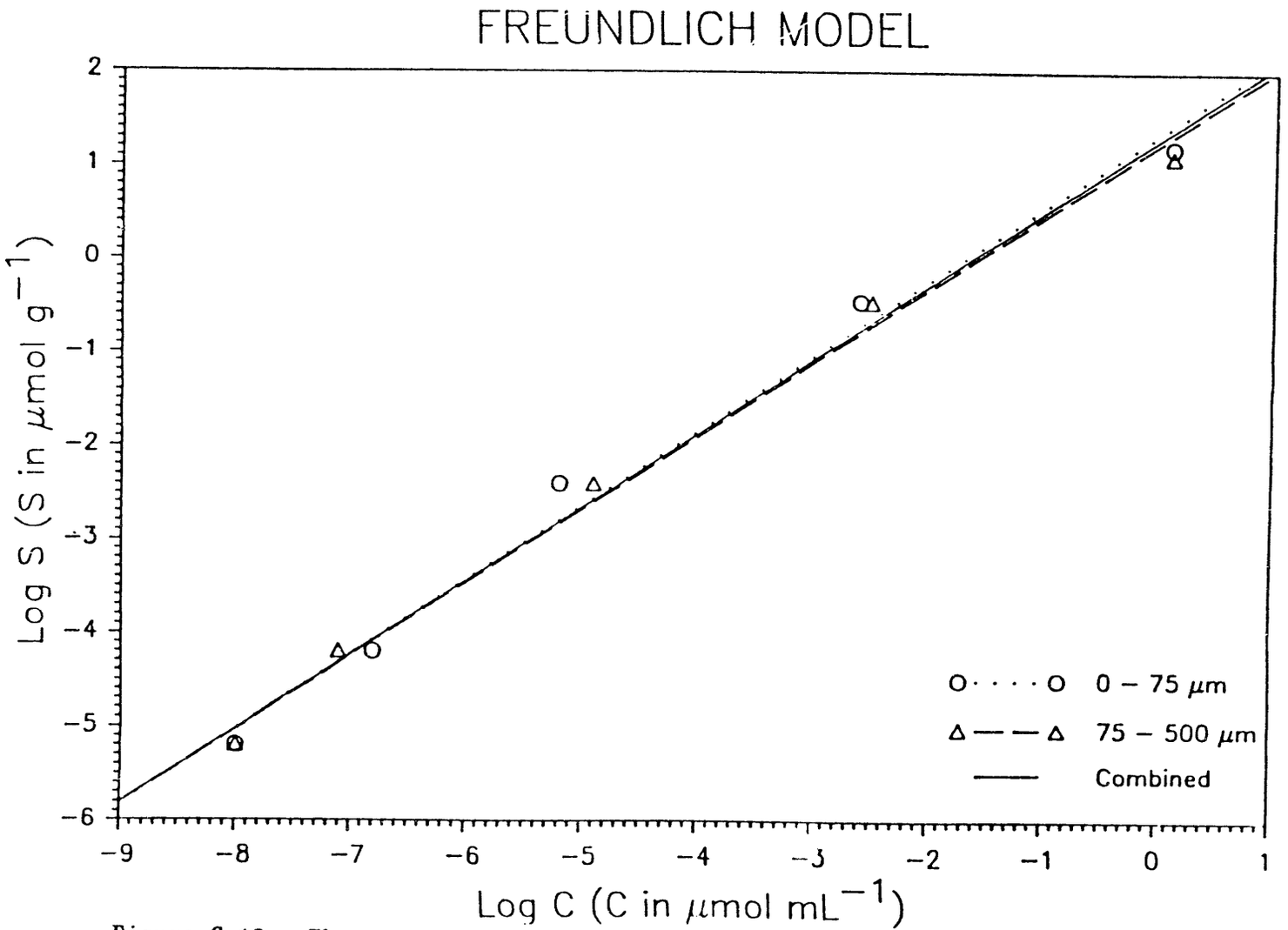

Figure C.18. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 44.0 and YM-22 Cs 21 air 75-500 amb 58.0; the variable being tested is particle size.

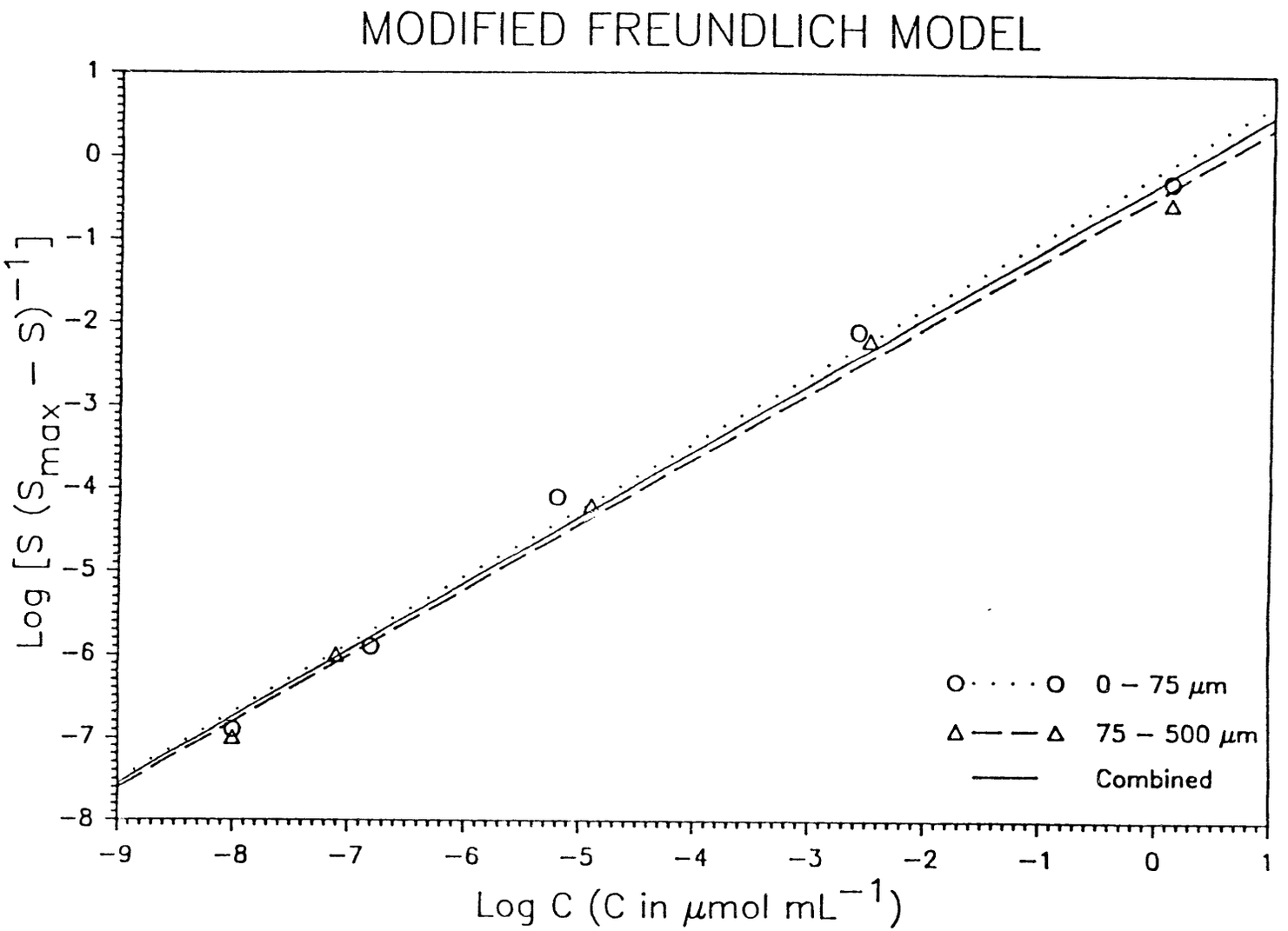

Figure C.19. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 44.0 and YM-22 Cs 21 air 75-500 amb 58.0; the variable being tested is particle size.

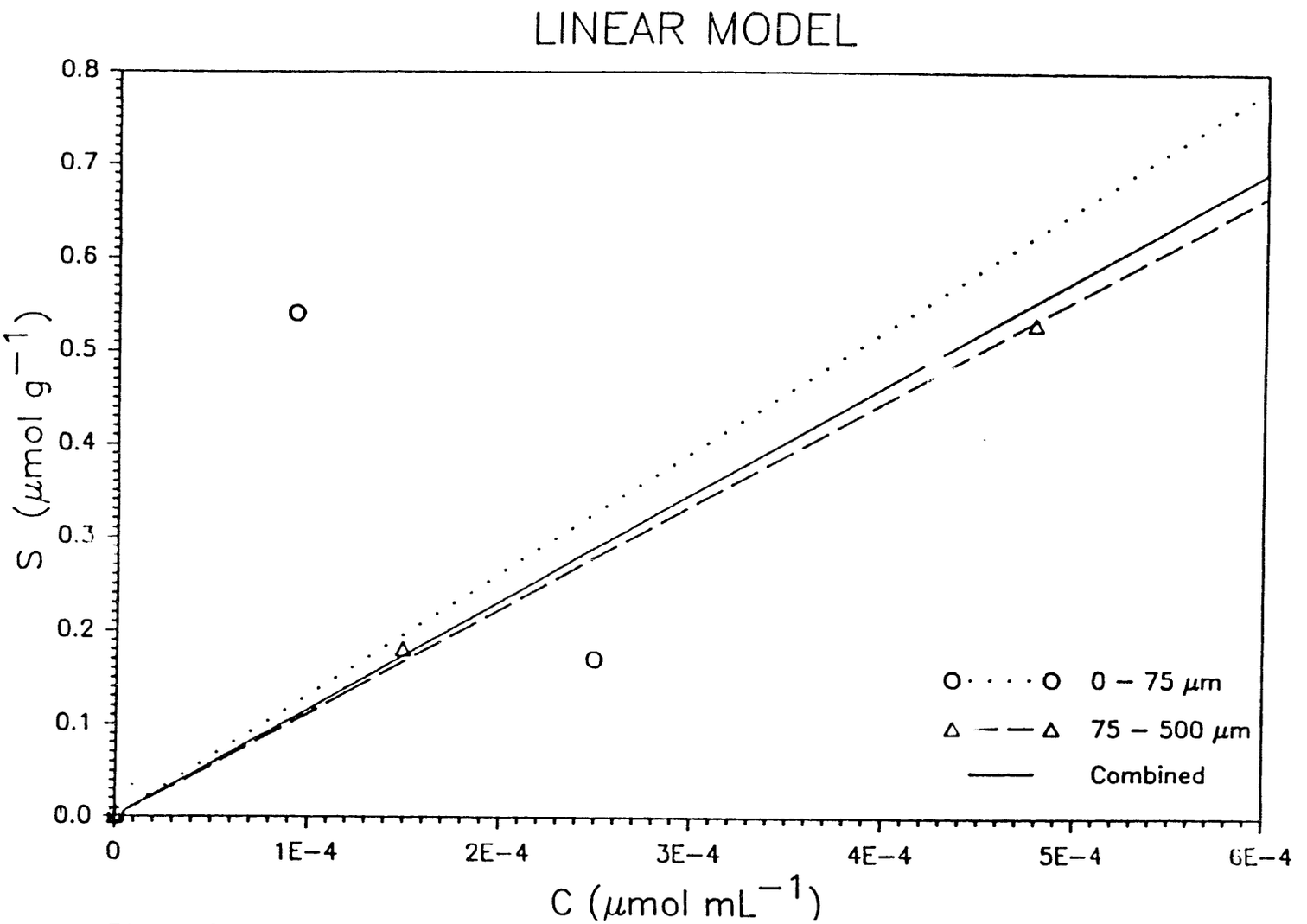

Figure C.20. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 44.0 and YM-22 Eu 21 air 75-500 amb 58.0; the variable being tested is particle size.

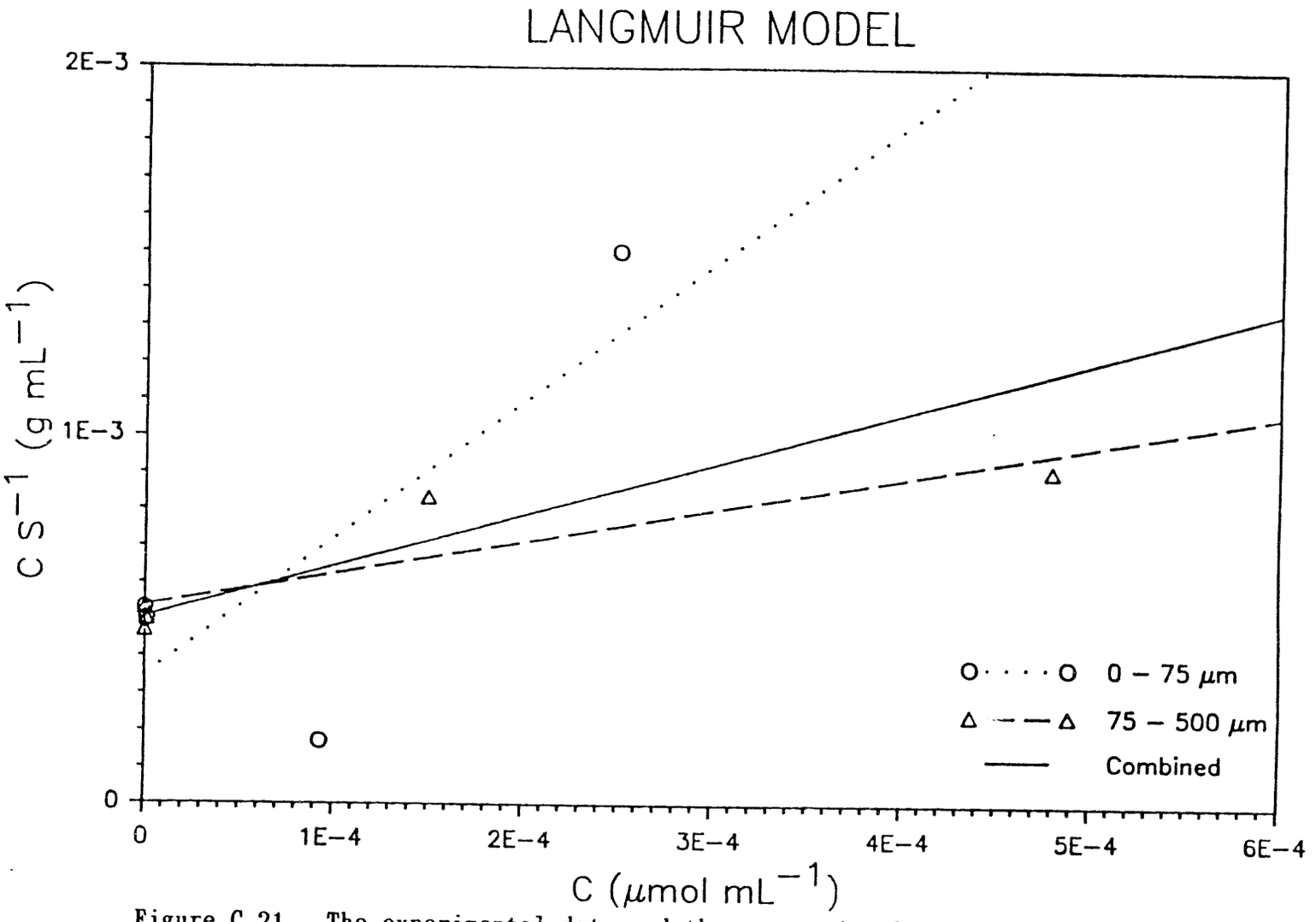

Figure C.21. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 44.0 and YM-22 Eu 21 air 75-500 amb 58.0; the variable being tested is particle size.

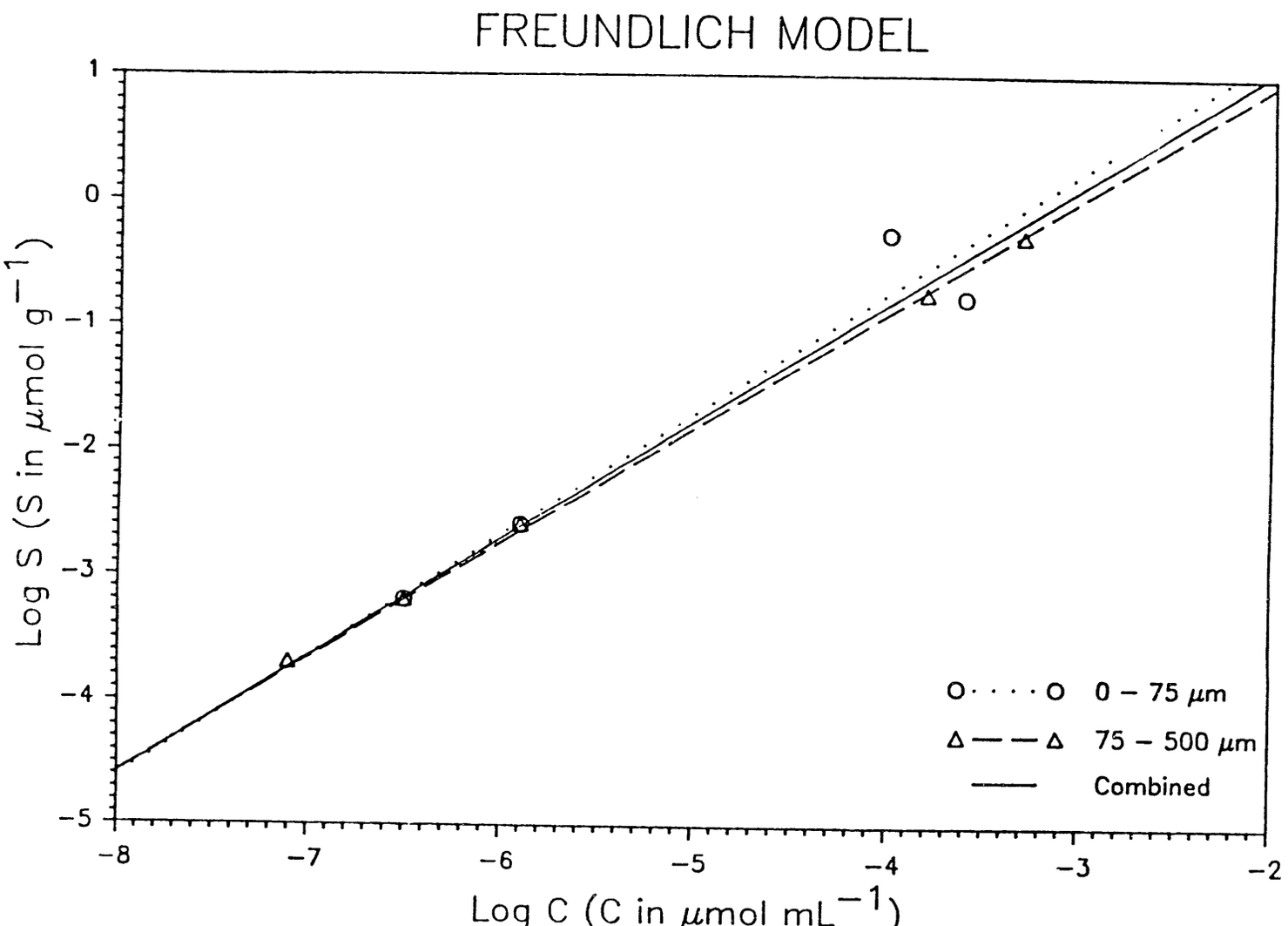

Figure C.22. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 44.0 and YM-22 Eu 21 air 75-500 amb 58.0; the variable being tested is particle size.

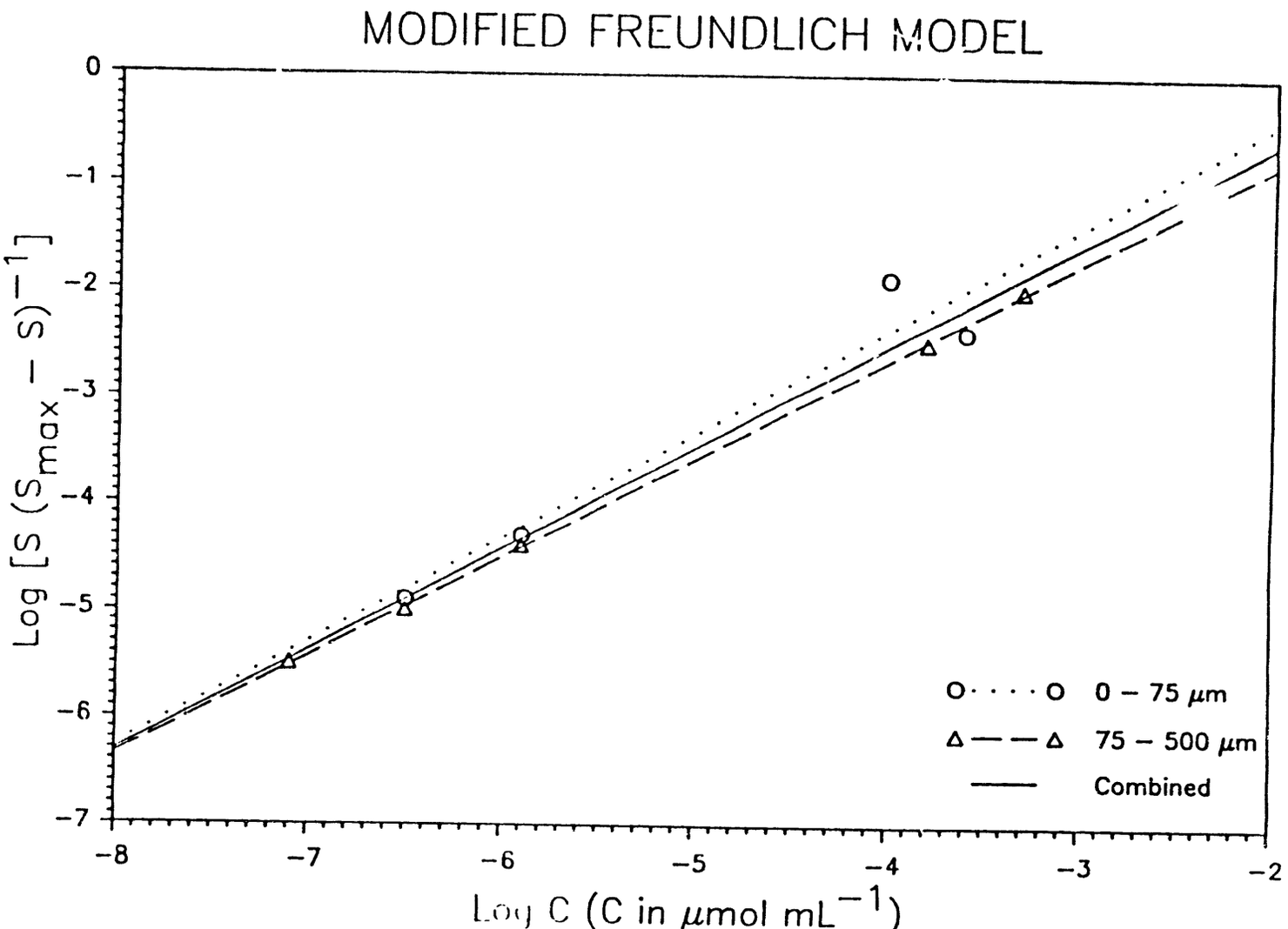

Figure C.23. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 44.0 and YM-22 Eu 21 air 75-500 amb 58.0; the variable being tested is particle size.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION

g4-1608 Pa 42 CO2 75-500 amb n.a. VERSUS g4-1608 Pa 42 CO2 75-500 amb n.a.

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=10.20<Ft=4.46 (Different)	Fc=0.64<Ft=4.46 (Same)	Fc=0.49<Ft=4.46 (Same)	n.a. n.a.
Intercept	n.a. n.a.	Fc=0.10<Ft=5.12 (Different)	Fc=0.02<Ft=5.12 (Same)	n.a. n.a.
Slope	n.a. n.a.	Fc=0.55<Ft=5.12 (Same)	Fc=0.06<Ft=5.12 (Same)	n.a. n.a.

g1-2840 Sr 21 air 75-500 amb 430.0 VERSUS g1-2840 Sr 21 air 75-500 amb 430.0

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.00<Ft=3.47 (Same)	Fc=0.45<Ft=3.47 (Same)	Fc=0.12<Ft=3.47 (Same)	Fc=0.13<Ft=3.47 (Same)
Intercept	n.a. n.a.	Fc= .07<Ft=4.30 Same)	Fc=0.17<Ft=4.30 (Same)	Fc=0.18<Ft=4.30 (Same)
Slope	Fc=0.00<Ft=4.30 (Same)	Fc=0.88<Ft=4.30 (San	Fc=0.02<Ft=4.30 (Same)	Fc=0.02<Ft=4.30 (Same)

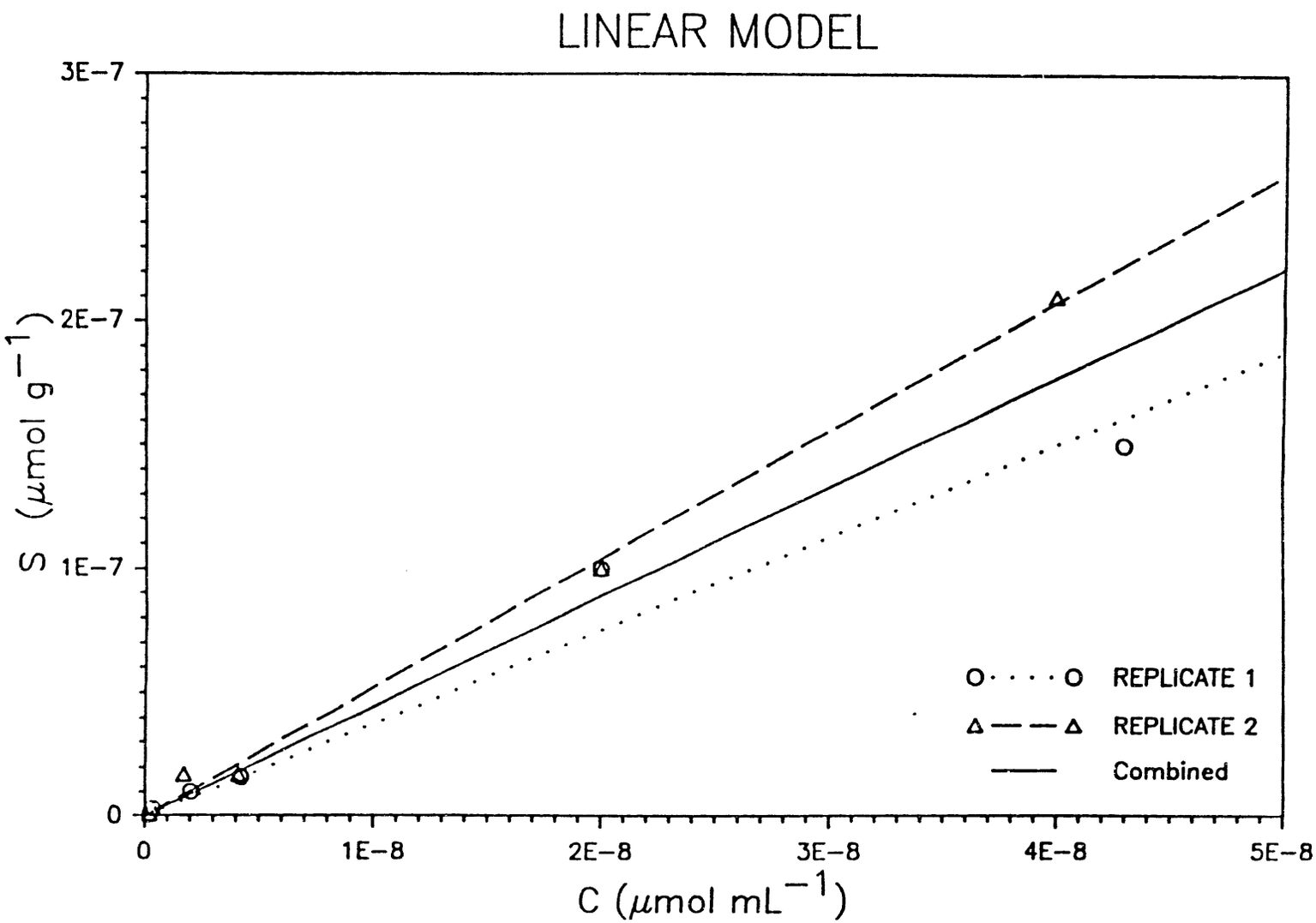

Figure C.24. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 1 and G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 2; the variable being tested is replication.

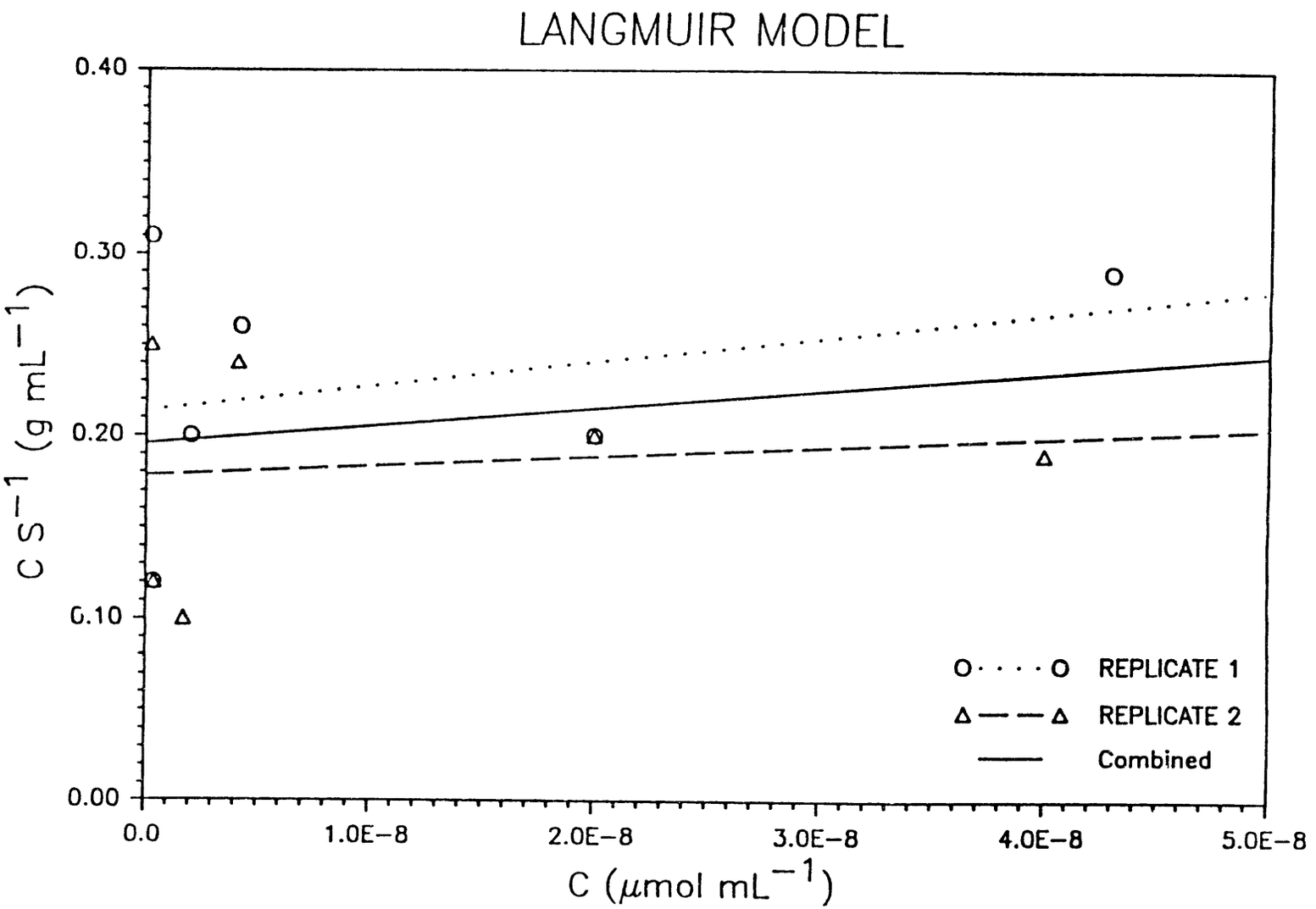

Figure C.25. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 1 and G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 2; the variable being tested is replication.

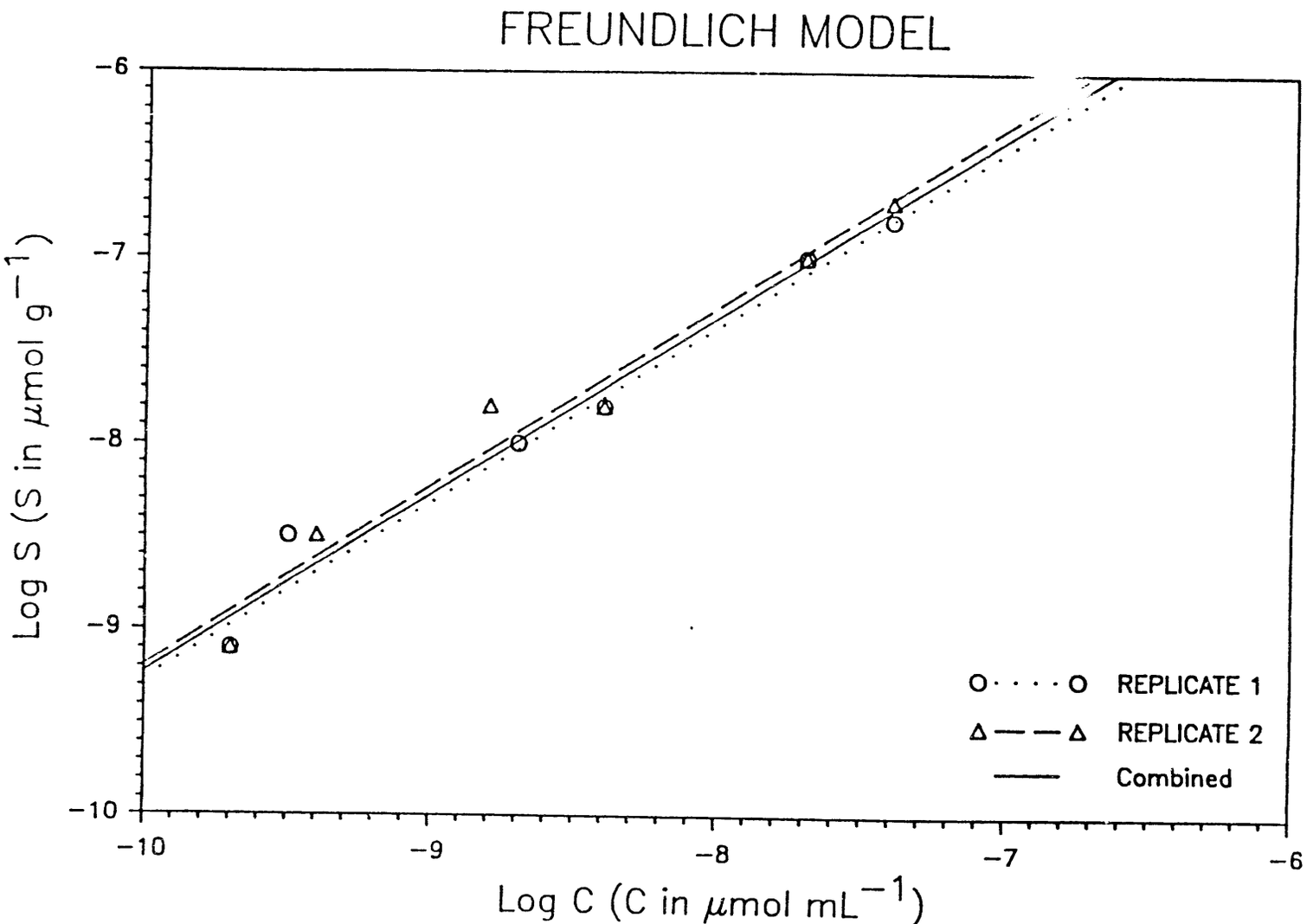

Figure C.26. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 1 and G4-1608 Pa 42 CO2 75-500 amb n.a. Replicate 2; the variable being tested is replication.

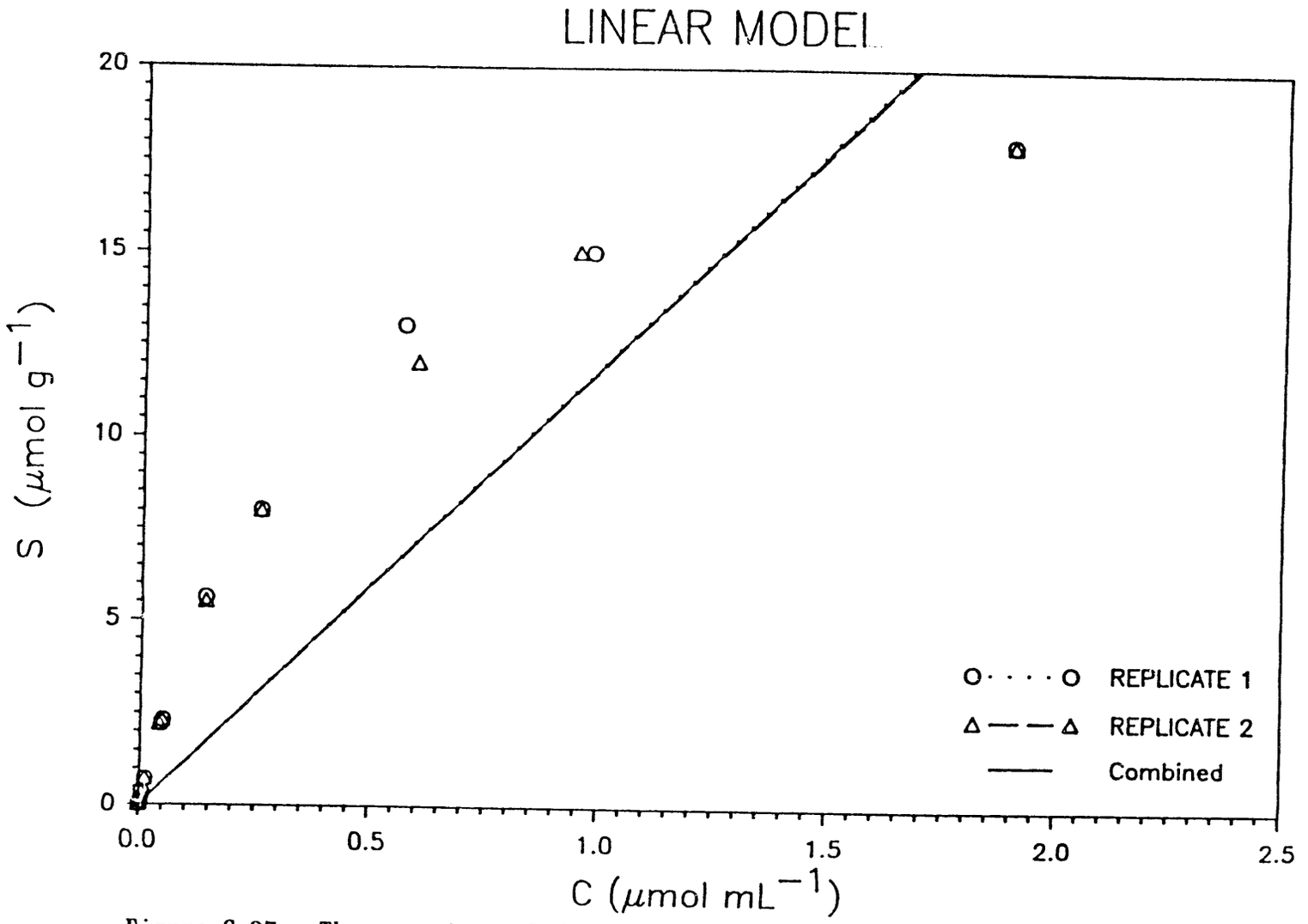

Figure C.27. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

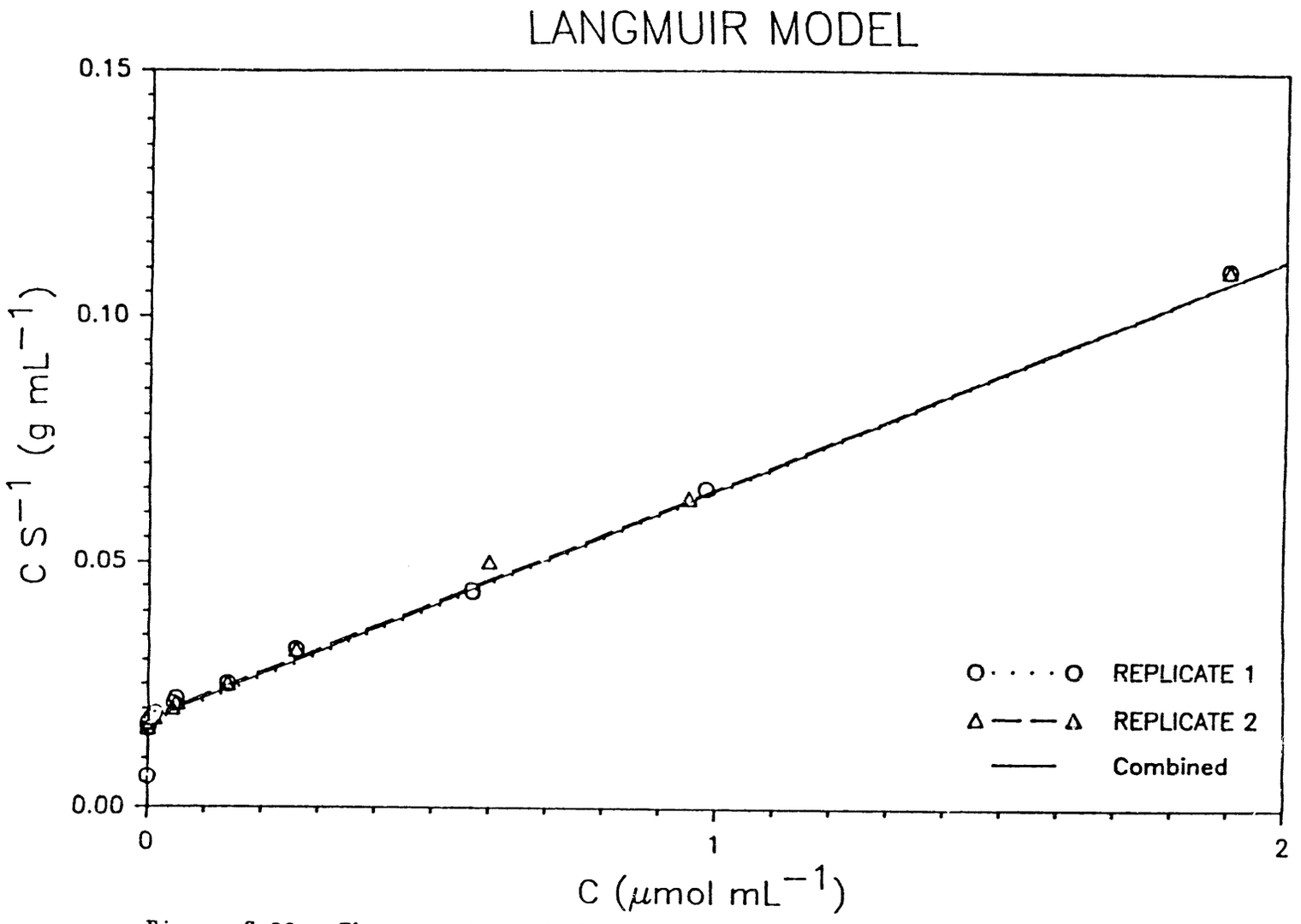

Figure C.28. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

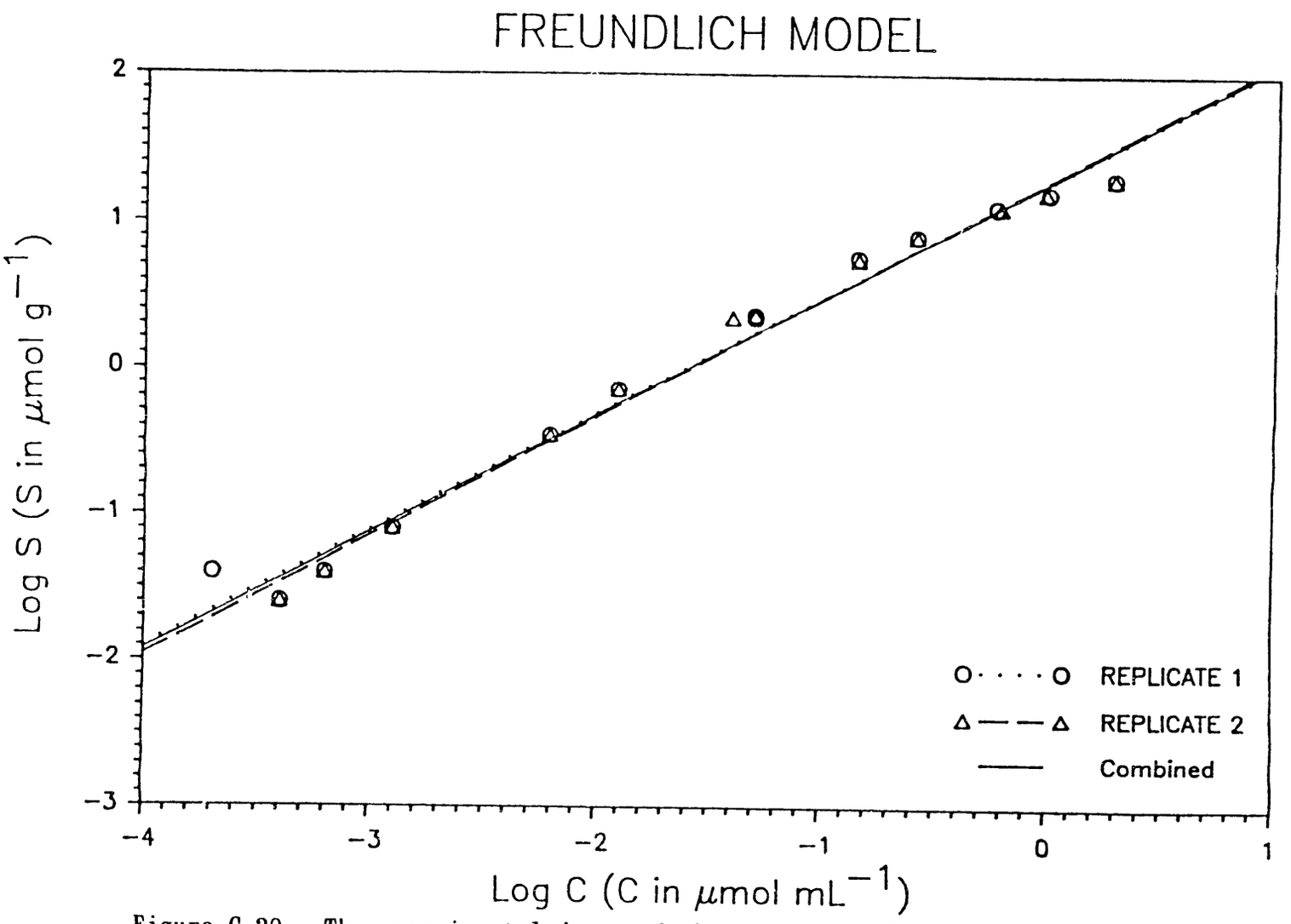

Figure C.29. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

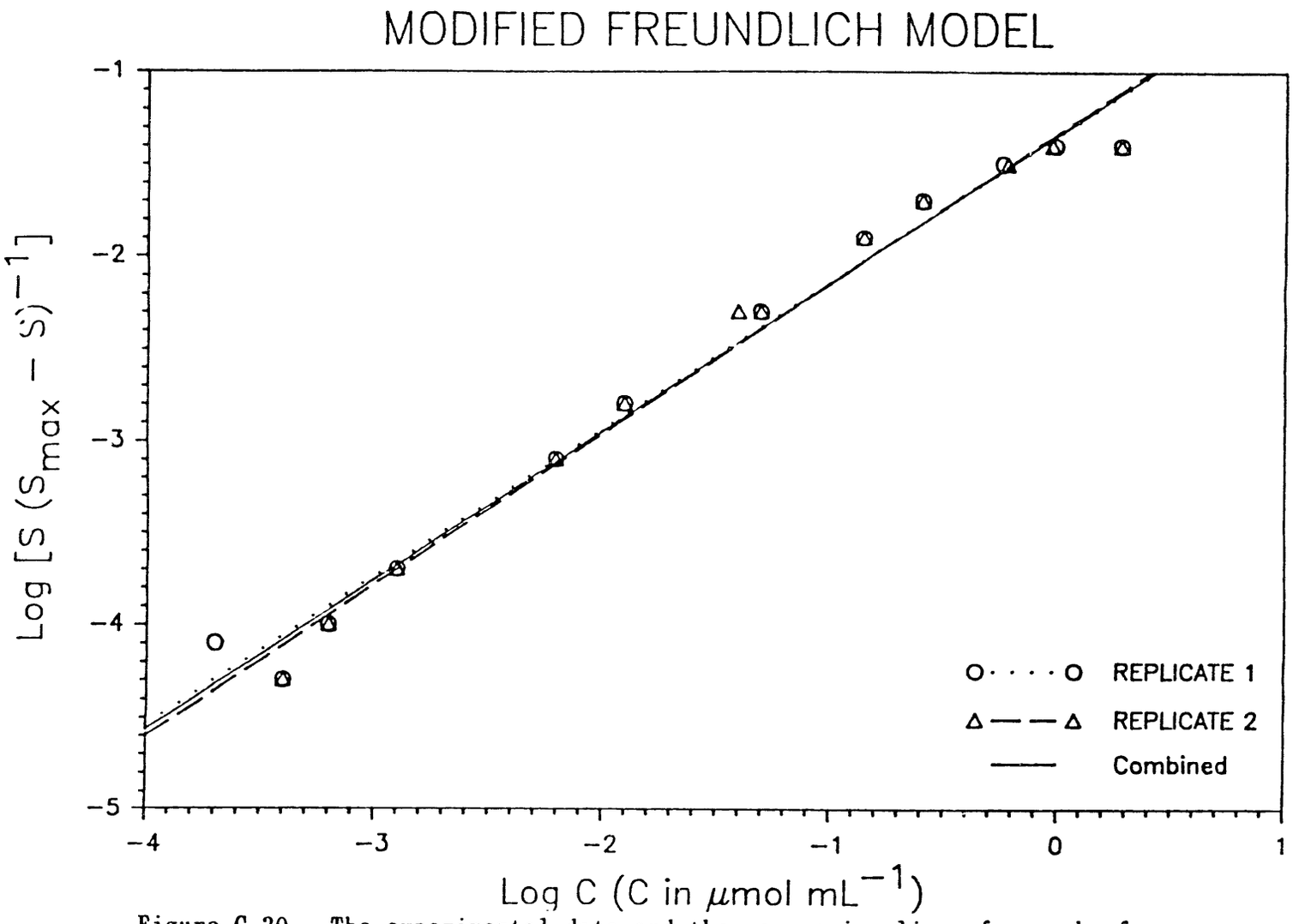

Figure C.30. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 430.0 Replicate 2; the variable being tested is replication.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS; ADSORPTION

ym-22 Sr 21 air - 75 amb 44.0 VERSUS ym-22 Sr 21 air 75-500 amb 58.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=2382.24>Ft=5.14 (Different)	Fc=46.93>Ft=5.14 (Different)	Fc=1.72<Ft=5.14 (Same)	n.a. n.a.
Intercept	n.a. n.a.	Fc=90.91>Ft=5.59 (Different)	Fc=3.53<Ft=5.59 (Same)	n.a. n.a.
Slope	Fc=0.00<Ft=5.59 (Same)	Fc=0.14<Ft=5.59 (Same)	Fc=3.79<Ft=5.59 (Same)	n.a. n.a.

ym-48 Tc 42 air 106-500 amb 484.0 VERSUS ym-49 Tc 42 air 106-500 amb 1170.0

Variable: Different Mineralogies in the Same Stratigraphic Unit

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.00<Ft=6.94 (Same)	Fc=2.44<Ft=6.94 (Same)	Fc=1.36<Ft=6.94 (Same)	Fc=1.20<Ft=6.94 (Same)
Intercept	n.a. n.a.	Fc=1.52<Ft=6.61 (Same)	Fc=0.03<Ft=6.61 (Same)	Fc=0.03<Ft=6.61 (Same)
Slope	Fc=0.00<Ft=6.61 (Same)	Fc=6.10<Ft=6.61 (Same)	Fc=0.90<Ft=6.61 (Same)	Fc=1.39<Ft=6.61 (Same)

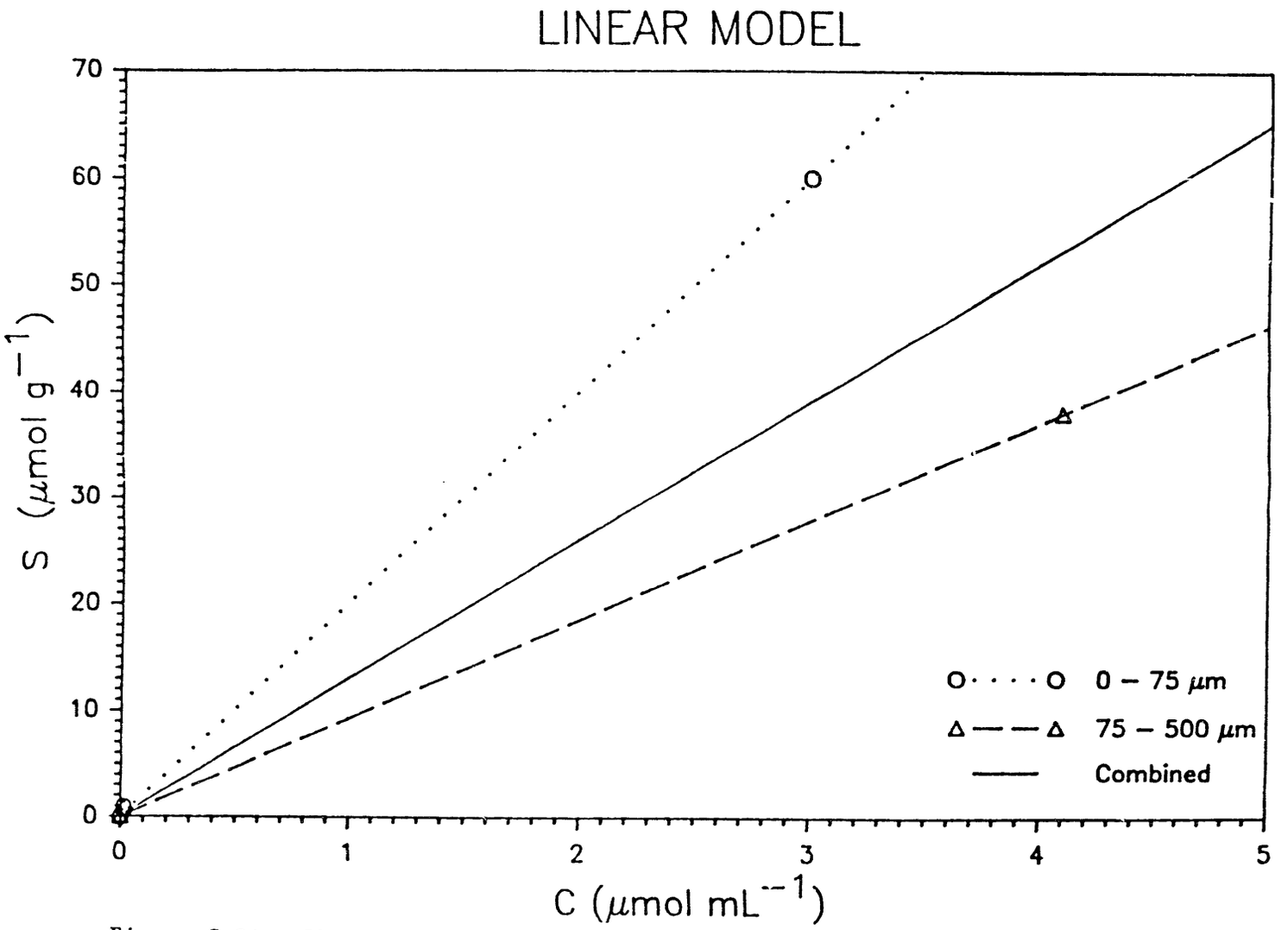

Figure C.31. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Sr 21 air -75 amb 44.0 and YM 22 Sr 21 air 75-500 amb 58.0; the variable being tested is particle size.

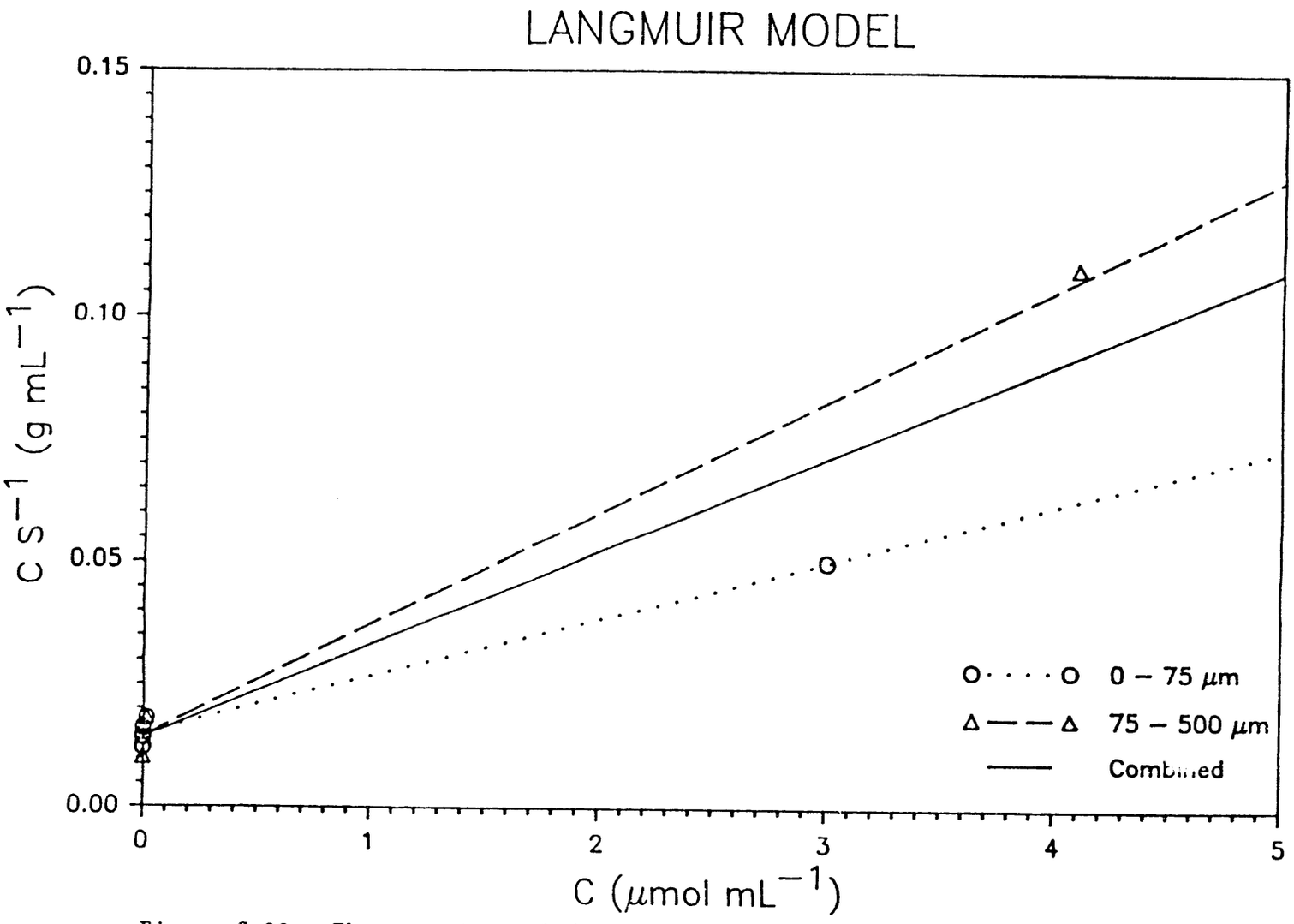

Figure C.32. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Sr 21 air -75 amb 44.0 and YM-22 Sr 21 air 75-500 amb 58.0; the variable being tested is particle size.

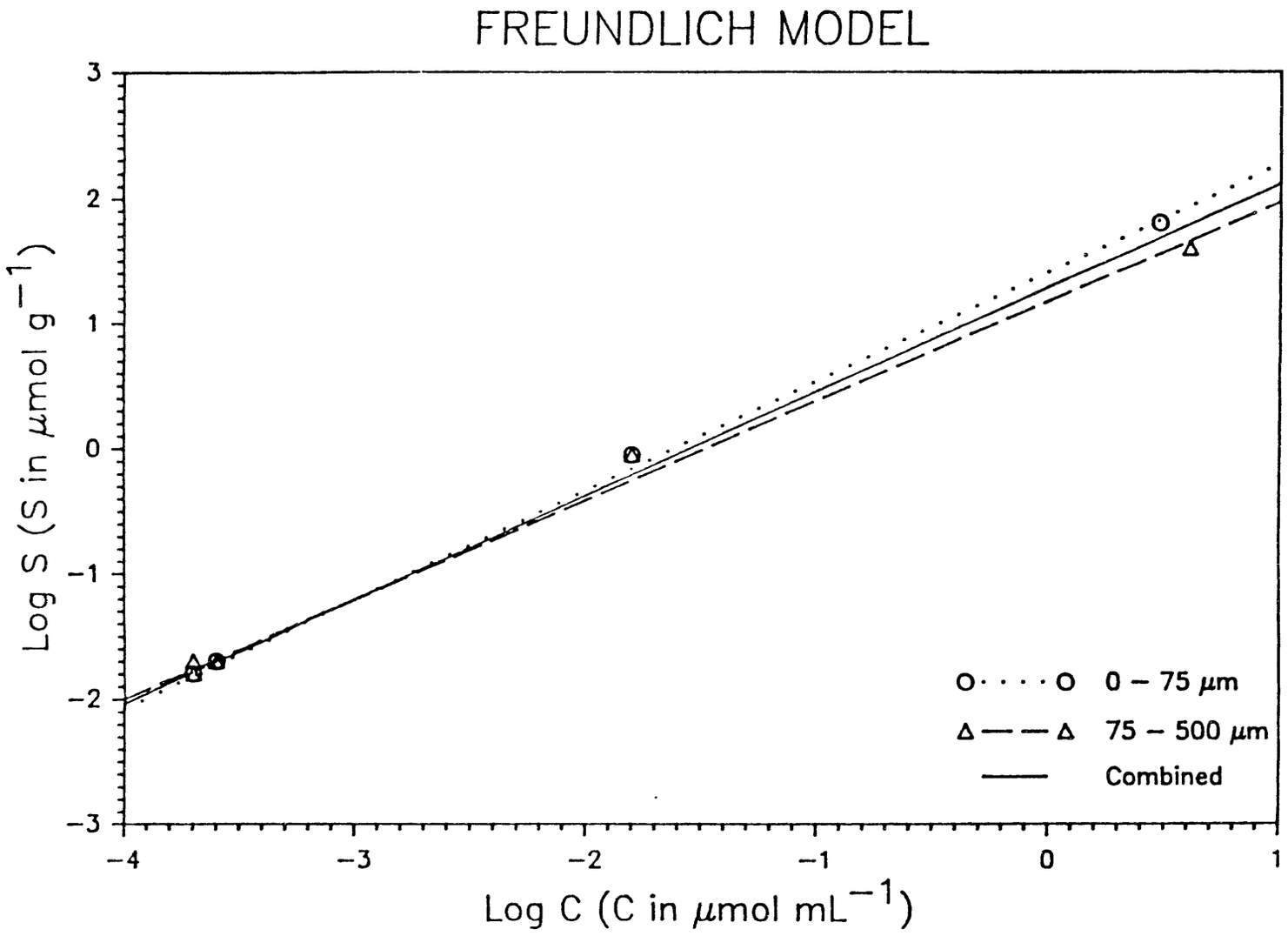

Figure C.33. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Sr 21 air -75 amb [illegible].0 and YM-22 Sr 21 air 75-500 amb 58.0; the variable being tested is particle size.

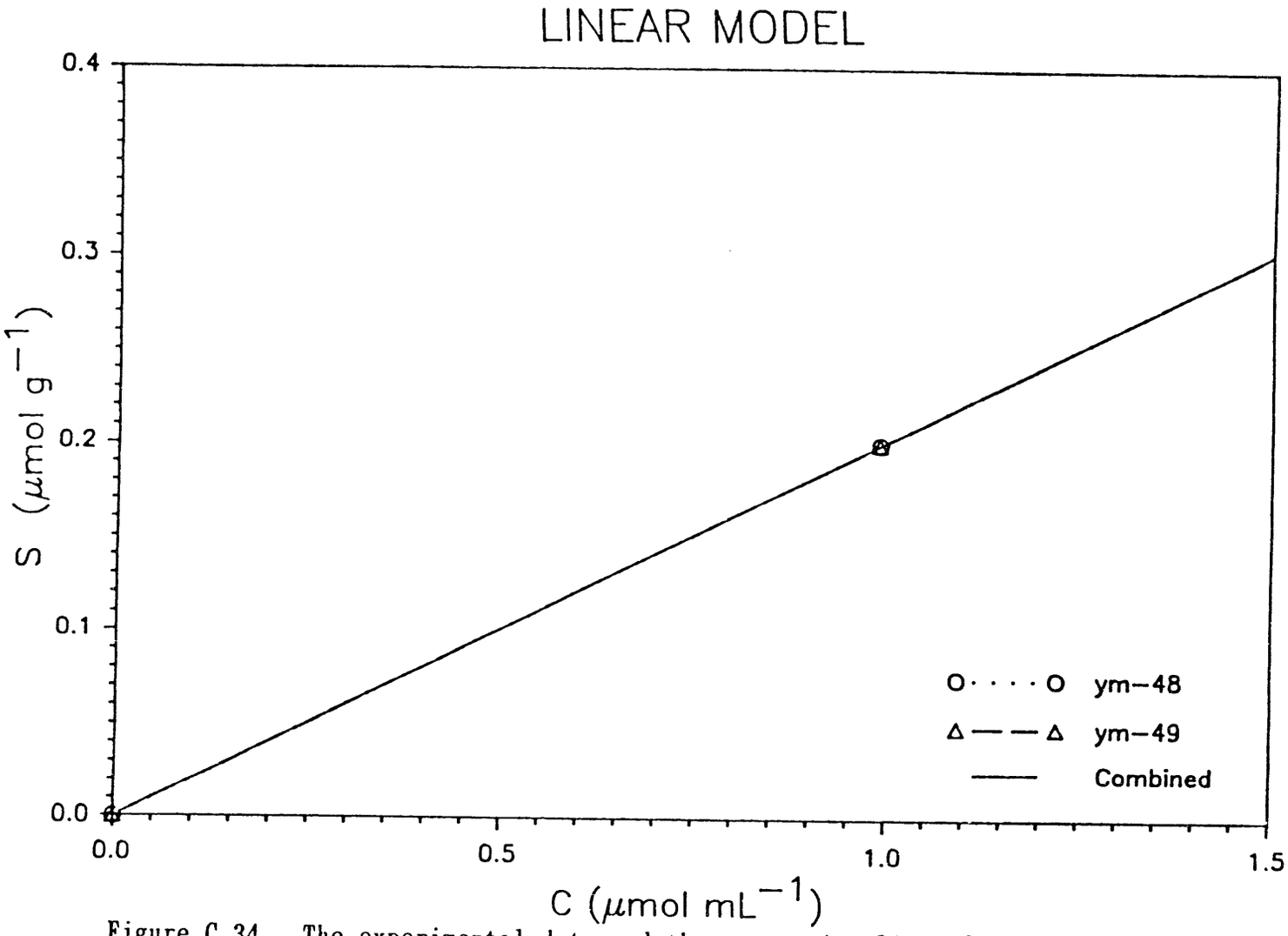

Figure C.34. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 adsorption; the variable being tested is mineralogy.

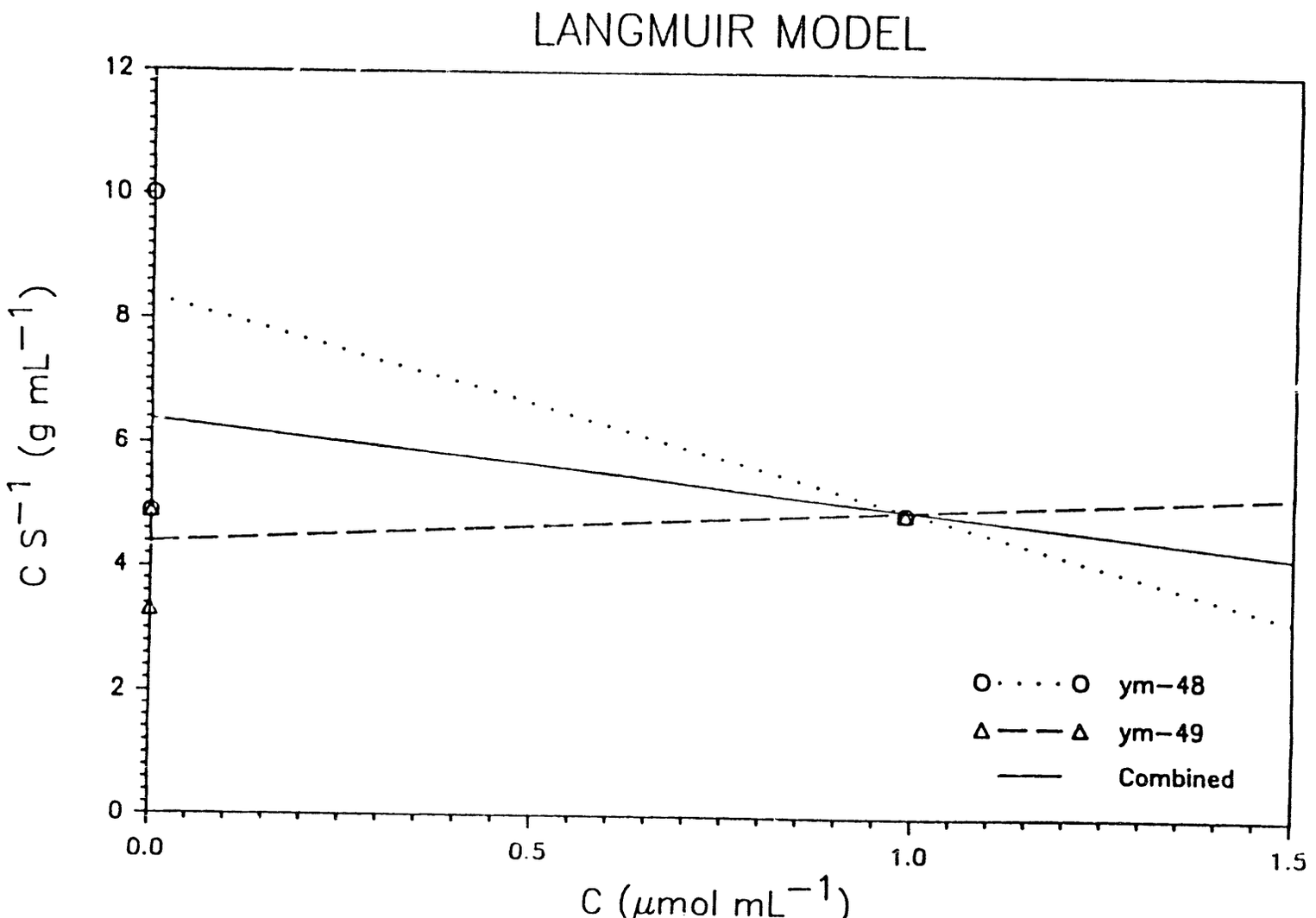

Figure C.35. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 adsorption; the variable being tested is mineralogy.

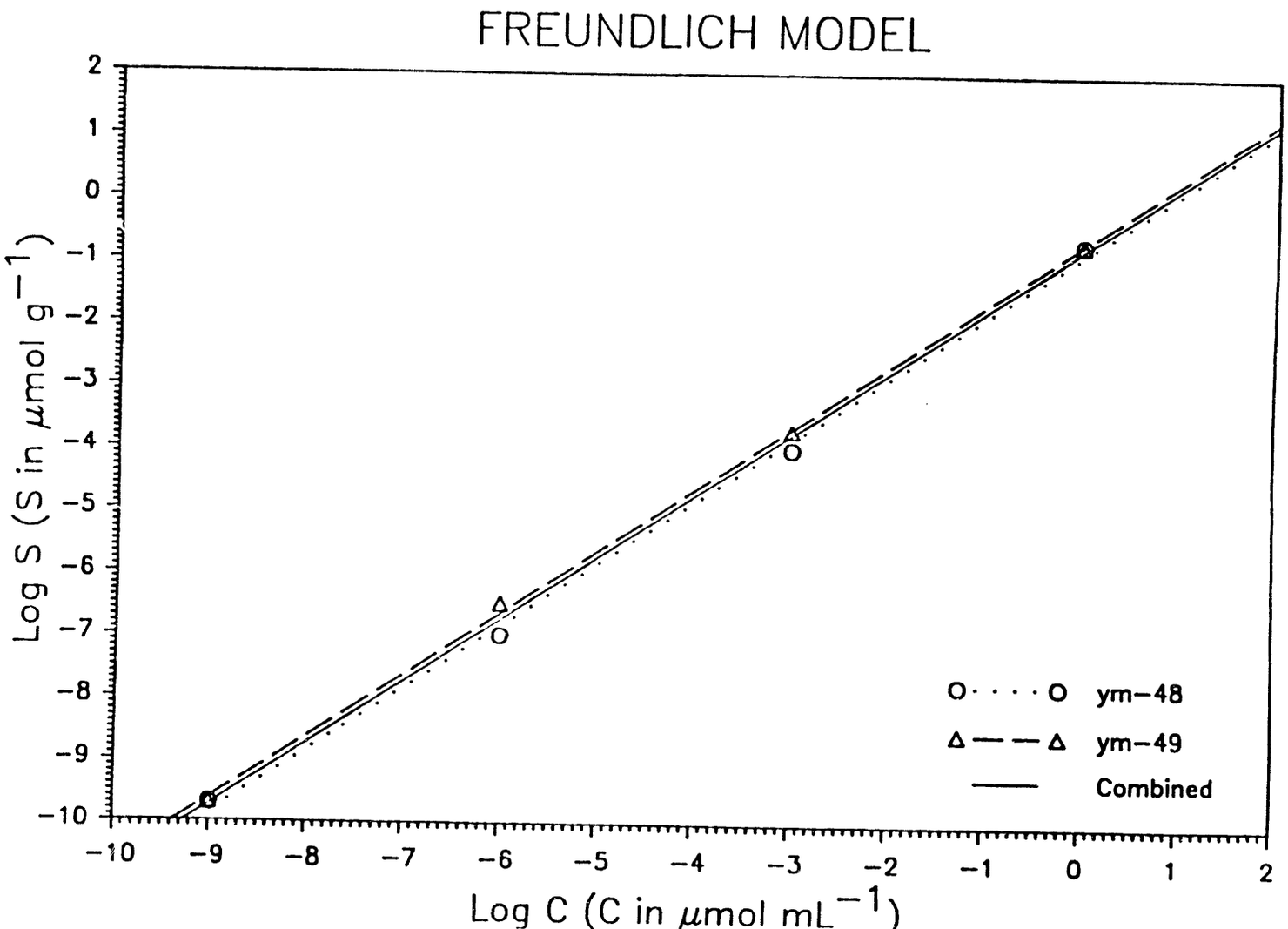

Figure C.36. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-48 Tc 42 air 106 500 amb 484.0 ad- sorption and YM-49 Tc 42 air 106-500 amb 1170.0 ad sorption; the variable being tested is mineralogy.

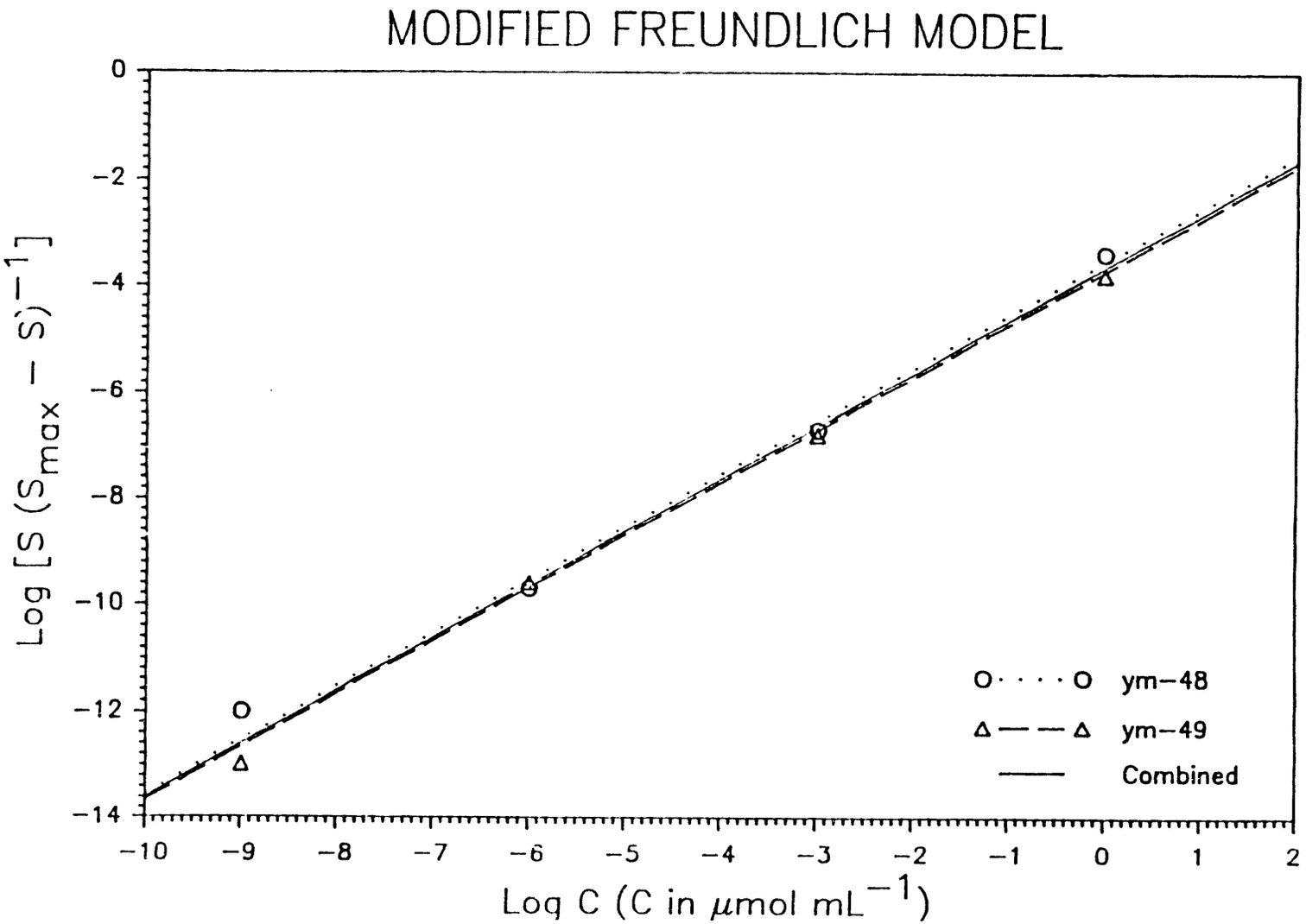

Figure C.37. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 ad- sorption and YM-49 Tc 42 air 106-500 amb 1170.0 adsorption; the variable being tested is mineralogy.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION

ym-22 Ba 21 air - 75 amb 58.0 VERSUS ym-22 Ba 21 air 75-500 amb 44.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=91.58>Ft=5.14 (Different)	Fc=6.82>Ft=5.14 (Different)	Fc=11.57>Ft=5.14 (Different)	Fc=1.99<Ft=5.14 (Same)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

gl-2840 Cs 21 air 75-500 amb 43.0 VERSUS gl-2840 Cs 21 air 75-500 amb 43.0

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.92<Ft=3.52 (Same)	Fc=0.02<Ft=3.52 (Same)	Fc=0.24<Ft=3.52 (Same)	Fc=0.24<Ft=3.52 (Same)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

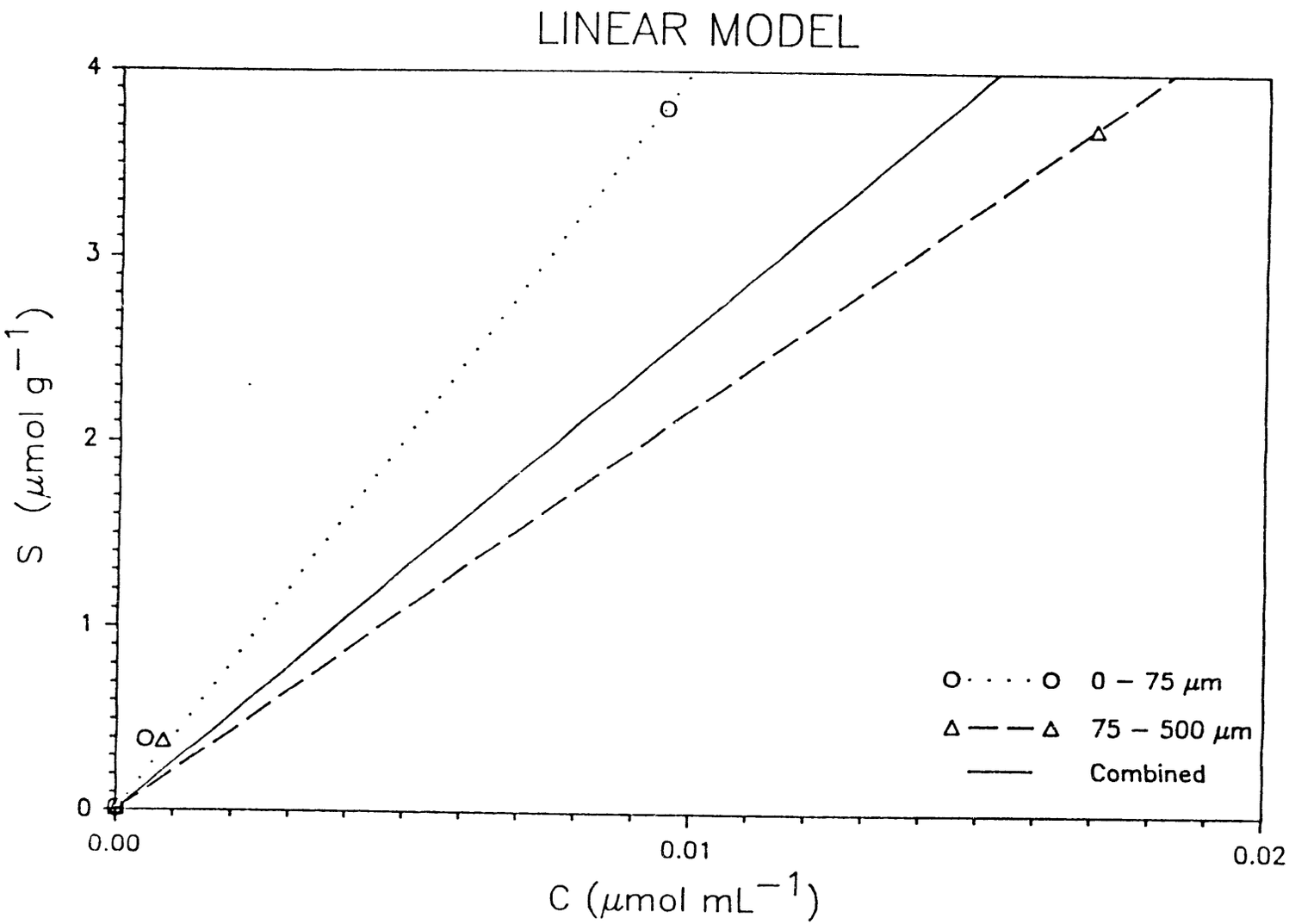

Figure C.38. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 58.0 and YM-22 Ba 21 air 75-500 amb 44.0; the variable being tested is particle size.

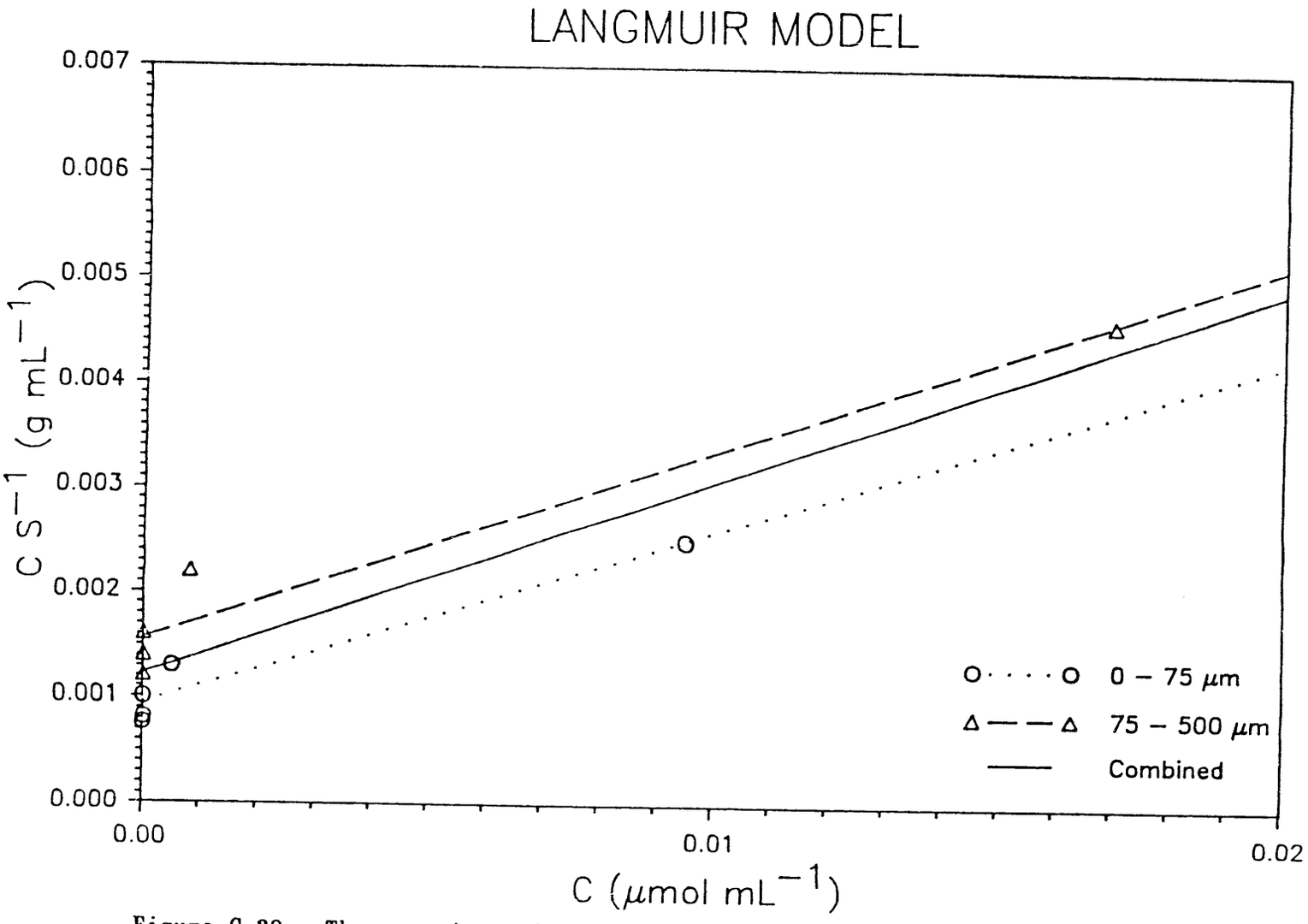

Figure C.39. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 58.0 and YM-22 Ba 21 air 75-500 amb 44.0; the variable being tested is particle size.

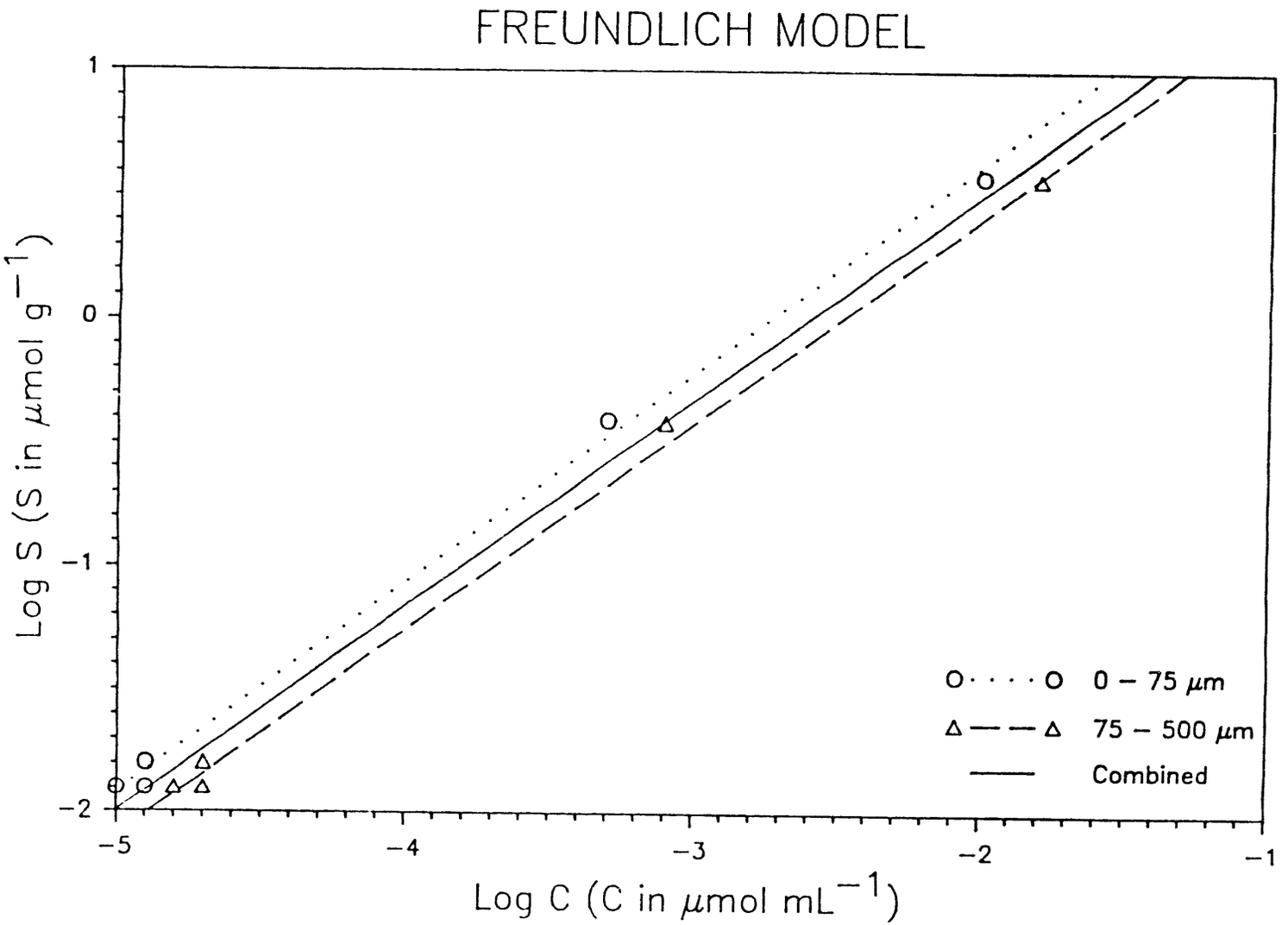

Figure C.40. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 58.0 and YM-22 Ba 21 air 75-500 amb 44.0; the variable being tested is particle size.

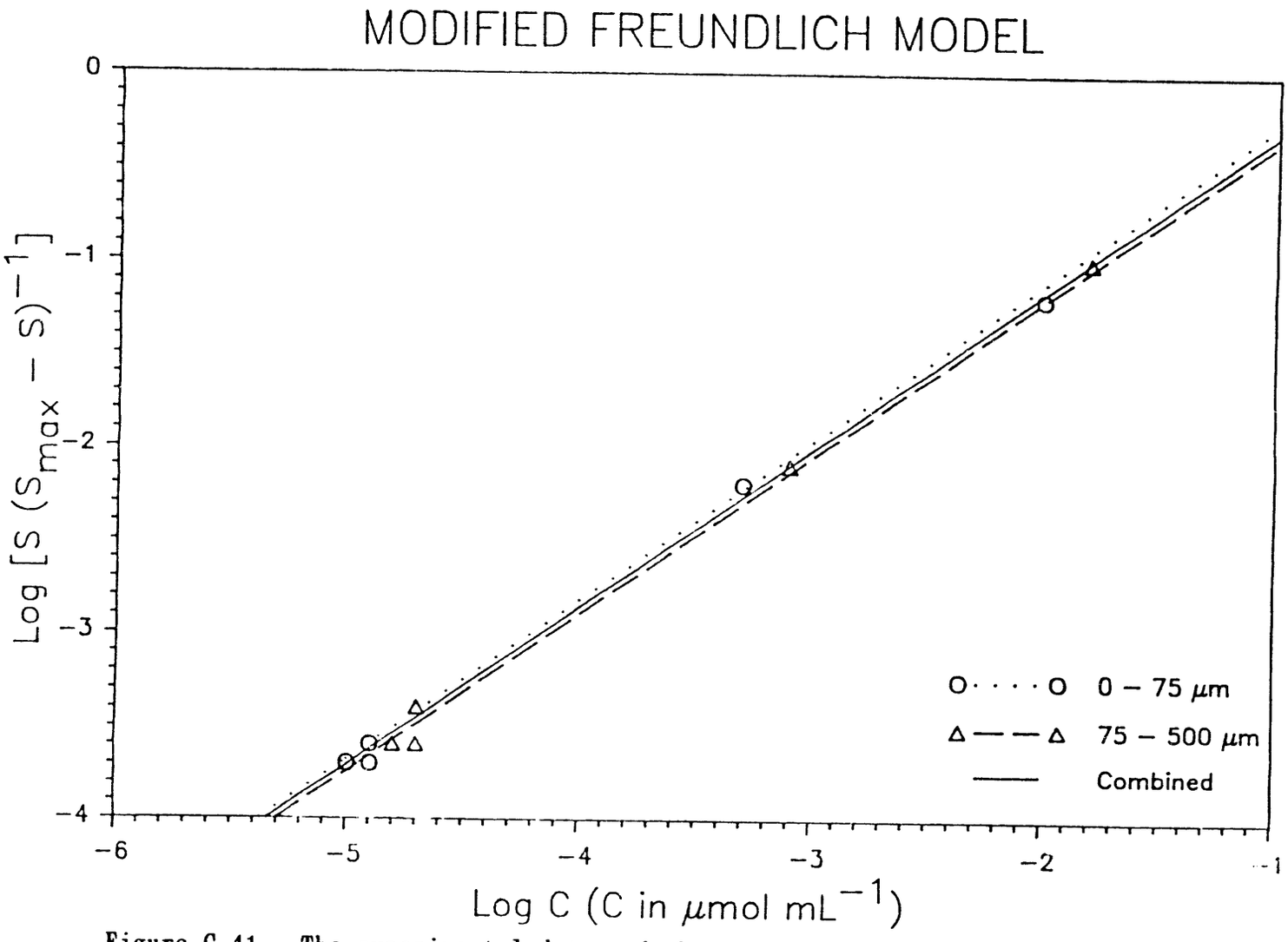

Figure C.41. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 58.0 and YM-22 Ba 21 air 75-500 amb 44.0; the variable being tested is particle size.

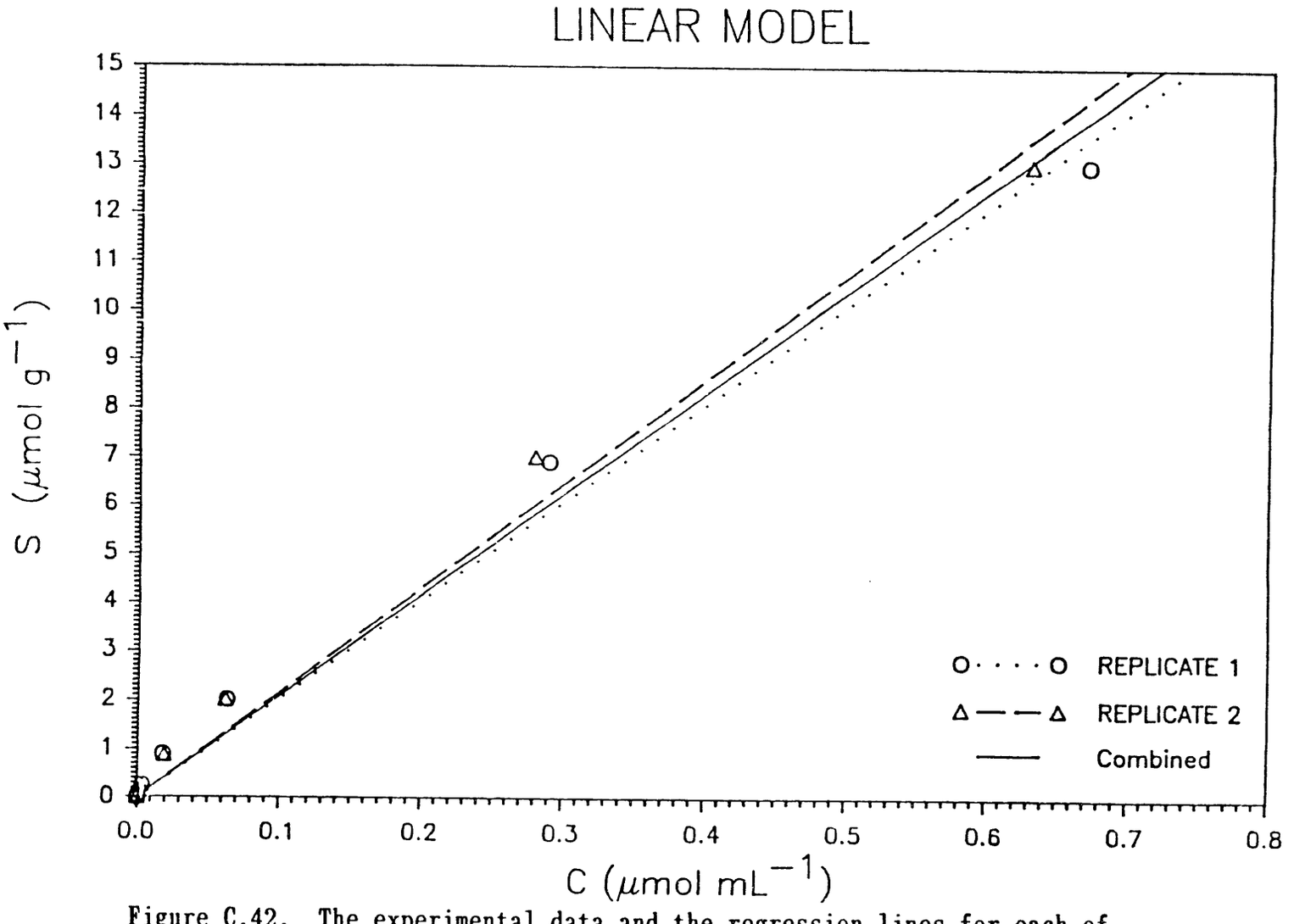

Figure C.42. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

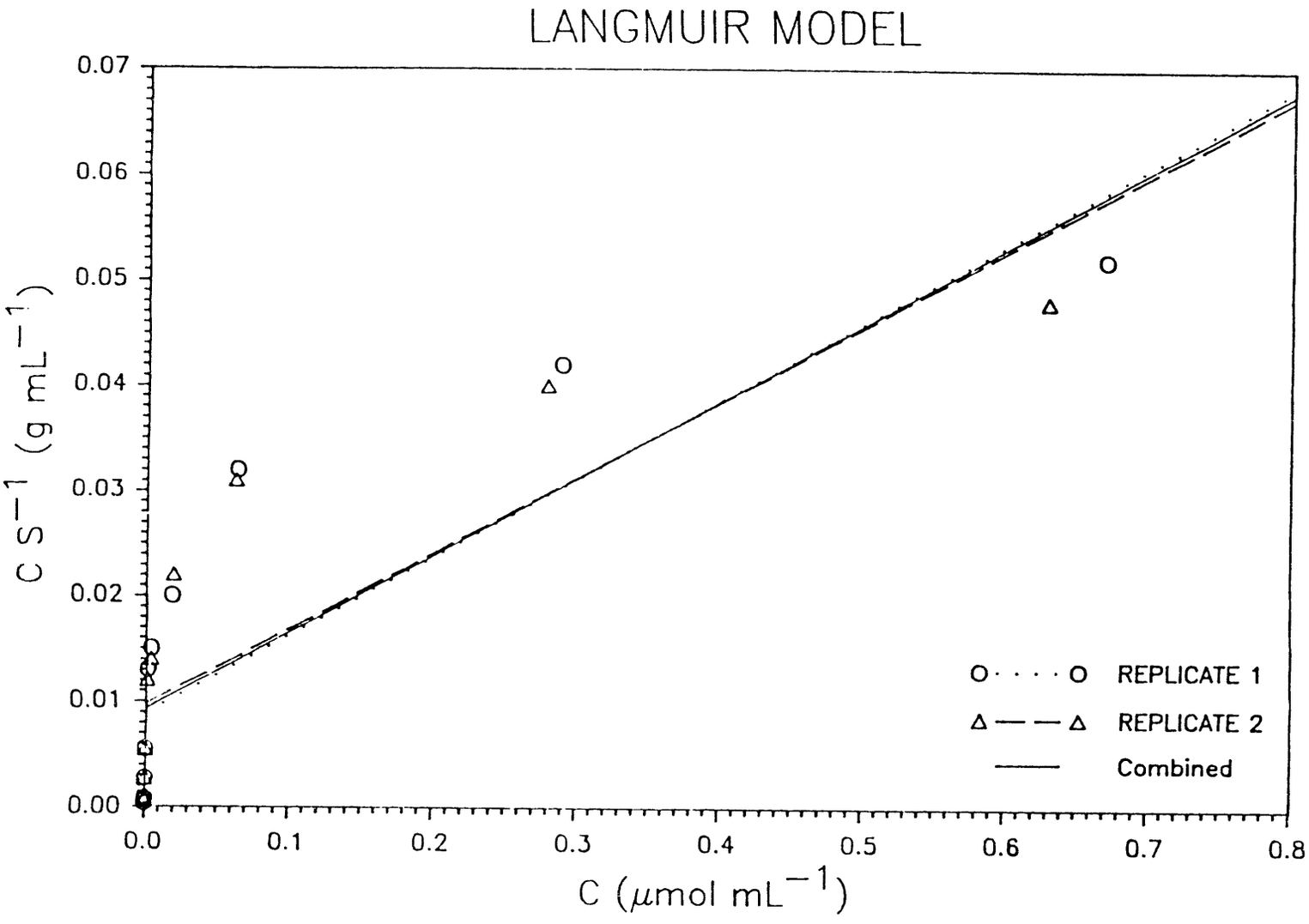

Figure C.43. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 CS 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

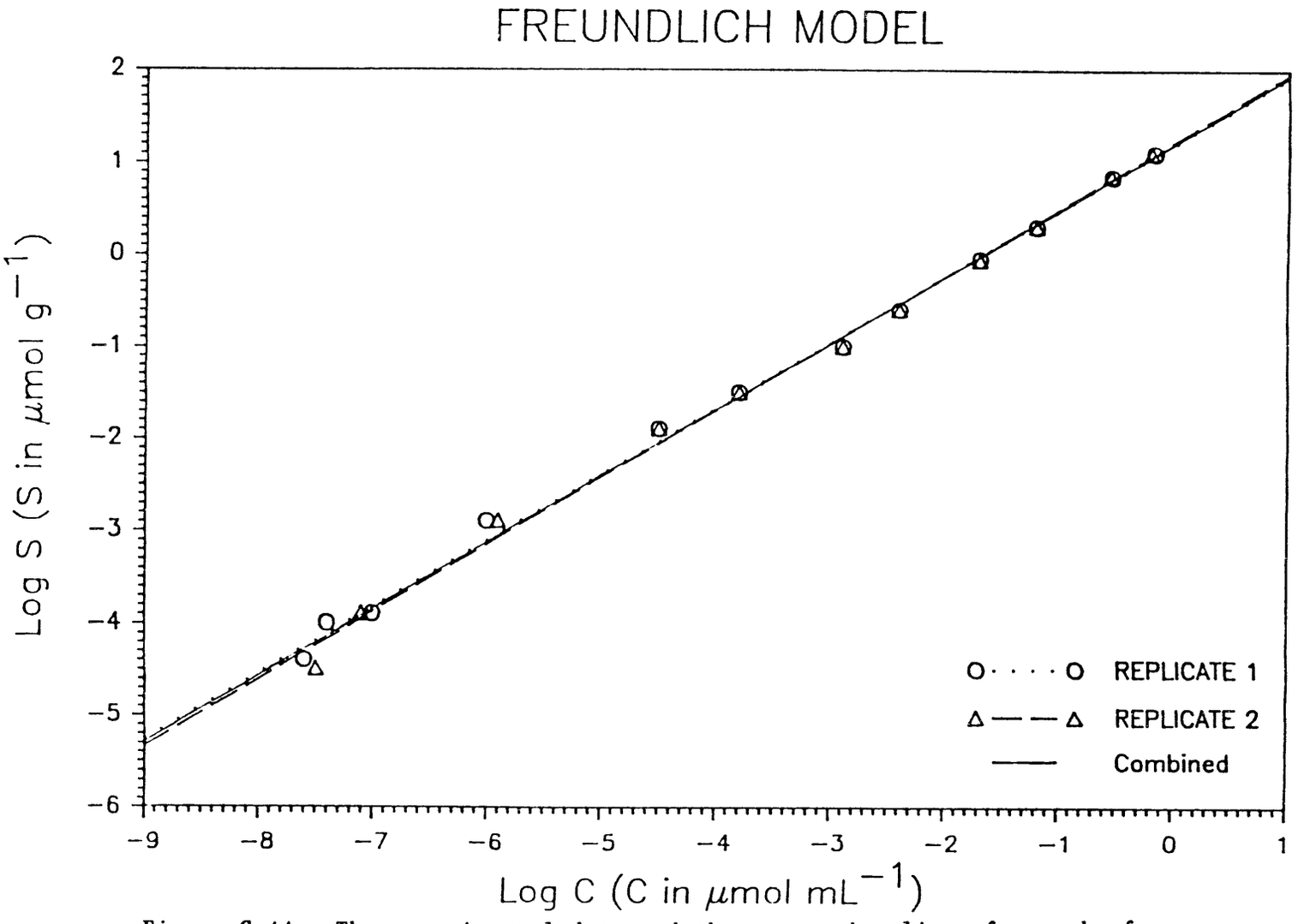

Figure C.44. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

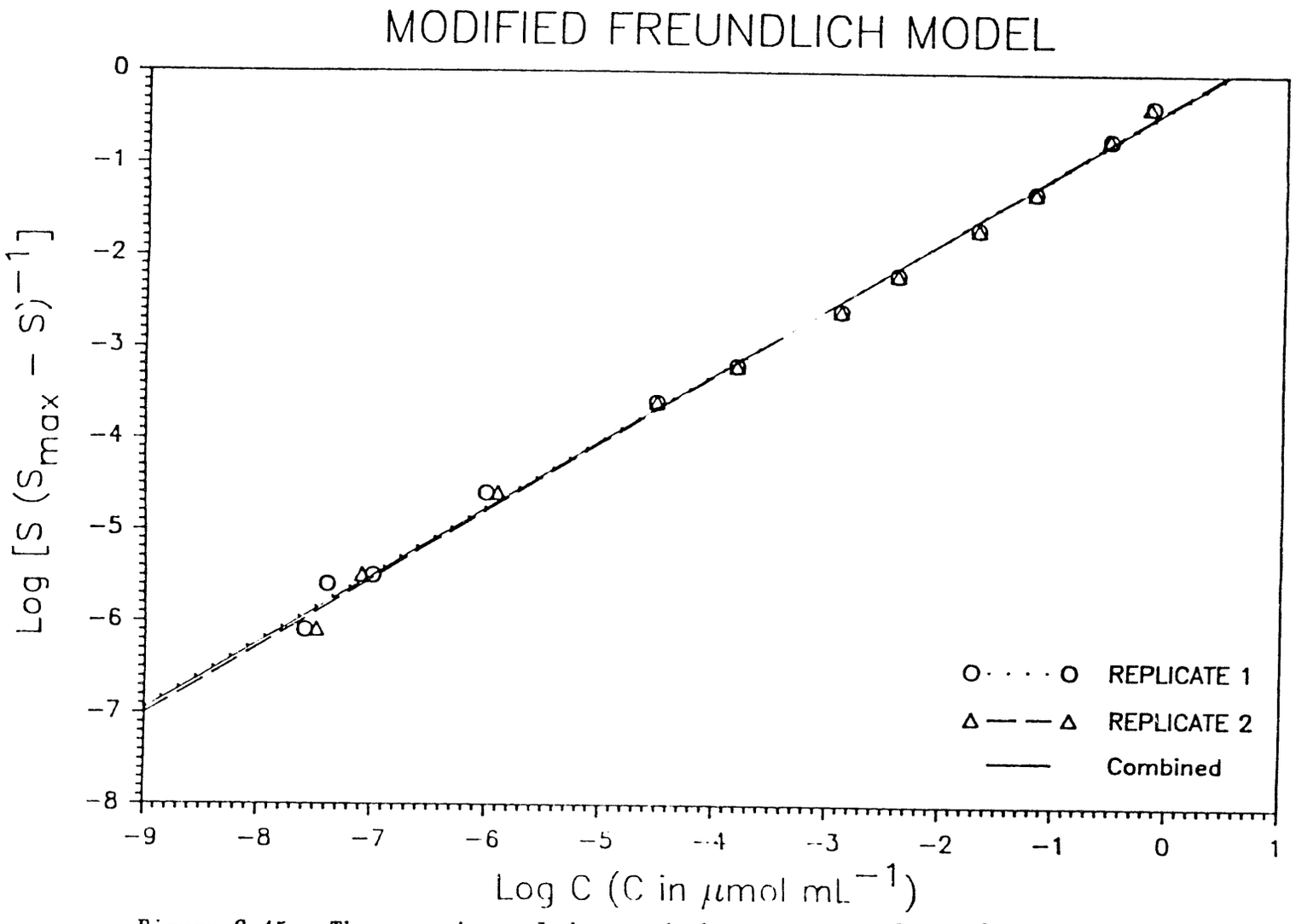

Figure C.45. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Cs 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION

ym-22 Cs 21 air - 75 amb 58.0 VERSUS ym-22 Cs 21 air 75-500 amb 44.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=30.43>Ft=5.14 (Different)	Fc=4.54<Ft=5.14 (Same)	Fc=0.05<Ft=5.14 (Same)	Fc=0.13<Ft=5.14 (Same)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

ym-22 Eu 21 air - 75 amb 58.0 VERSUS ym-22 Eu 21 air 75-500 amb 44.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.03<Ft=5.79 (Same)	Fc=1.79<Ft=5.79 (Same)	Fc=0.20<Ft=5.79 (Same)	Fc=0.06<Ft=5.79 (Same)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

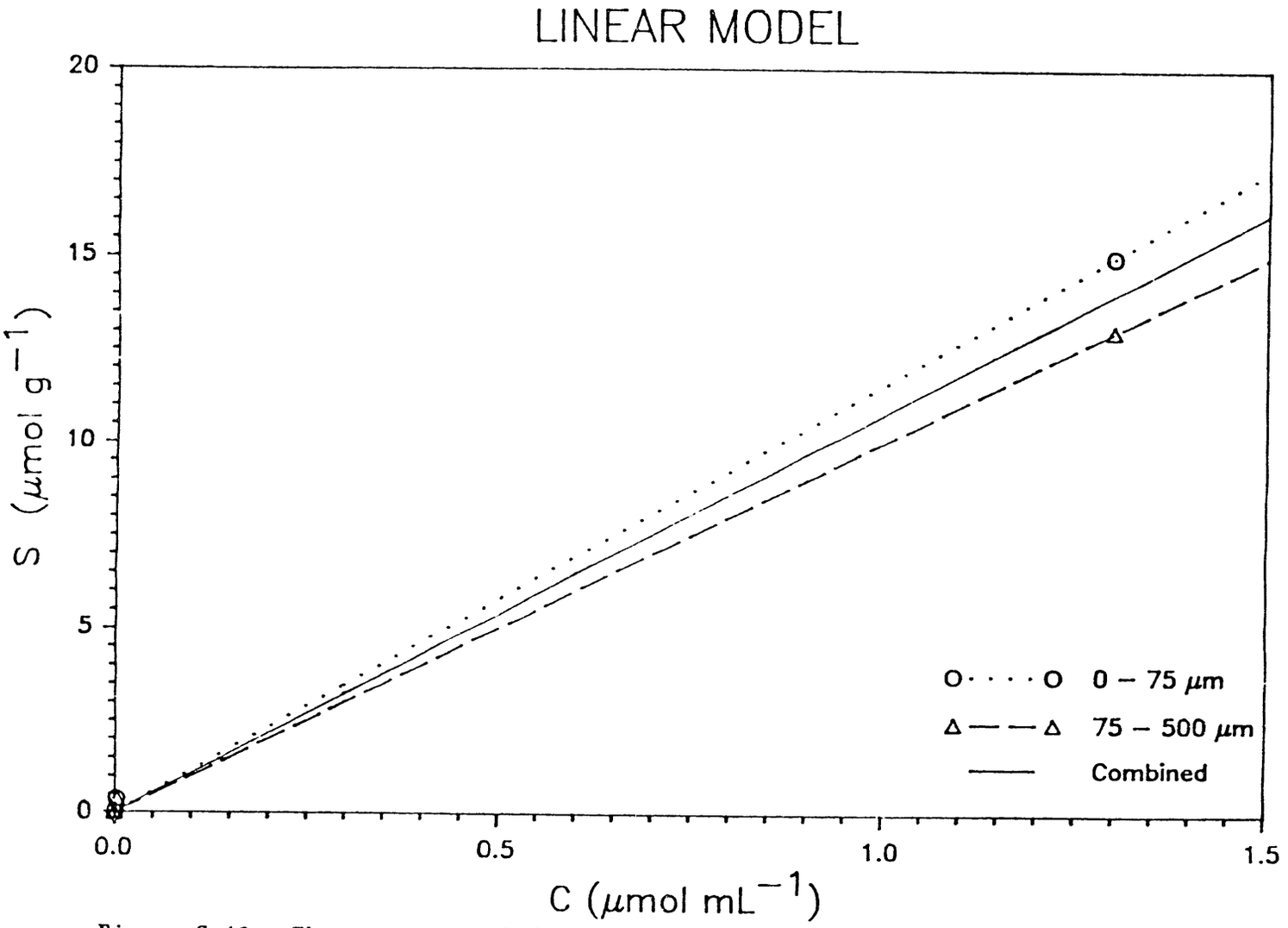

Figure C.46. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 58.0 and YM-22 Cs 21 air 75-500 amb 44.0; the variable being tested is particle size.

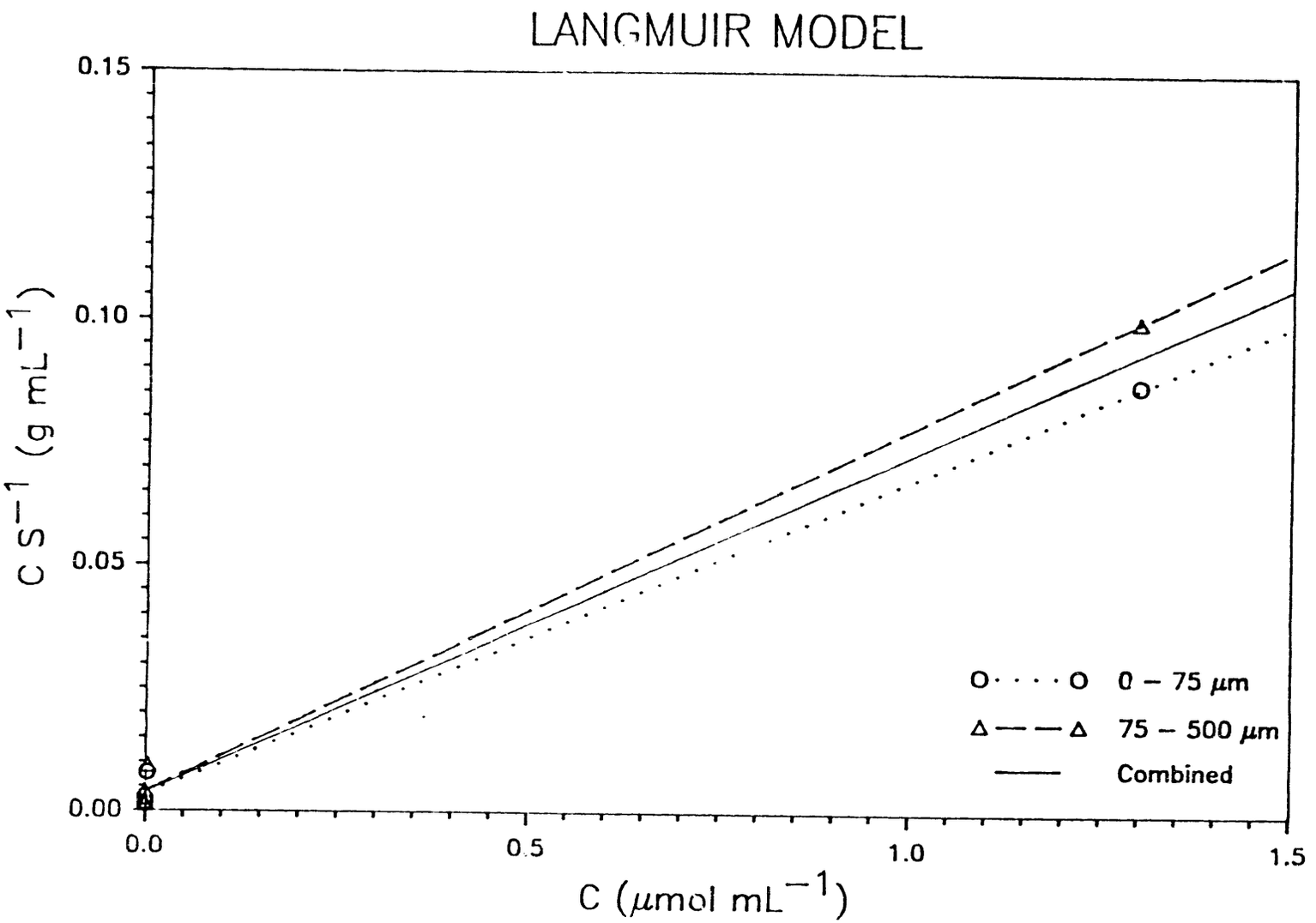

Figure C.47. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 58.0 and YM-22 Cs 21 air 75-500 amb 44.0; the variable being tested is particle size.

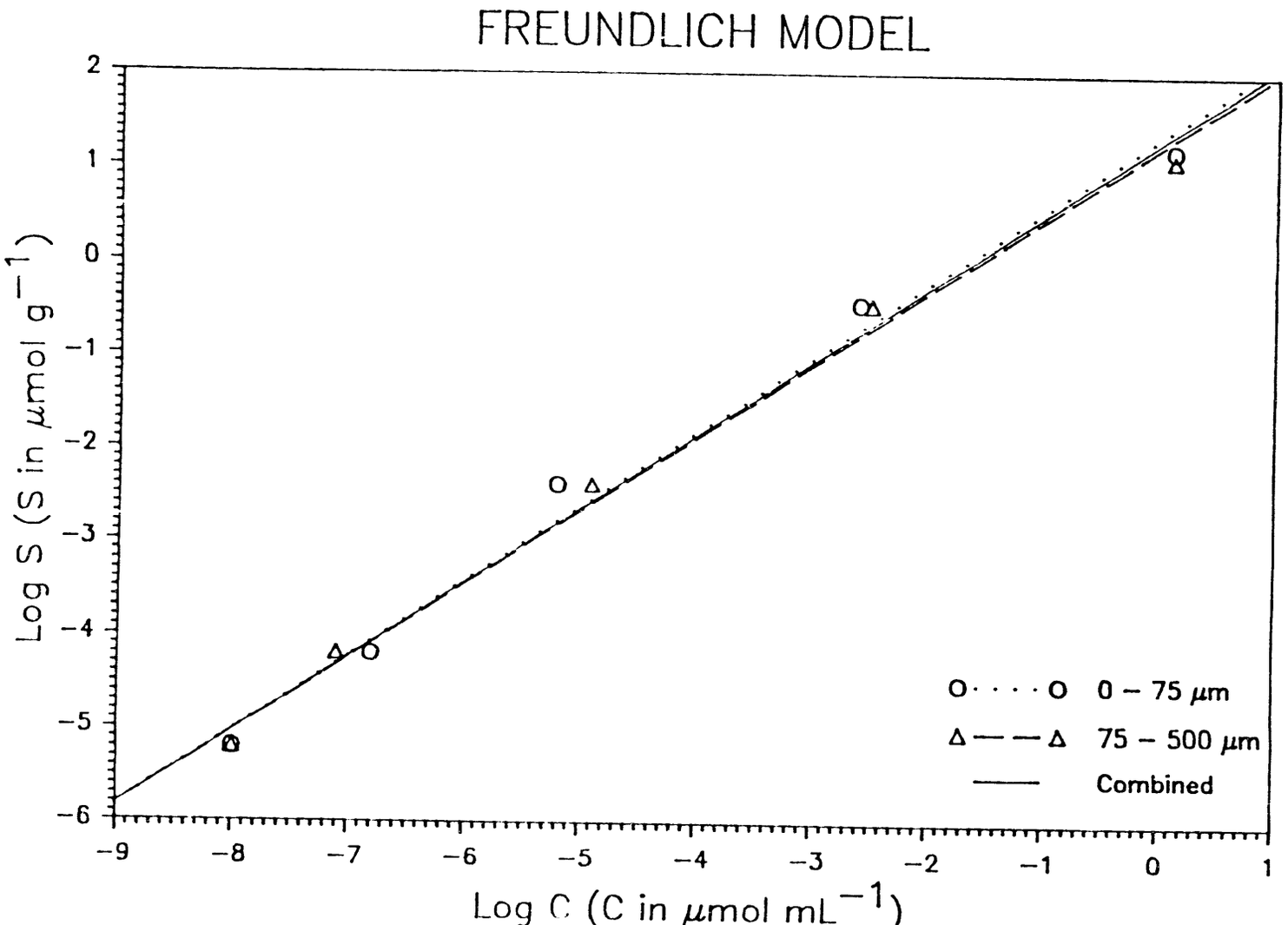

Figure C.48. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 58.0 and YM-22 Cs 21 air 75-500 amb 44.0; the variable being tested is particle size.

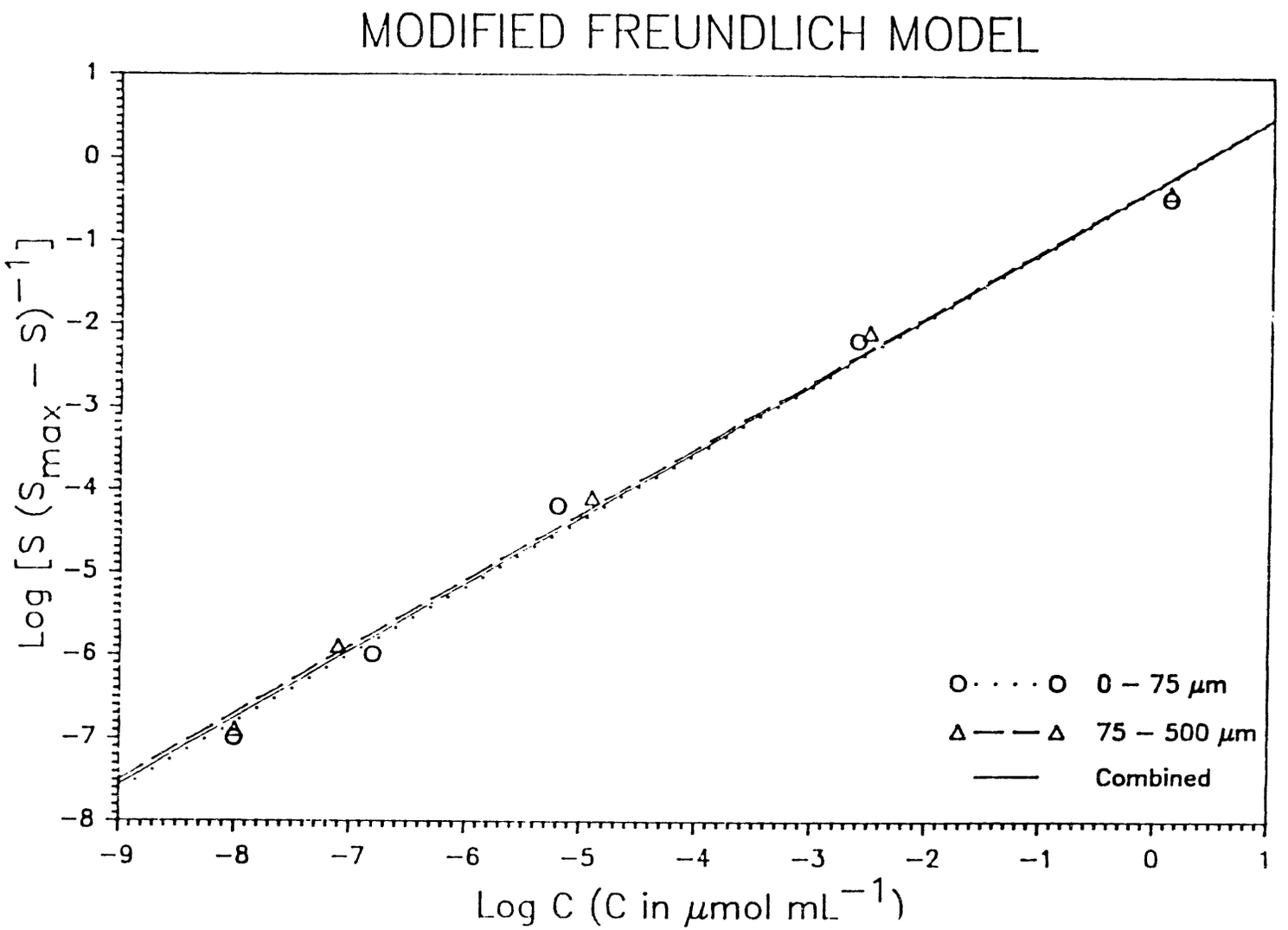

Figure C.49. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 58.0 and YM-22 Cs 21 air 75-500 amb 44.0; the variable being tested is particle size.

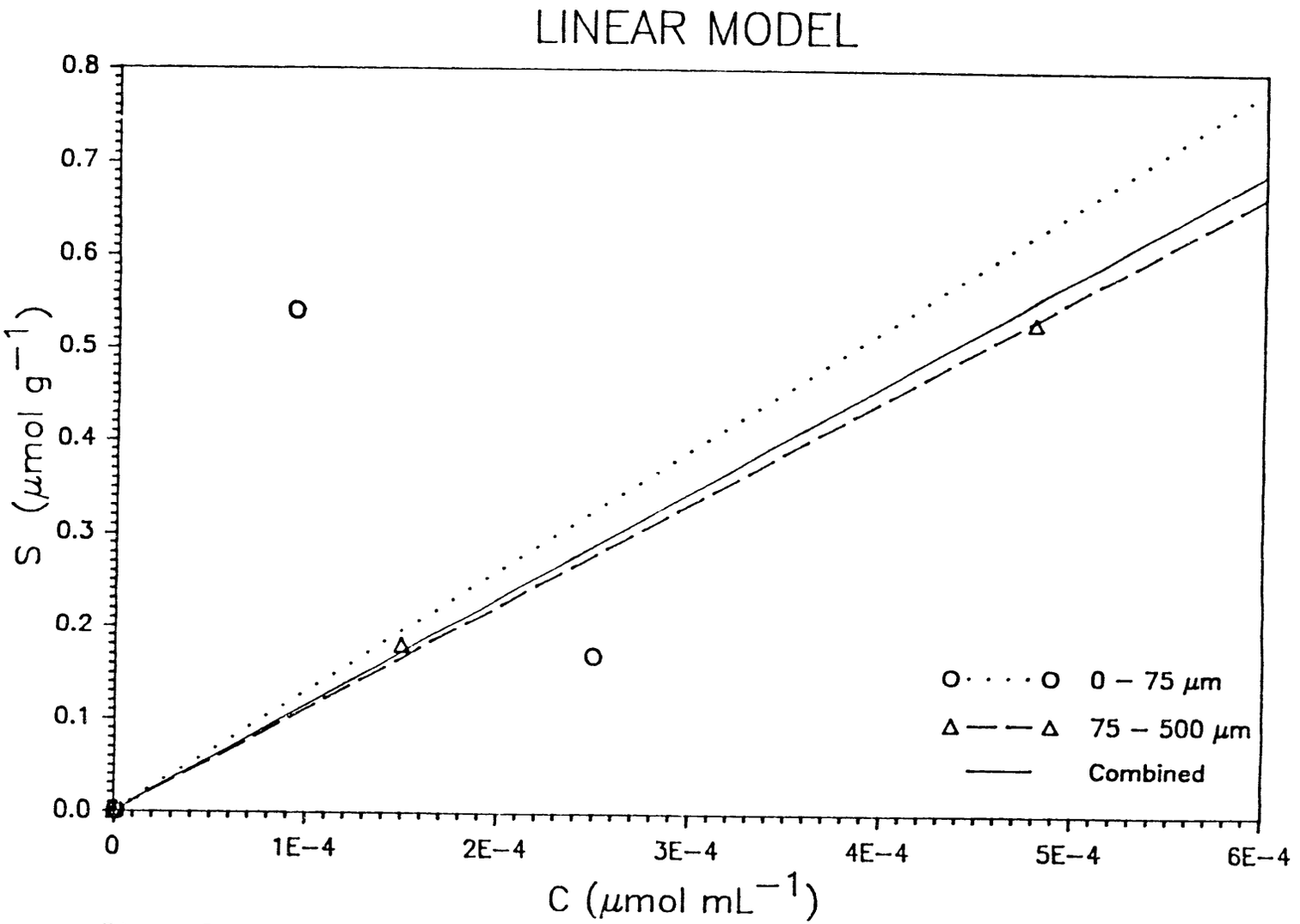

Figure C.50. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 58.0 and YM-22 Eu 21 air 75-500 amb 44.0; the variable being tested is particle size.

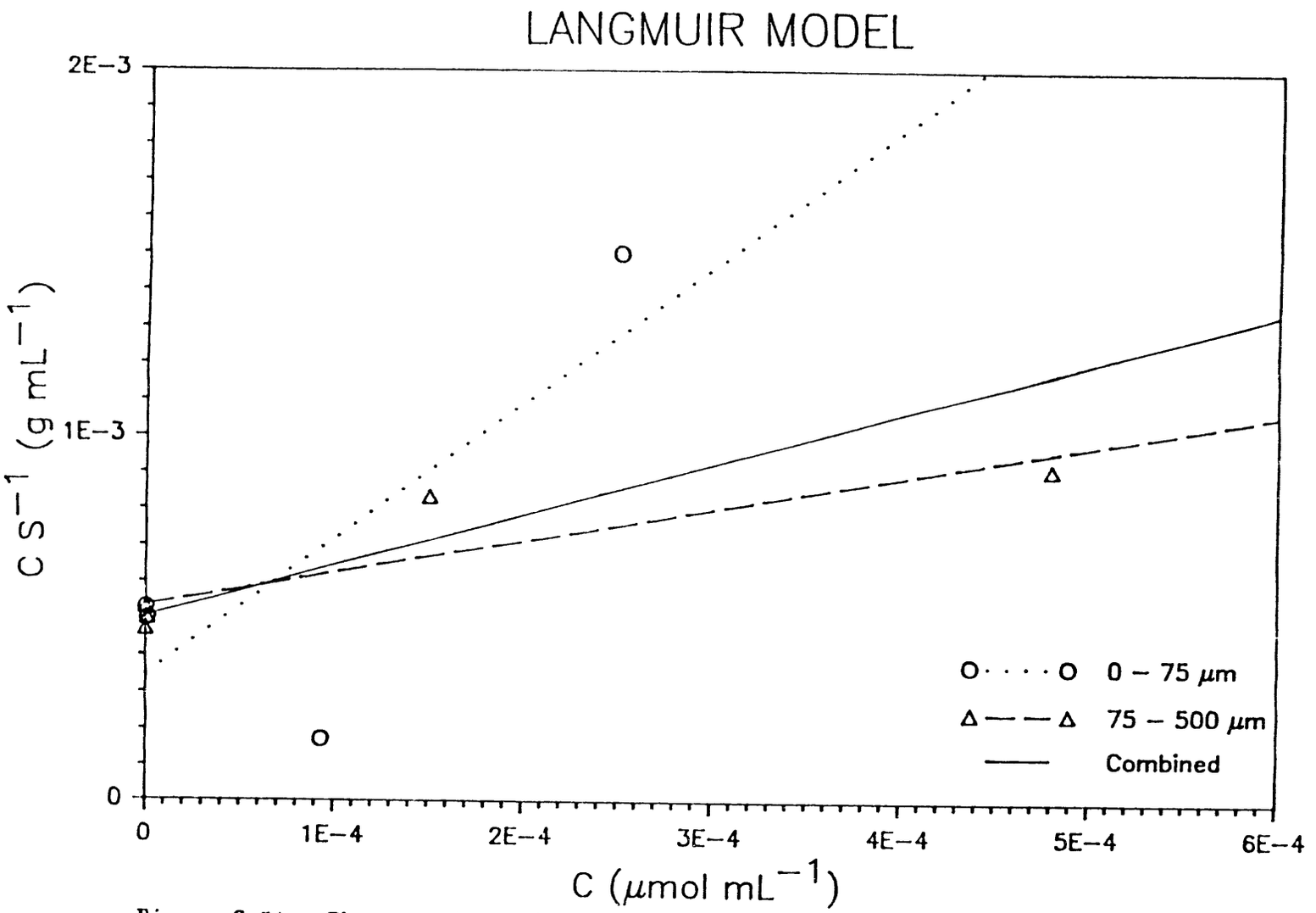

Figure C.51. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 58.0 and YM-22 Eu 21 air 75-500 amb 44.0; the variable being tested is particle size.

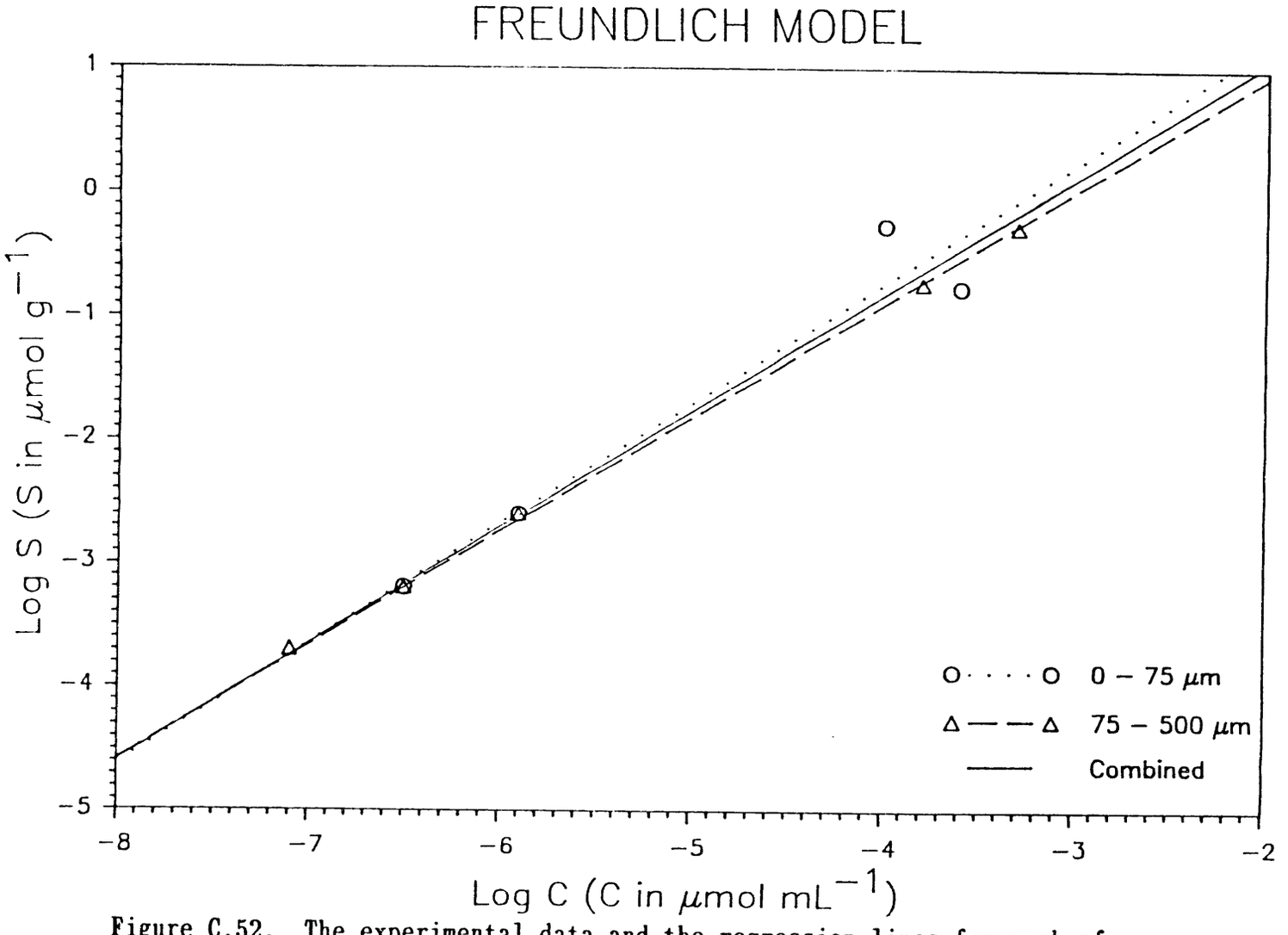

Figure C.52. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 58.0 and YM-22 Eu 21 air 75-500 amb 44.0; the variable being tested is particle size.

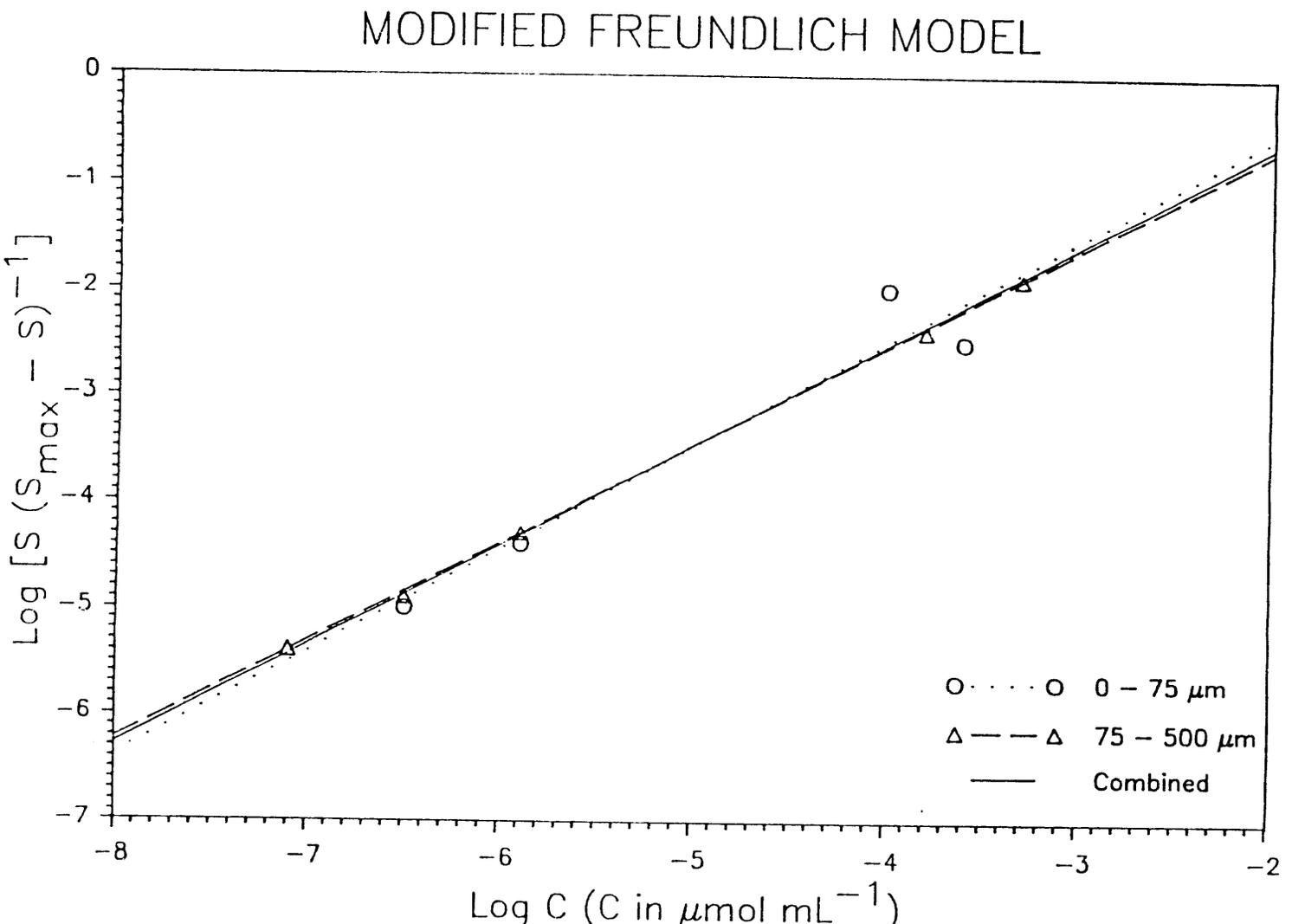

Figure C.53. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 58.0 and YM-22 Eu 21 air 75-500 amb 44.0; the variable being tested is particle size.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION

gl-2840 Sr 21 air 75-500 amb 43.0 VERSUS gl-2840 Sr 21 air 75-500 amb 43.0

Variable: Replication

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.00<Ft=3.47 (Same)	Fc=0.45<Ft=3.47 (Same)	Fc=0.12<Ft=3.47 (Same)	Fc=0.33<Ft=3.47 (Same)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

ym-22 Ba 21 air - 75 amb 14.0 VERSUS ym-22 Ba 21 air 75-500 amb 8.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=91.58>Ft=5.14 (Different)	Fc=6.82>Ft=5.14 (Different)	Fc=11.57>Ft=5.14 (Different)	Fc=3.05<Ft=5.14 (Same)
Intercept	n.a. n.a.	Fc=0.31<Ft=5.59 (Same)	Fc=0.12<Ft=5.59 (Same)	Fc=1.42<Ft=5.59 (Same)
Slope	Fc=0.00<Ft=5.59 (Same)	Fc=11.51>Ft=5.59 (Different)	Fc=3.44<Ft=5.59 (Same)	Fc=3.38<Ft=5.59 (Same)

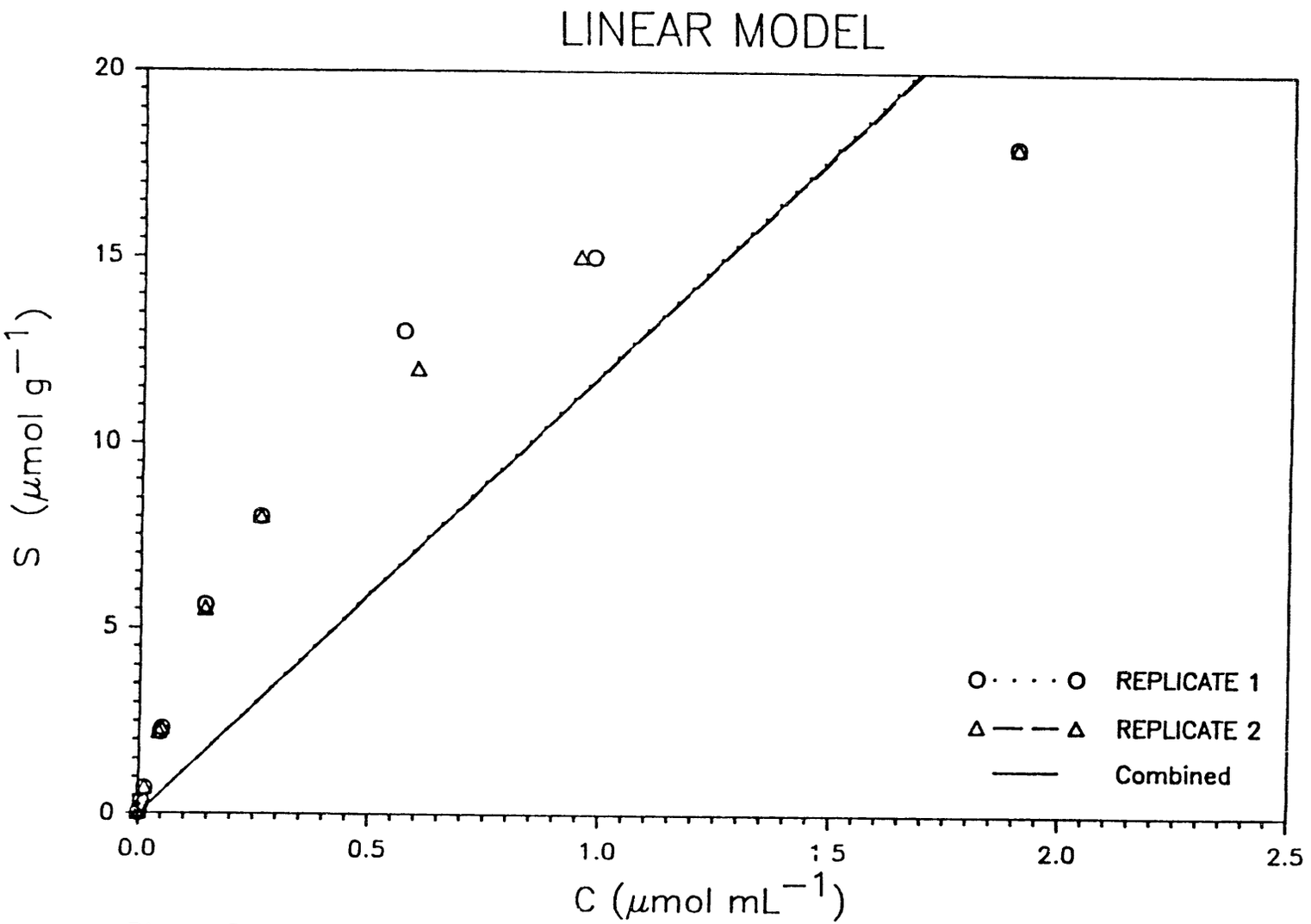

Figure C.54. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

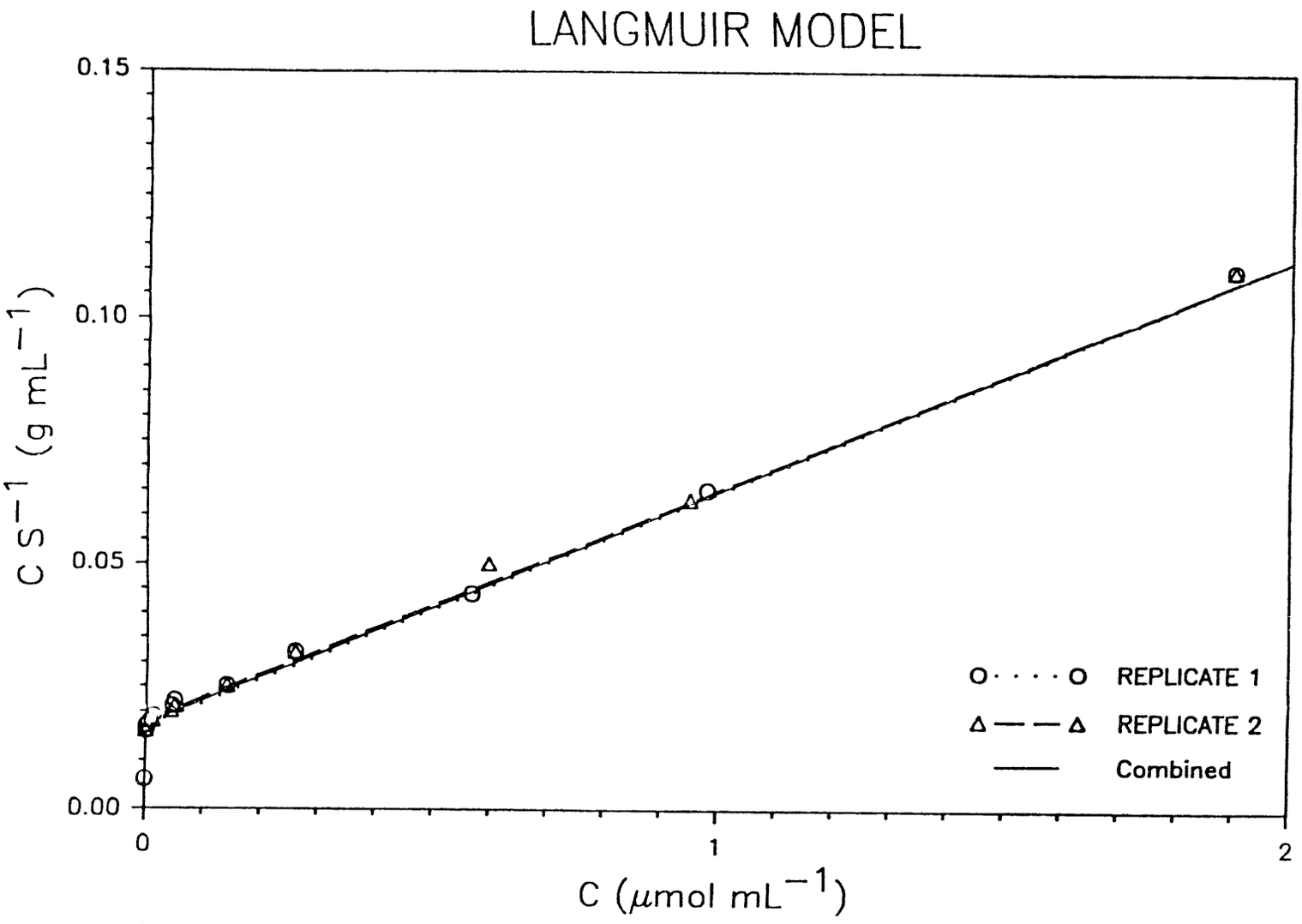

Figure C.55. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

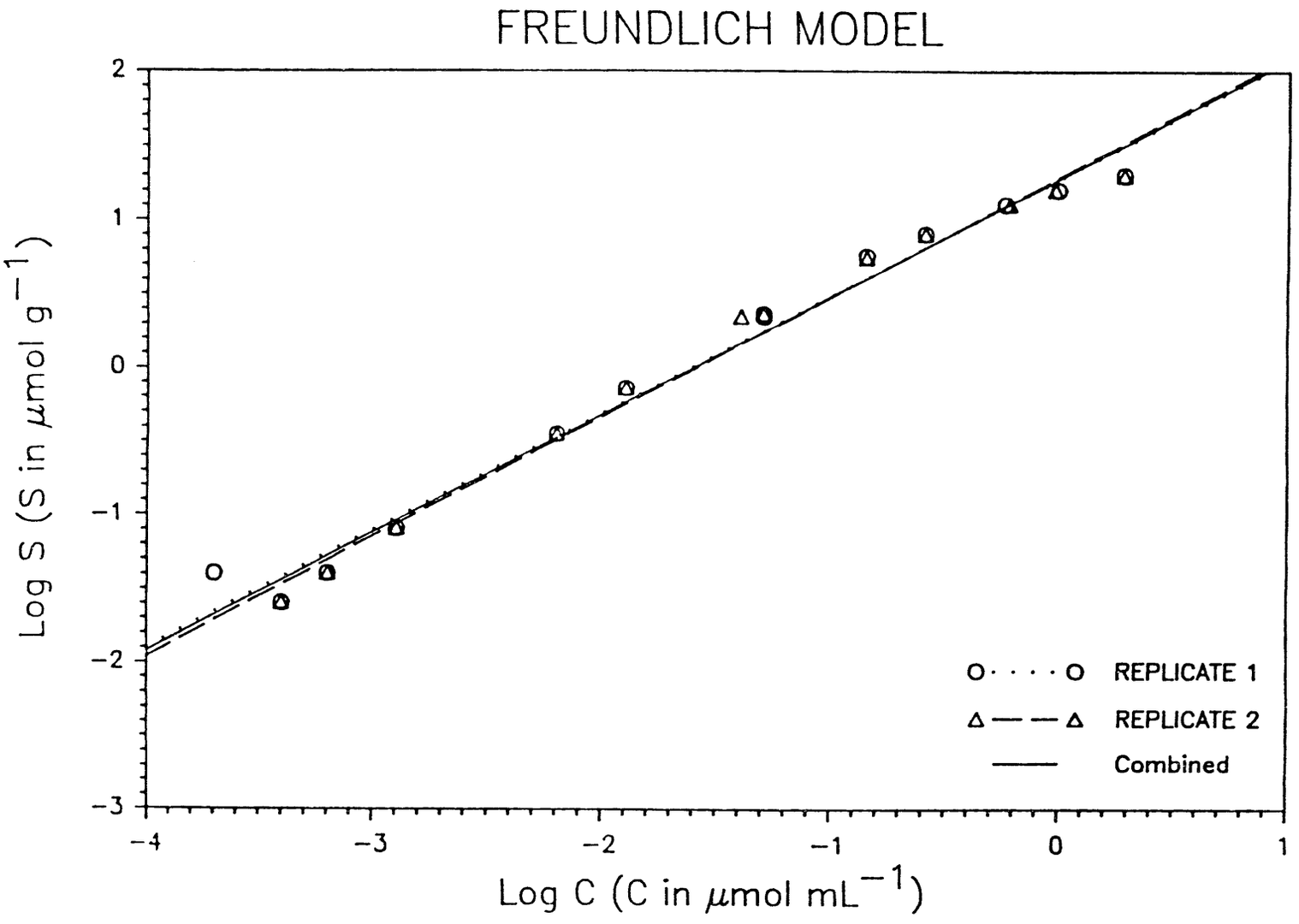

Figure C.56. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

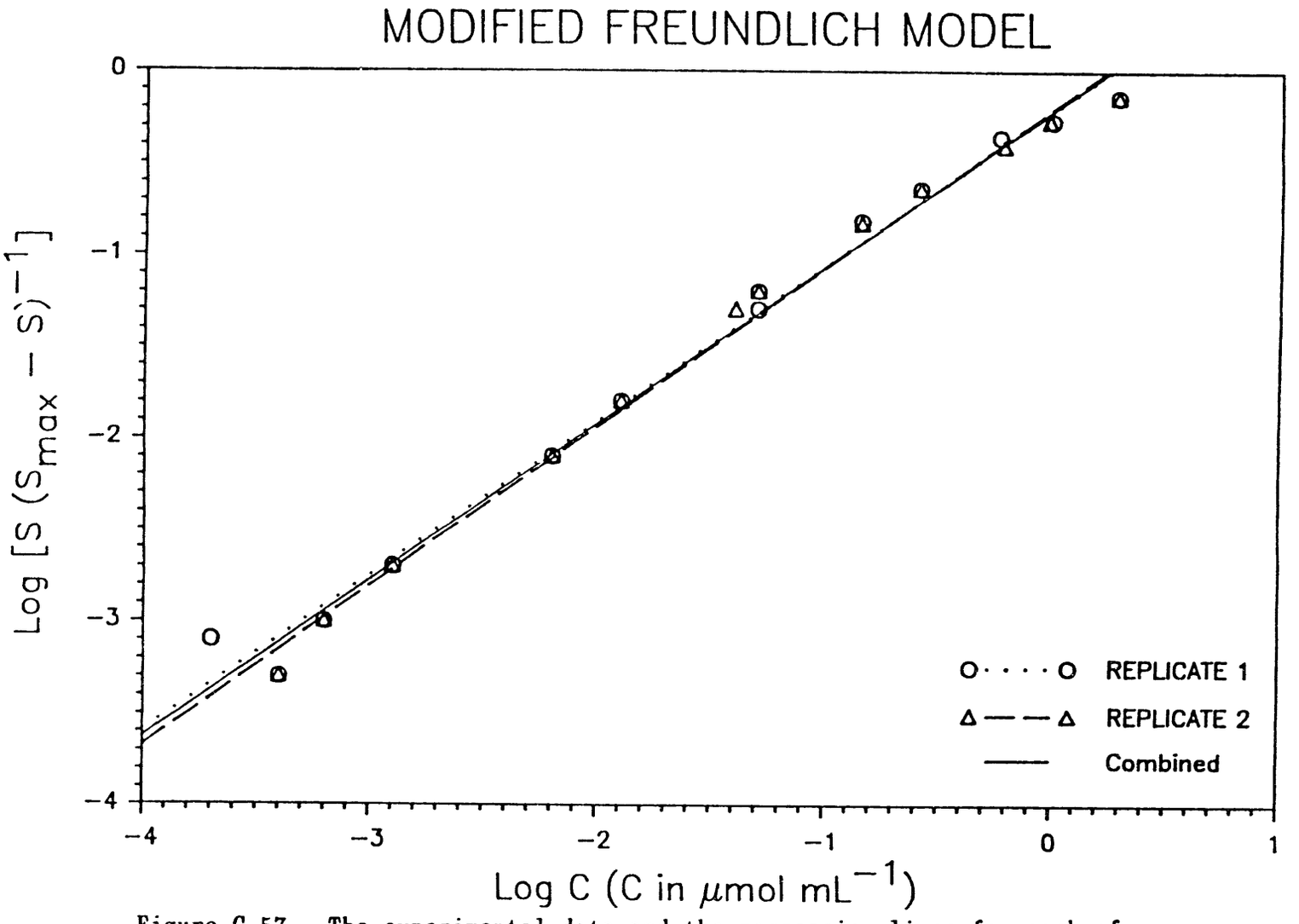

Figure C.57. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 1 and G1-2840 Sr 21 air 75-500 amb 43.0 Replicate 2; the variable being tested is replication.

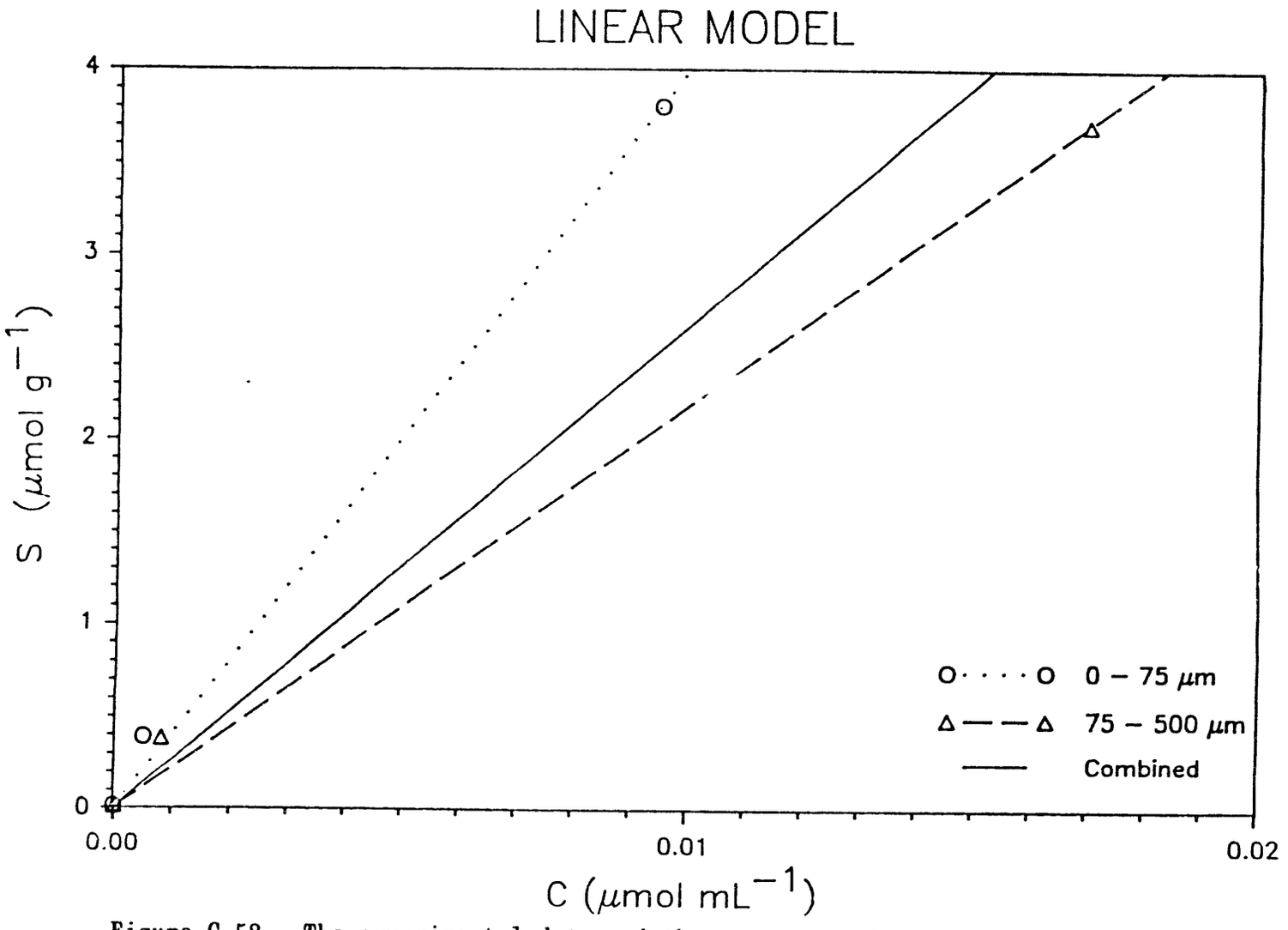

Figure C.58. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 14.0 and YM-22 Ba 21 air 75-500 amb 8.0; the variable being tested is particle size.

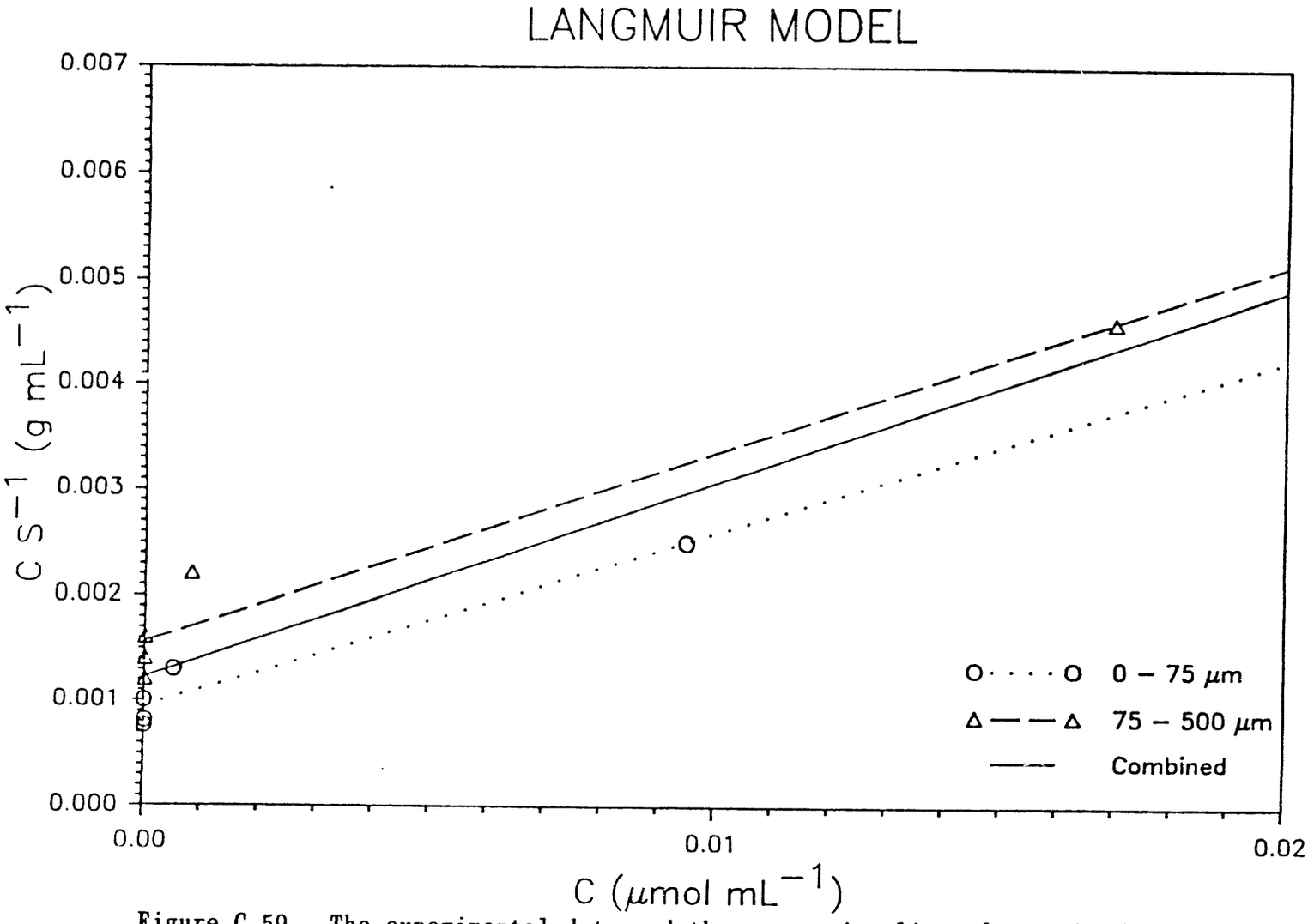

Figure C.59. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 14.0 and YM-22 Ba 21 air 75-500 amb 8.0; the variable being tested is particle size.

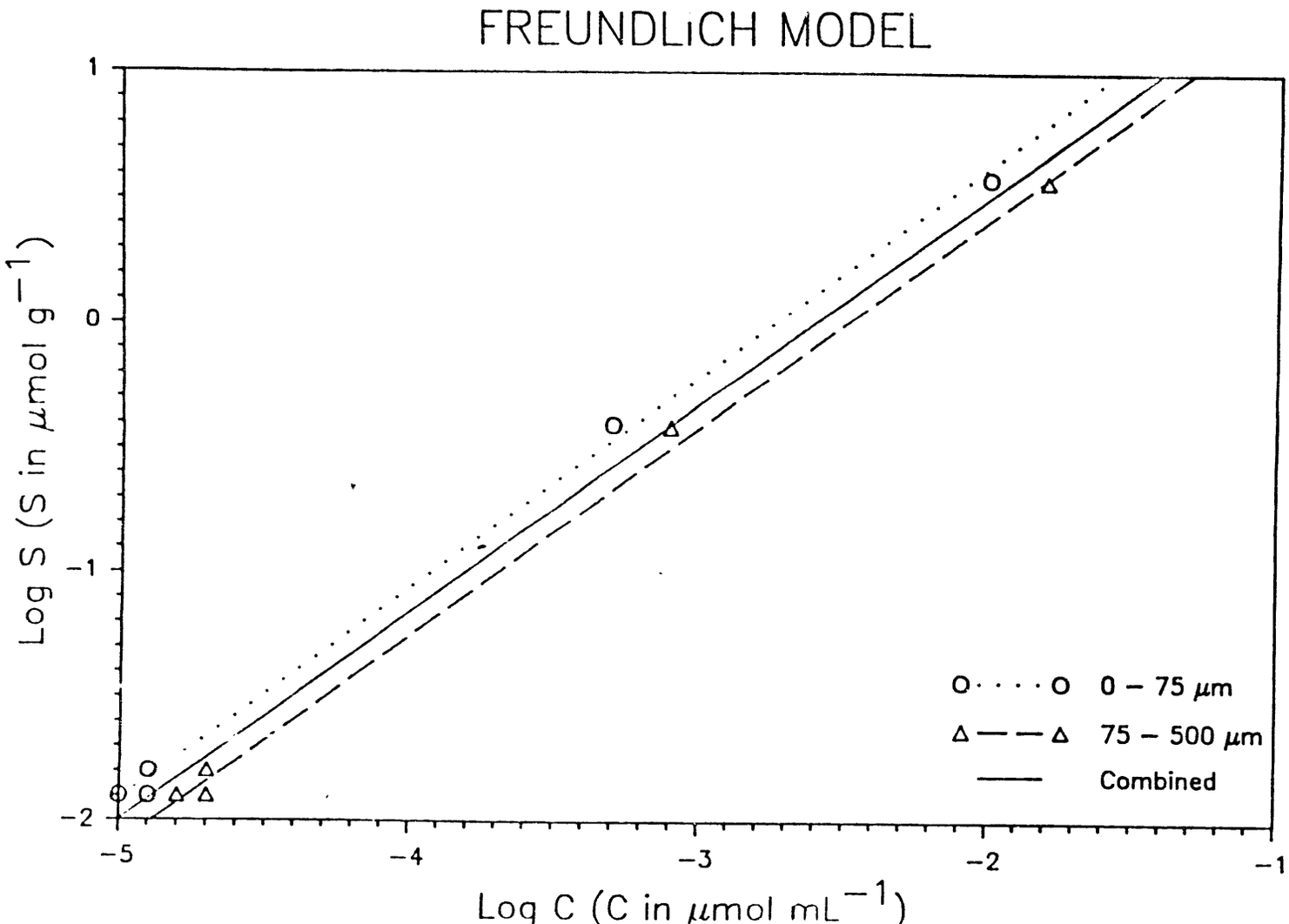

Figure C.60. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. the two data sets are YM-22 Ba 21 air -75 amb 14.0 and YM-22 Ba 21 air 75-500 amb 8.0; the variable being tested is particle size.

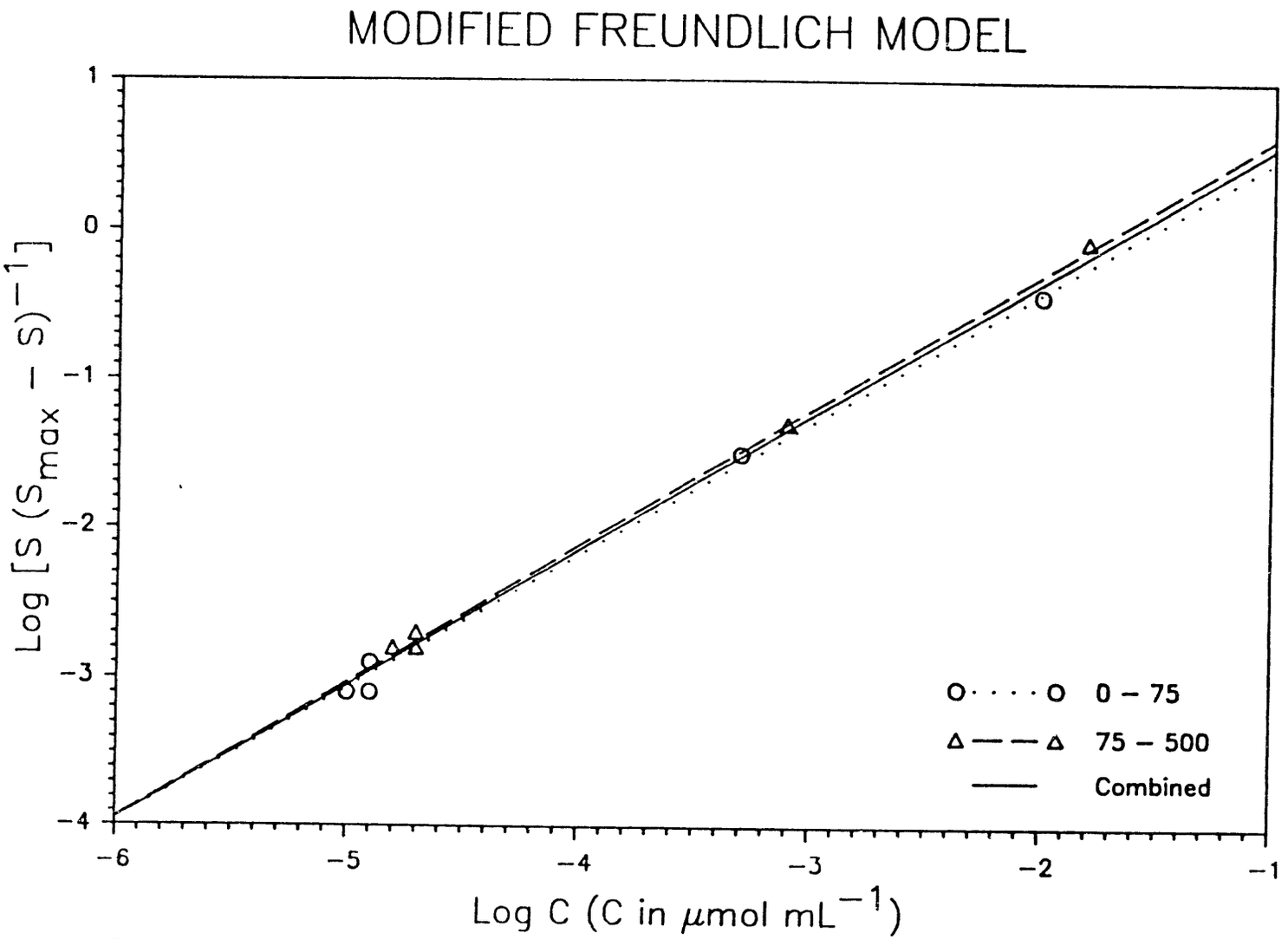

Figure C.61. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Ba 21 air -75 amb 14.0 and YM-22 Ba 21 air 75-500 amb 8.0; the variable being tested is particle size.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS; ADSORPTION

ym-22 Cs 21 air - 75 amb 14.0 VERSUS ym-22 Cs 21 air 75-500 amb 8.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=233.80>Ft=6.94 (Different)	Fc=0.19<Ft=6.94 (Same)	Fc=0.24<Ft=6.94 (Same)	Fc=1.48<Ft=6.94 (Same)
Intercept	n.a. n.a.	Fc=0.03<Ft=6.61 (Same)	Fc=0.40<Ft=6.61 (Same)	Fc=0.39<Ft=6.61 (Same)
Slope	Fc=0.00<Ft=6.61 (Same)	Fc=0.28<Ft=6.61 (Same)	Fc=0.56<Ft=6.61 (Same)	Fc=0.00<Ft=6.61 (Same)

ym-22 Eu 21 air - 75 amb 14.0 VERSUS ym-22 Eu 21 air 75-500 amb 8.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.03<Ft=5.79 (Same)	Fc=1.79<Ft=5.79 (Same)	Fc=0.20<Ft=5.79 (Same)	Fc=0.29<Ft=5.79 (Same)
Intercept	n.a. n.a.	Fc=4.05<Ft=5.99 (Same)	Fc=0.13<Ft=5.99 (Same)	Fc=0.12<Ft=5.99 (Same)
Slope	Fc=0.00<Ft=6.61 (Same)	Fc=0.62<Ft=6.61 (Same)	Fc=0.21<Ft=6.61 (Same)	Fc=0.02<Ft=6.61 (Same)

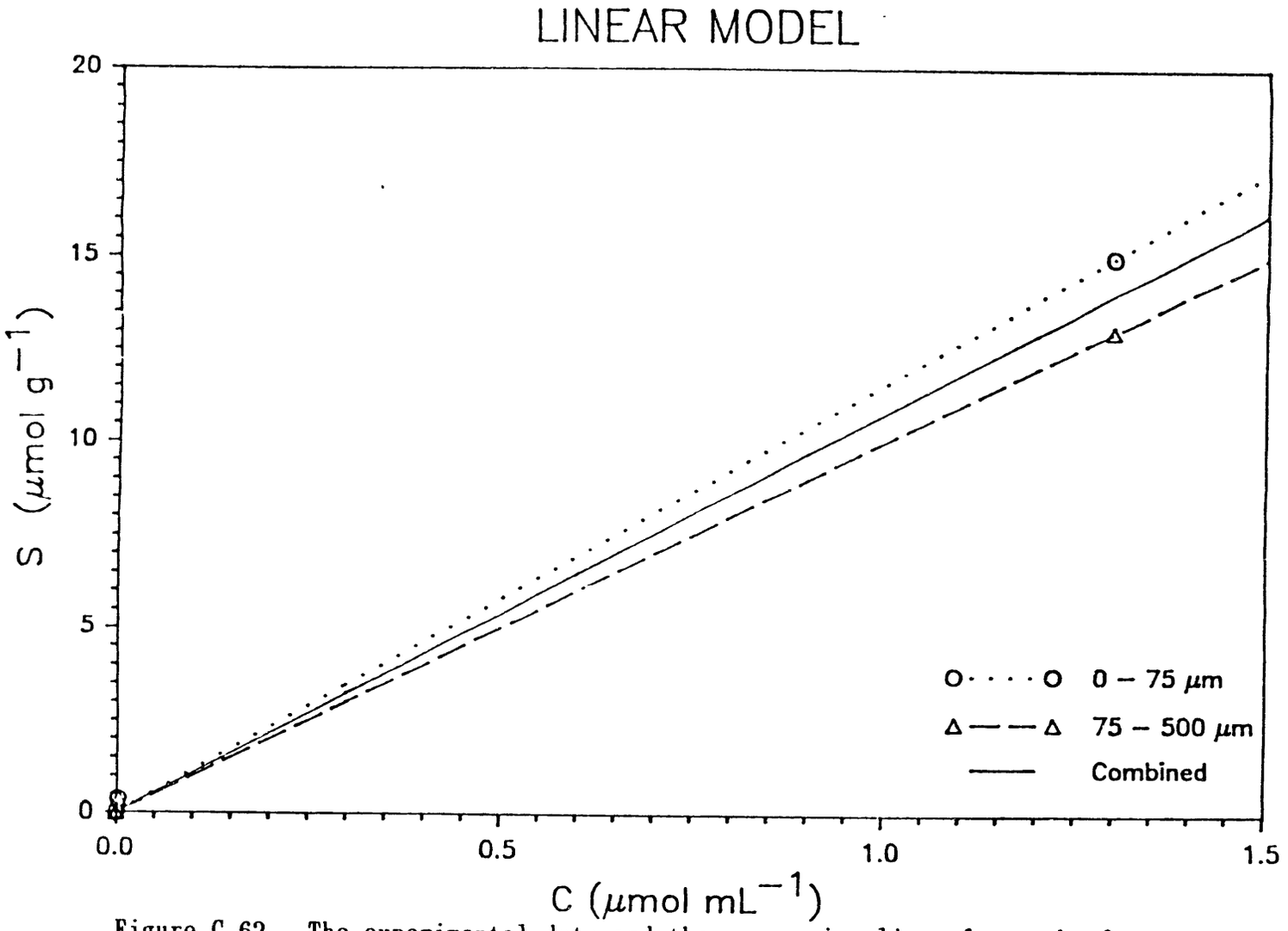

Figure C.62. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 14.0 and YM-22 Cs 21 air 75-500 amb 8.0; the variable being tested is particle size.

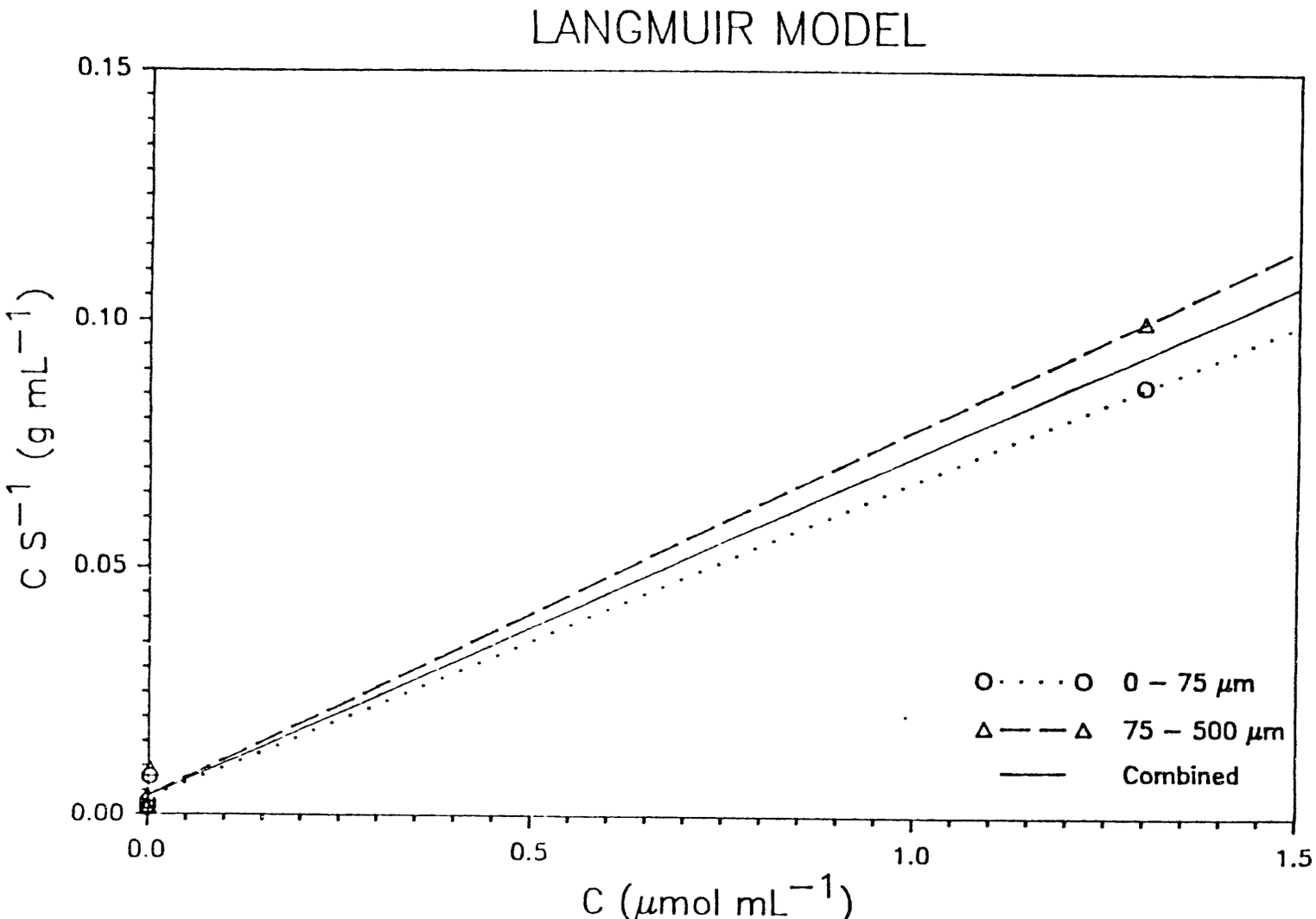

Figure C.63. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 14.0 and YM-22 Cs 21 air 75-500 amb 8.0; the variable being tested is particle size.

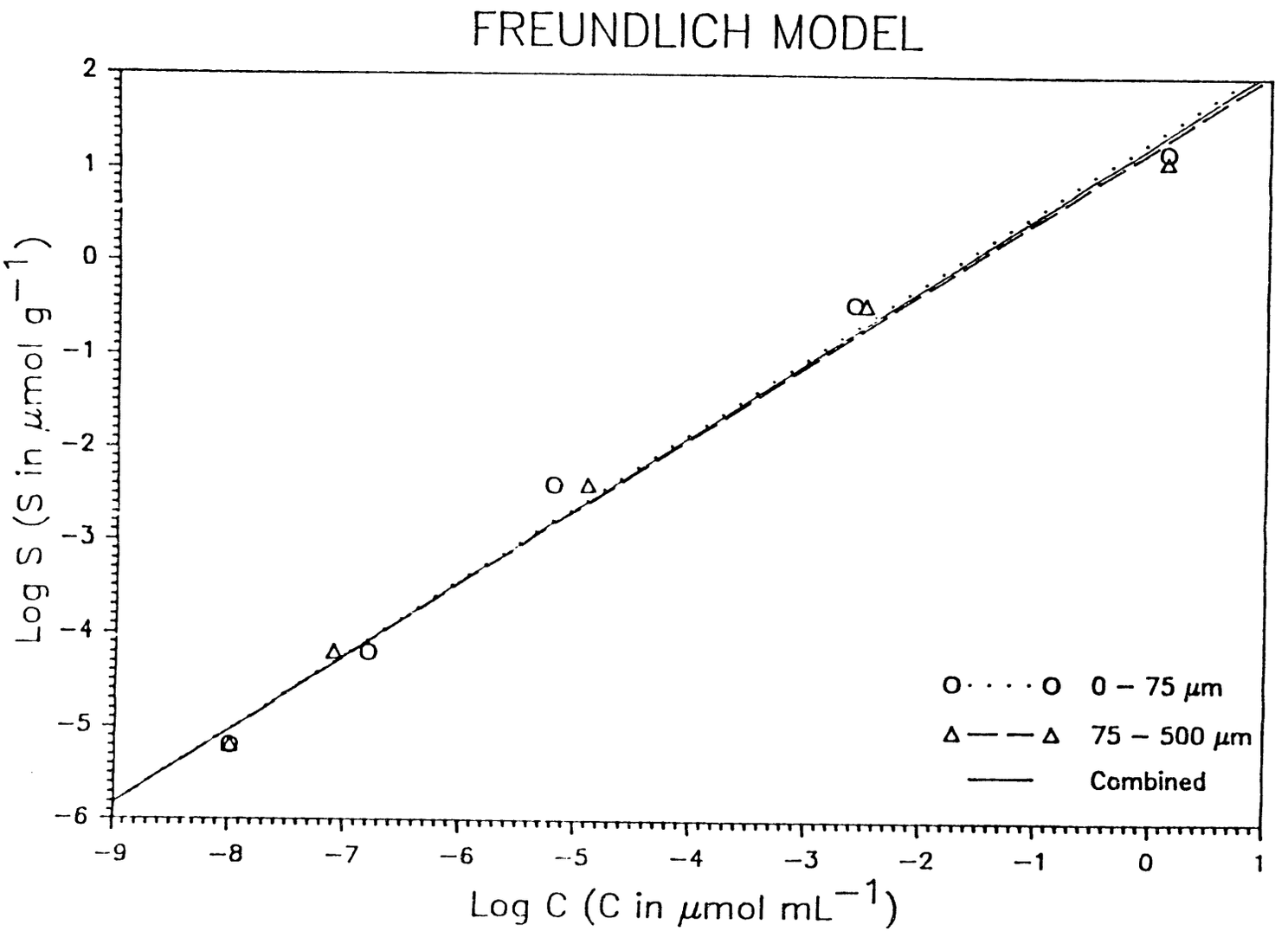

Figure C.64. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 14.0 and YM-22 Cs 21 air 75-500 amb 8.0; the variable being tested is particle size.

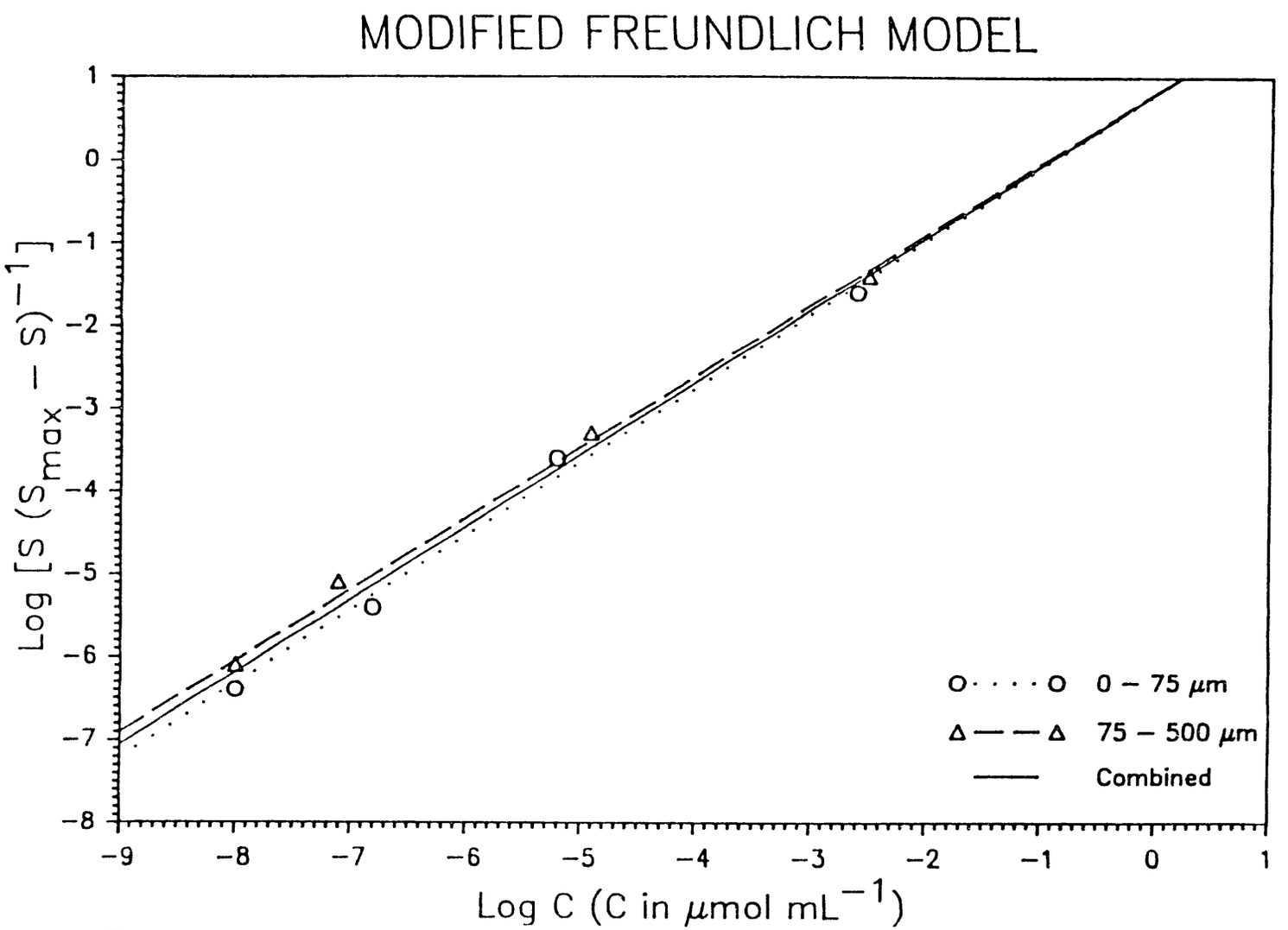

Figure C.65. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Cs 21 air -75 amb 14.0 and YM-22 Cs 21 air 75-500 amb 8.0; the variable being tested is particle size.

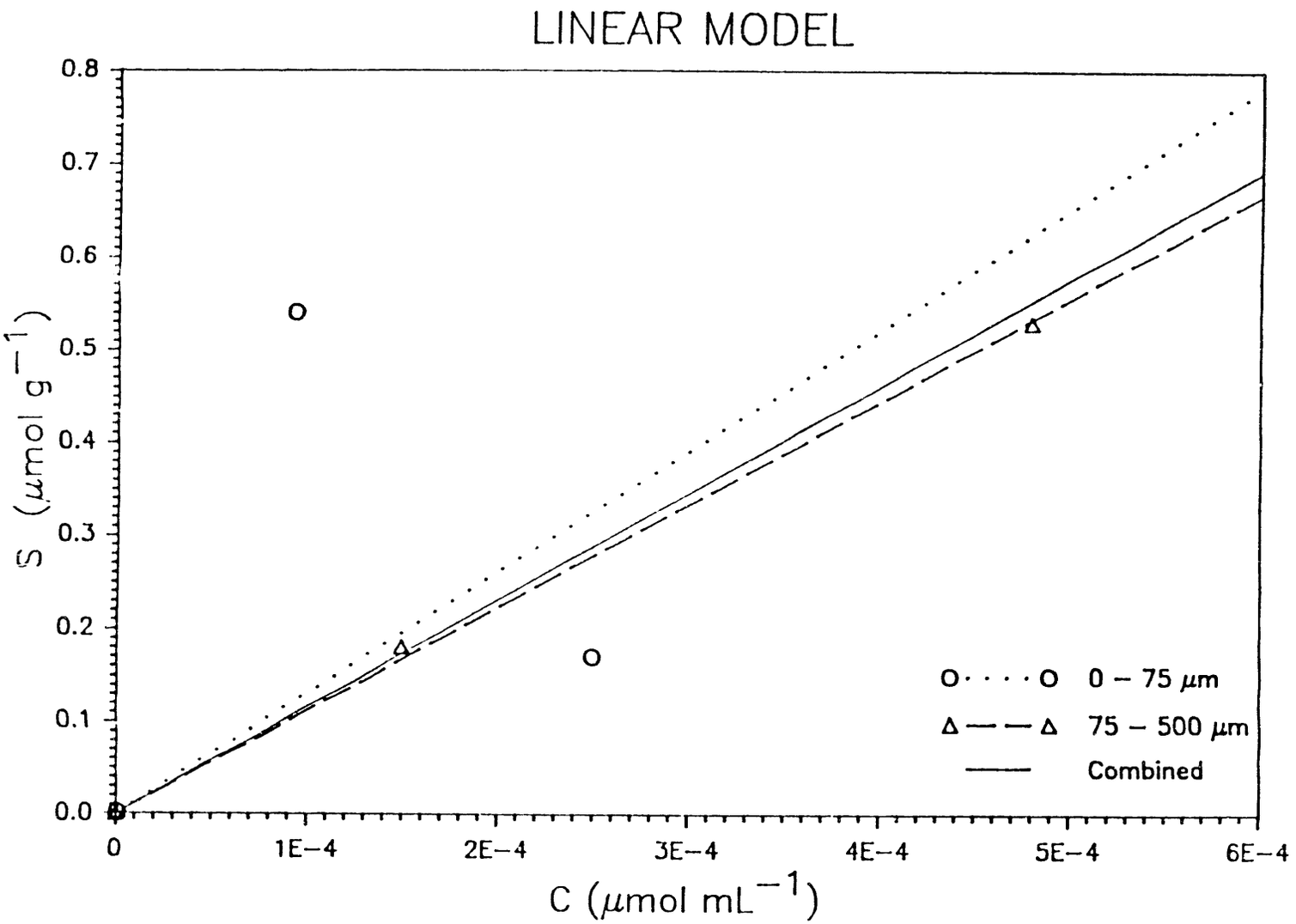

Figure C.66. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM 22 Eu 21 air -75 amb 14.0 and YM-22 Eu 21 air 75-500 amb 8.0; the variable being tested is particle size.

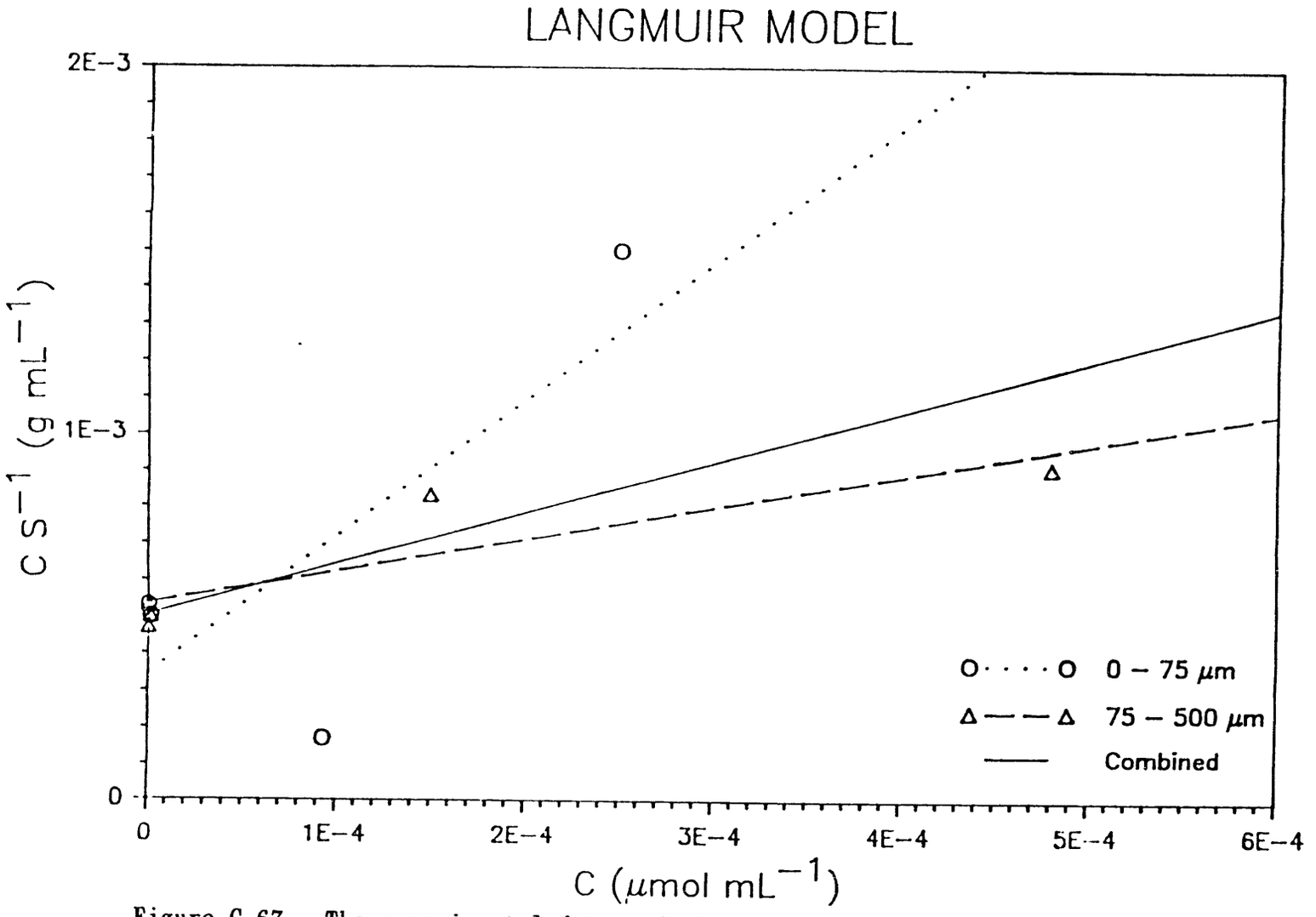

Figure C.67. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 14.0 and YM-22 Eu 21 air 75-500 amb 8.0; the variable being tested is particle size.

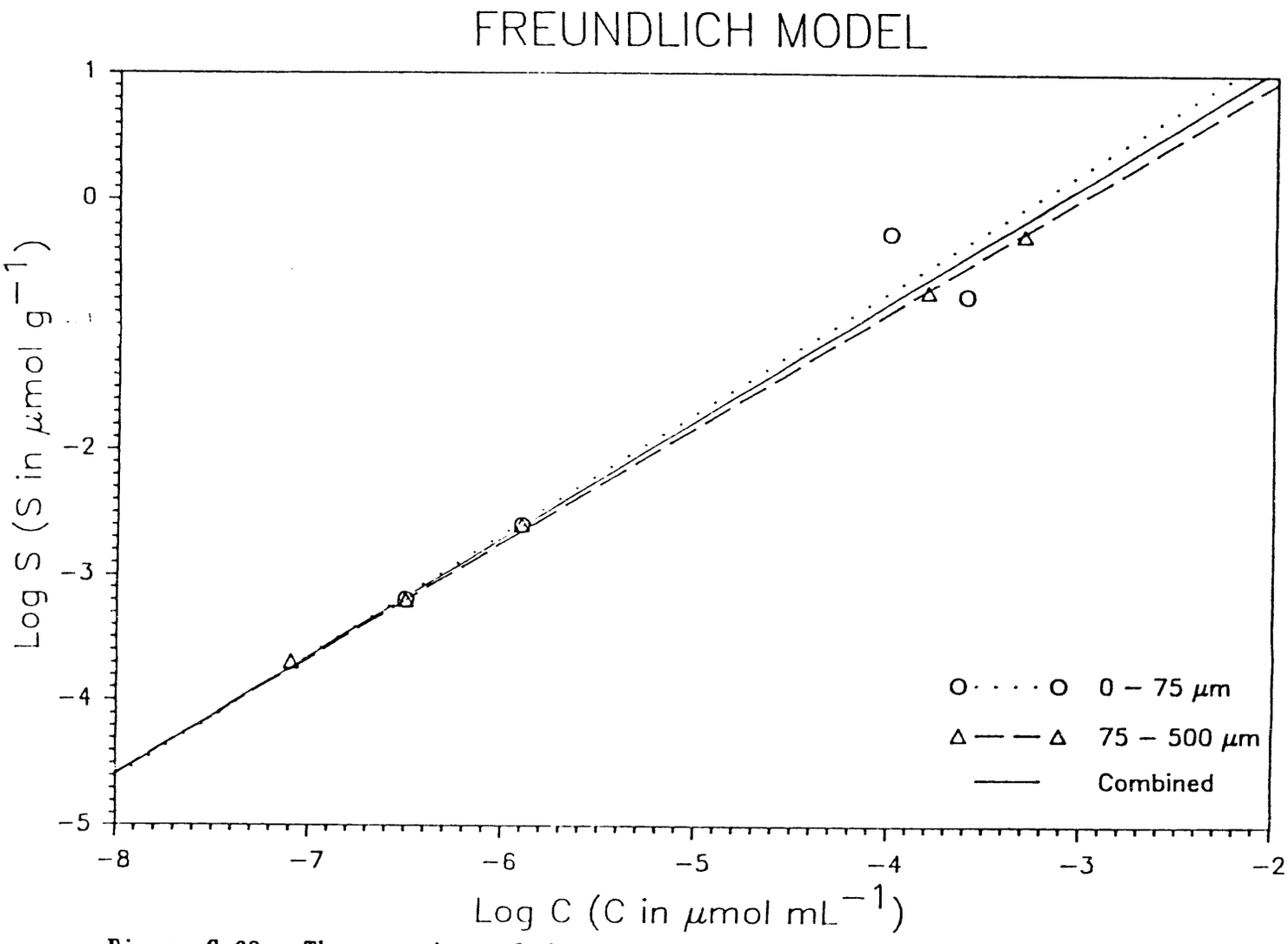

Figure C.68. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 14.0 and YM-22 Eu 21 air 75-500 amb 8.0; the variable being tested is particle size.

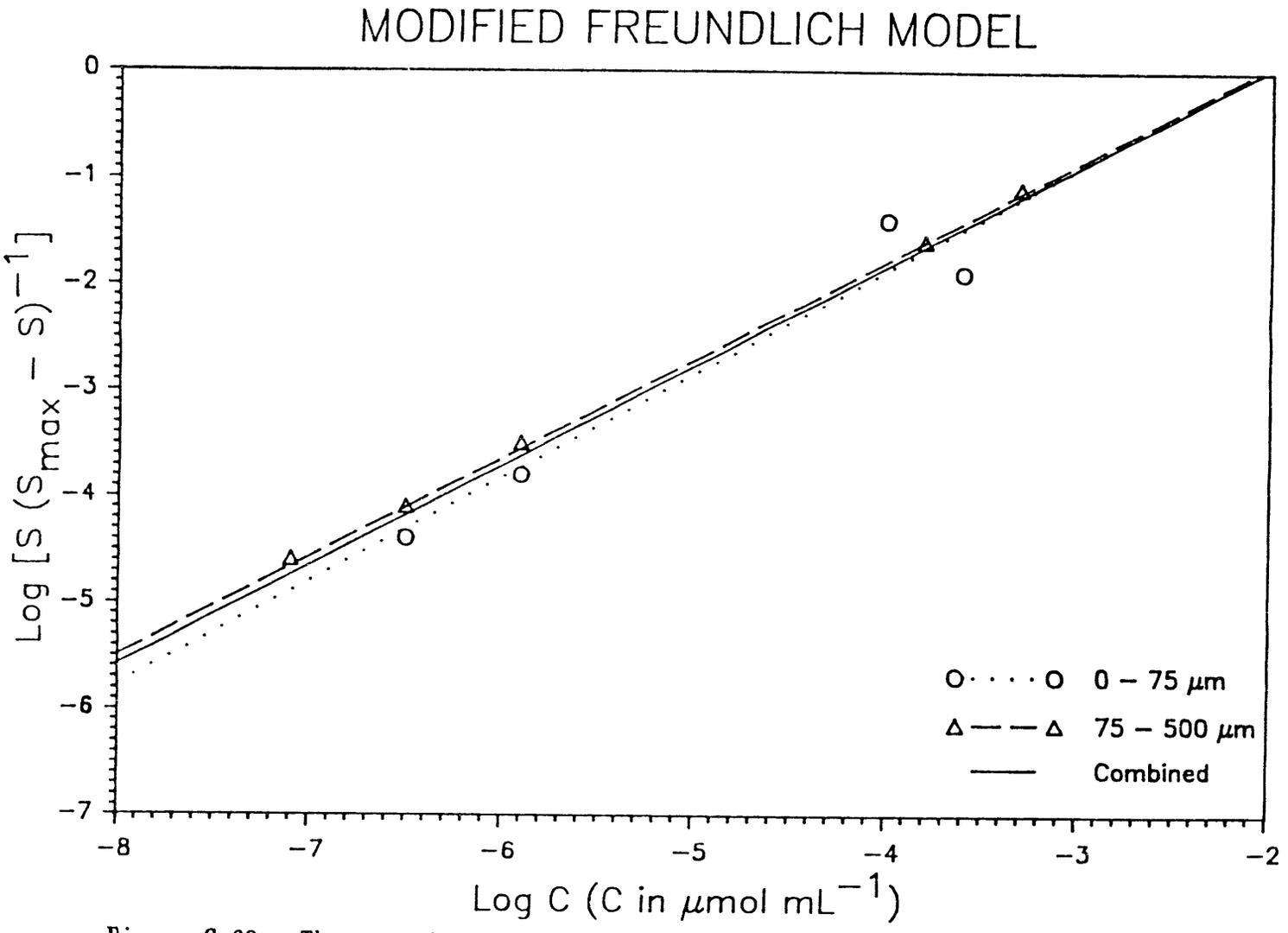

Figure C.69. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Eu 21 air -75 amb 14.0 and YM-22 Eu 21 air 75-500 amb 8.0; the variable being tested is particle size.

TABLE C.I (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION

ym-22 Sr 21 air - 75 amb 14.0 VERSUS ym-22 Sr 21 air 75-500 amb 8.0

Variable: Particle Size

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=0.00<Ft=6.94 (Same)	Fc=0.11<Ft=6.94 (Same)	Fc=0.14<Ft=6.94 (Same)	Fc=16.14>Ft=6.94 (Different)
Intercept	n.a. n.a.	Fc=0.07<Ft=6.61 (Same)	Fc=0.10<Ft=6.61 (Same)	Fc=0.01<Ft=6.61 (Same)
Slope	Fc=0.00<Ft=6.61 (Same)	Fc=0.28<Ft=6.61 (Same)	Fc=0.03<Ft=6.61 (Same)	Fc=2.12<Ft=6.61 (Same)

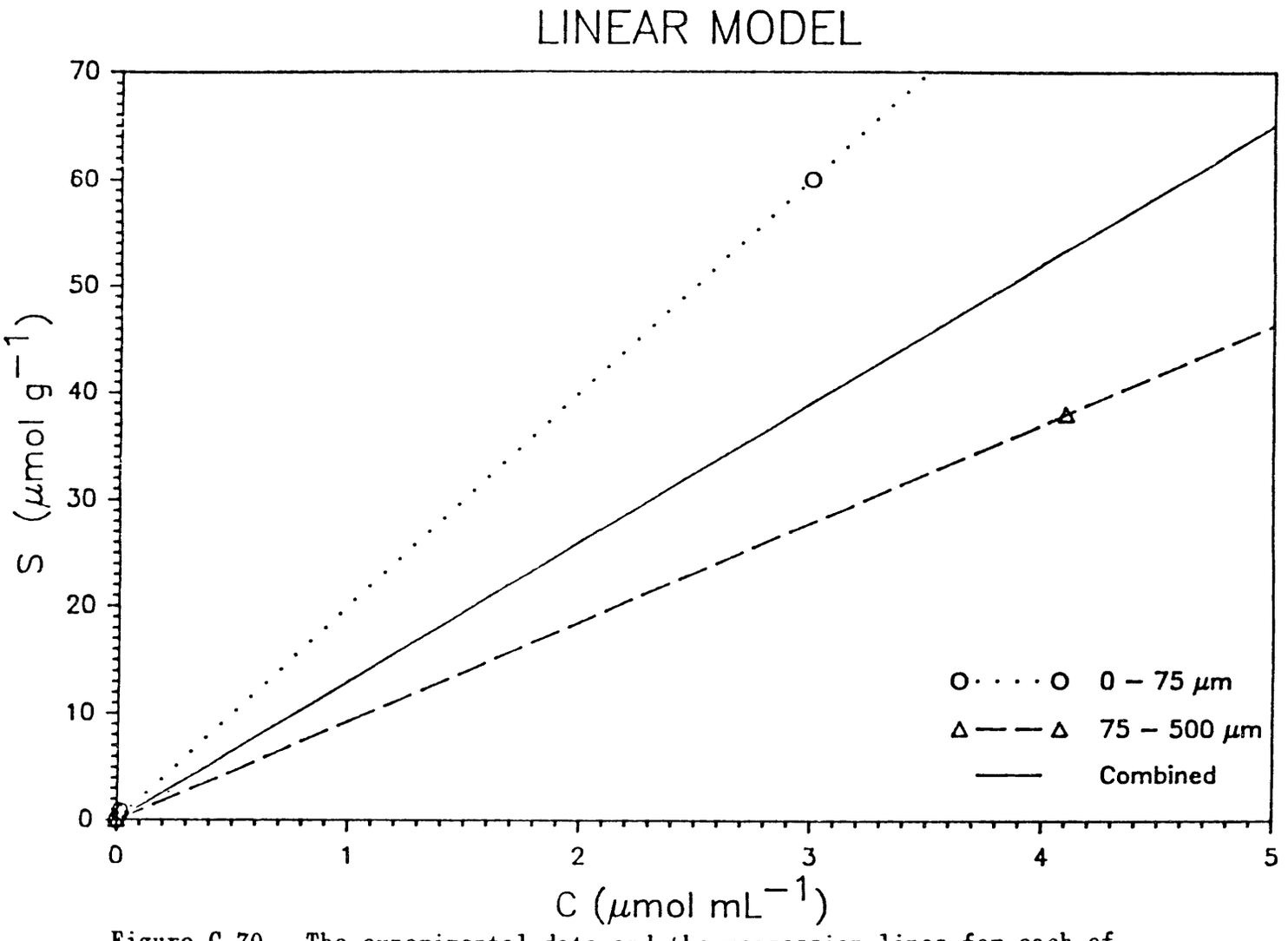

Figure C.70. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-22 Sr 21 air -75 amb 14.0 and YM-22 Sr 21 air 75-500 amb 8.0; the variable being tested is particle size.

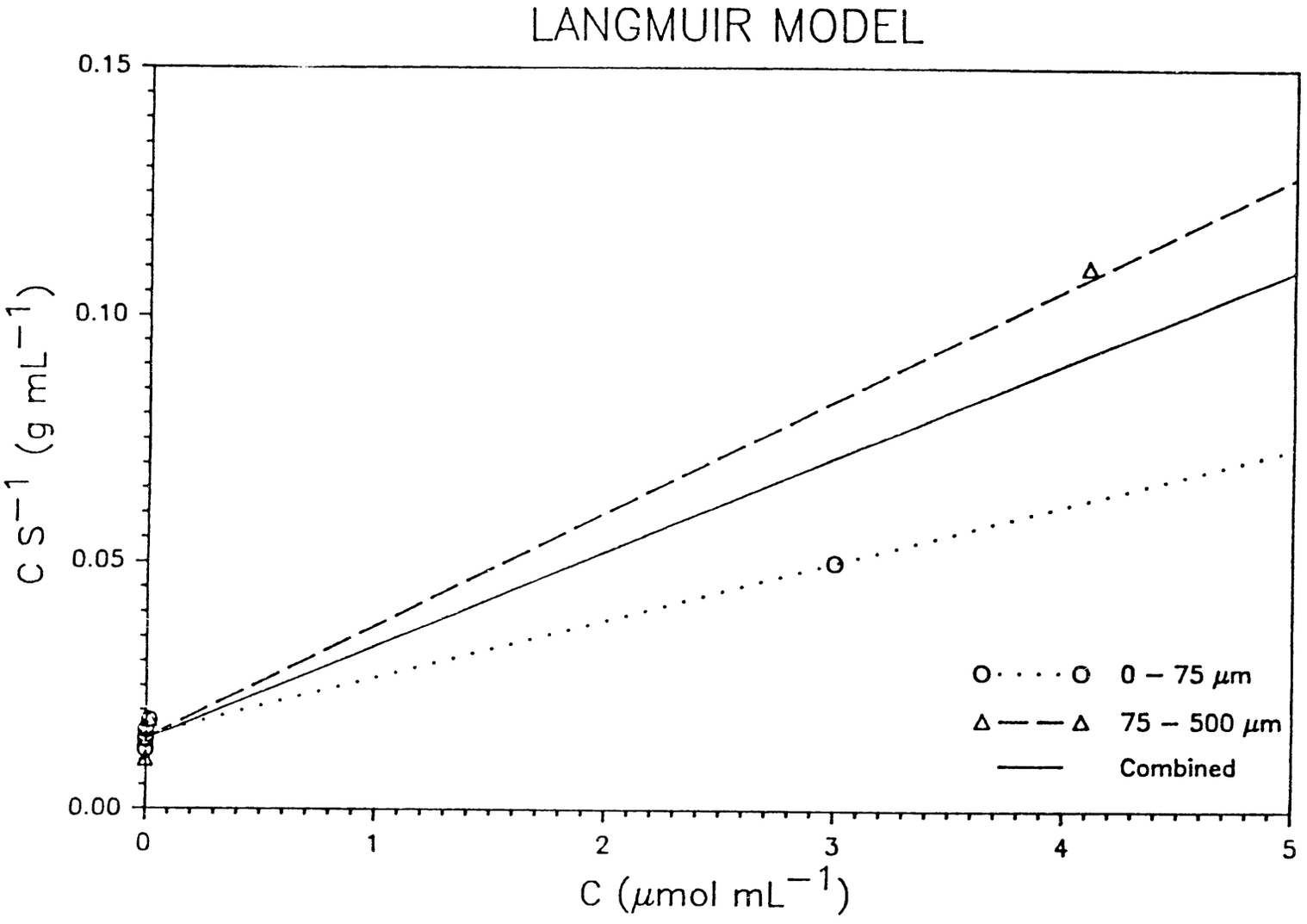

Figure C.71. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-22 Sr 21 air -75 amb 14.0 and YM-22 Sr 21 air 75-500 amb 8.0; the variable being tested is particle size.

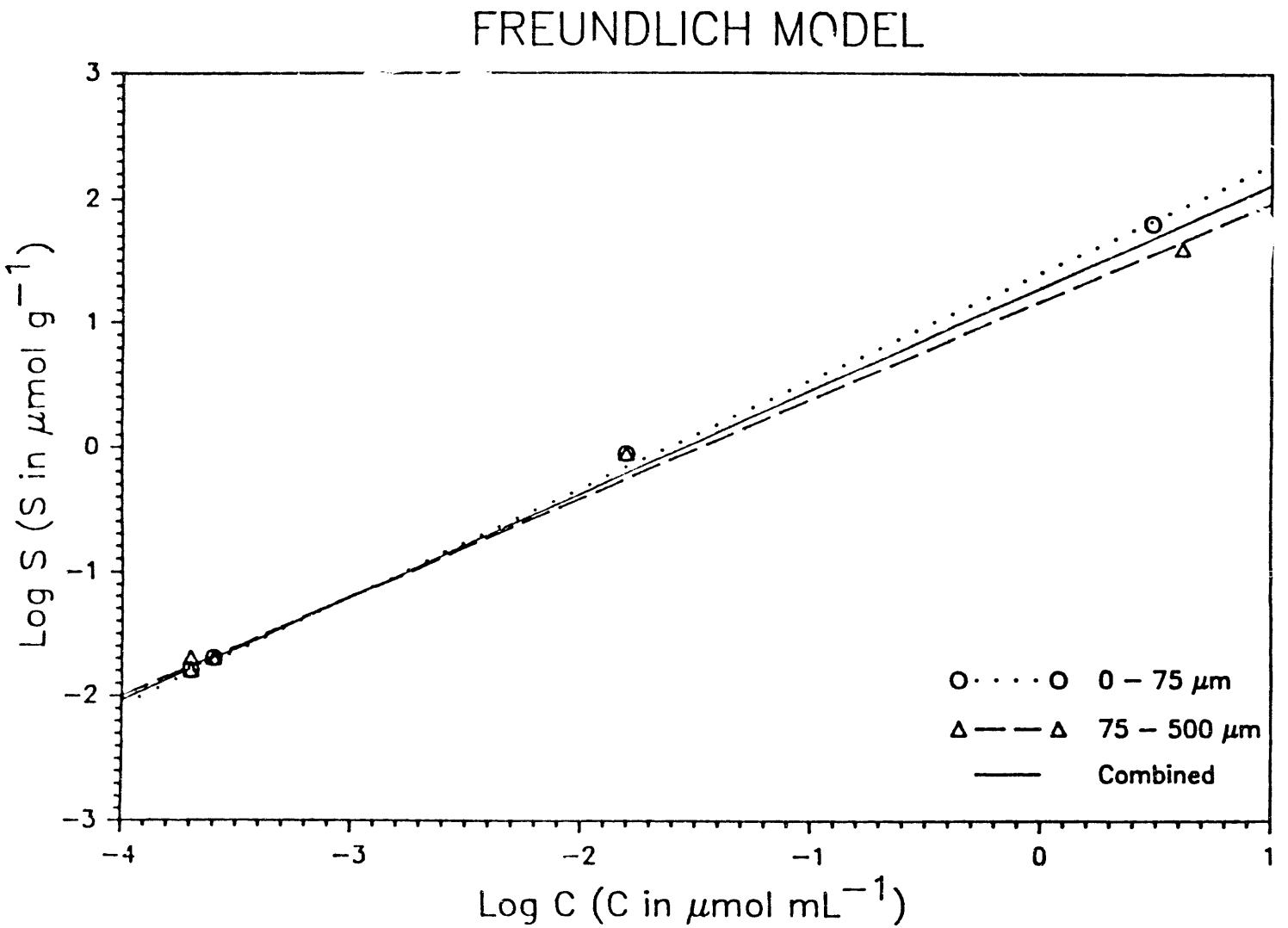

Figure C.72. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-22 Sr 21 air -75 amb 14.0 and YM-22 Sr 21 air 75-500 amb 8.0; the variable being tested is particle size.

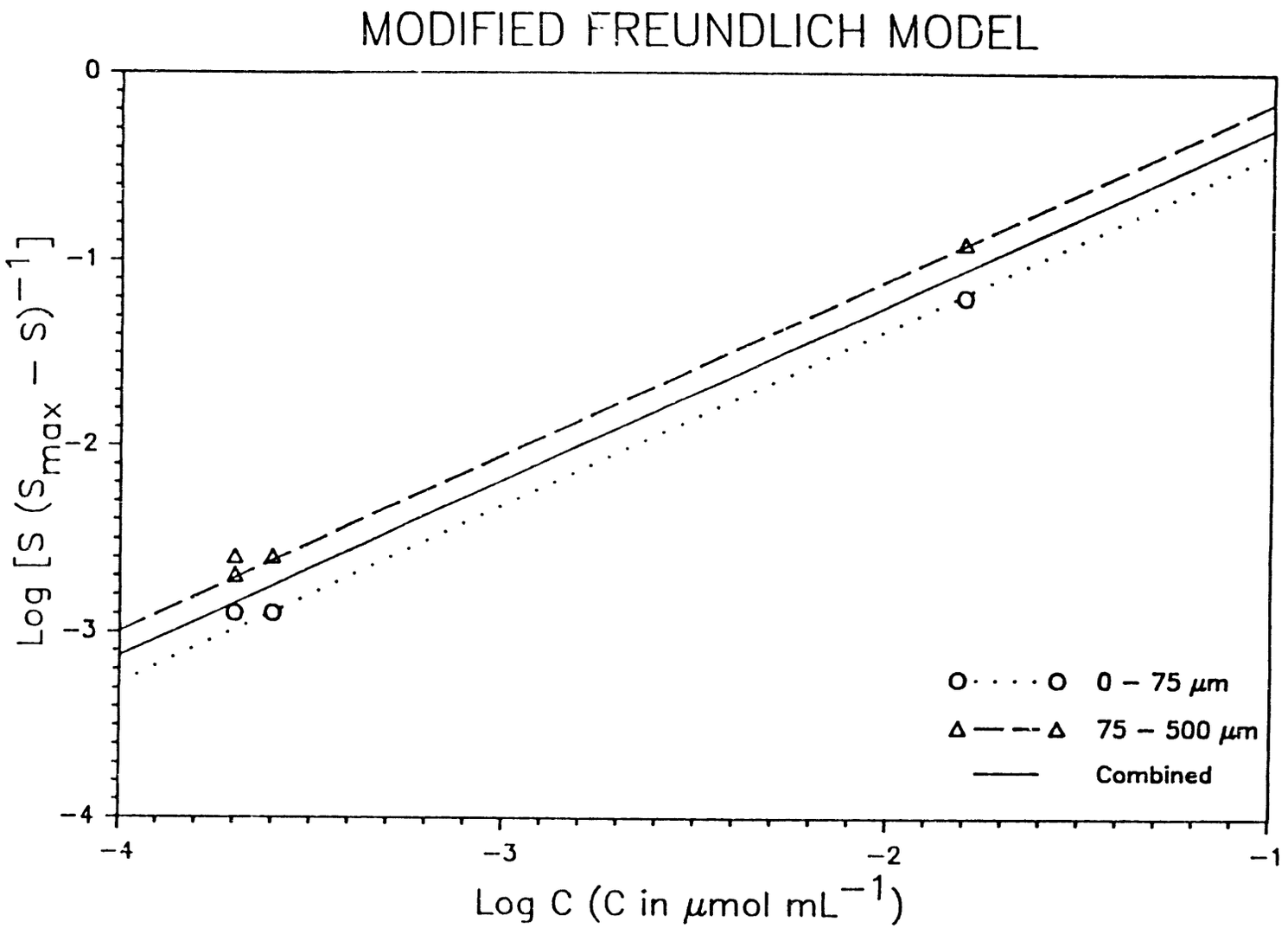

Figure C.73. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-22 Sr 21 air -75 amb 14.0 and YM-22 Sr 21 air 75-500 amb 8.0; the variable being tested is particle size.

TABLE C.II

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS; DESORPTION

ym-48 Tc 63 air 106-500 amb 484.0 VERSUS ym-49 Tc 63 air 106-500 amb 1170.0

Variable: Different Mineralogies in the Same Stratigraphic Unit

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=316565.89>Ft=6.94 (Different)	Fc=0.57<Ft=6.94 (Same)	Fc=0.69<Ft=6.94 (Same)	Fc=7.53>Ft=6.94 (Same)
Intercept	n.a. n.a.	Fc=0.94<Ft=6.61 (Same)	Fc=0.95<Ft=6.61 (Same)	Fc=0.95<Ft=6.61 (Same)
Slope	Fc=-0.33<Ft=6.61 (Same)	Fc=1.17<Ft=6.61 (Same)	Fc=0.07<Ft=6.61 (Same)	Fc=10.89>Ft=6.61 (Different)

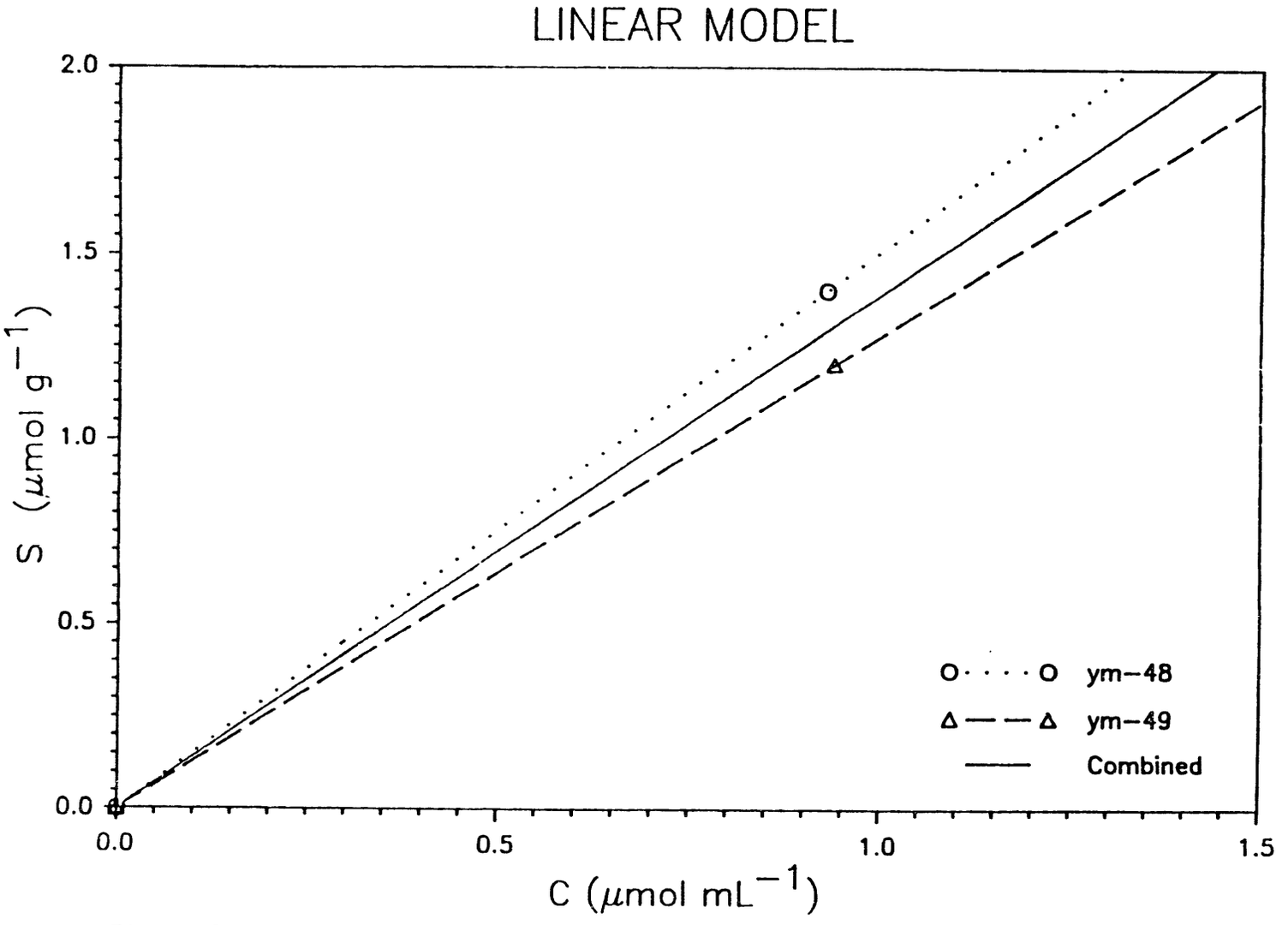

Figure C.74. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-48 Tc 63 air 106-500 amb 484.0 desorption and YM-49 Tc 63 air 106-500 amb 1170.0 desorption; the variable being tested is mineralogy.

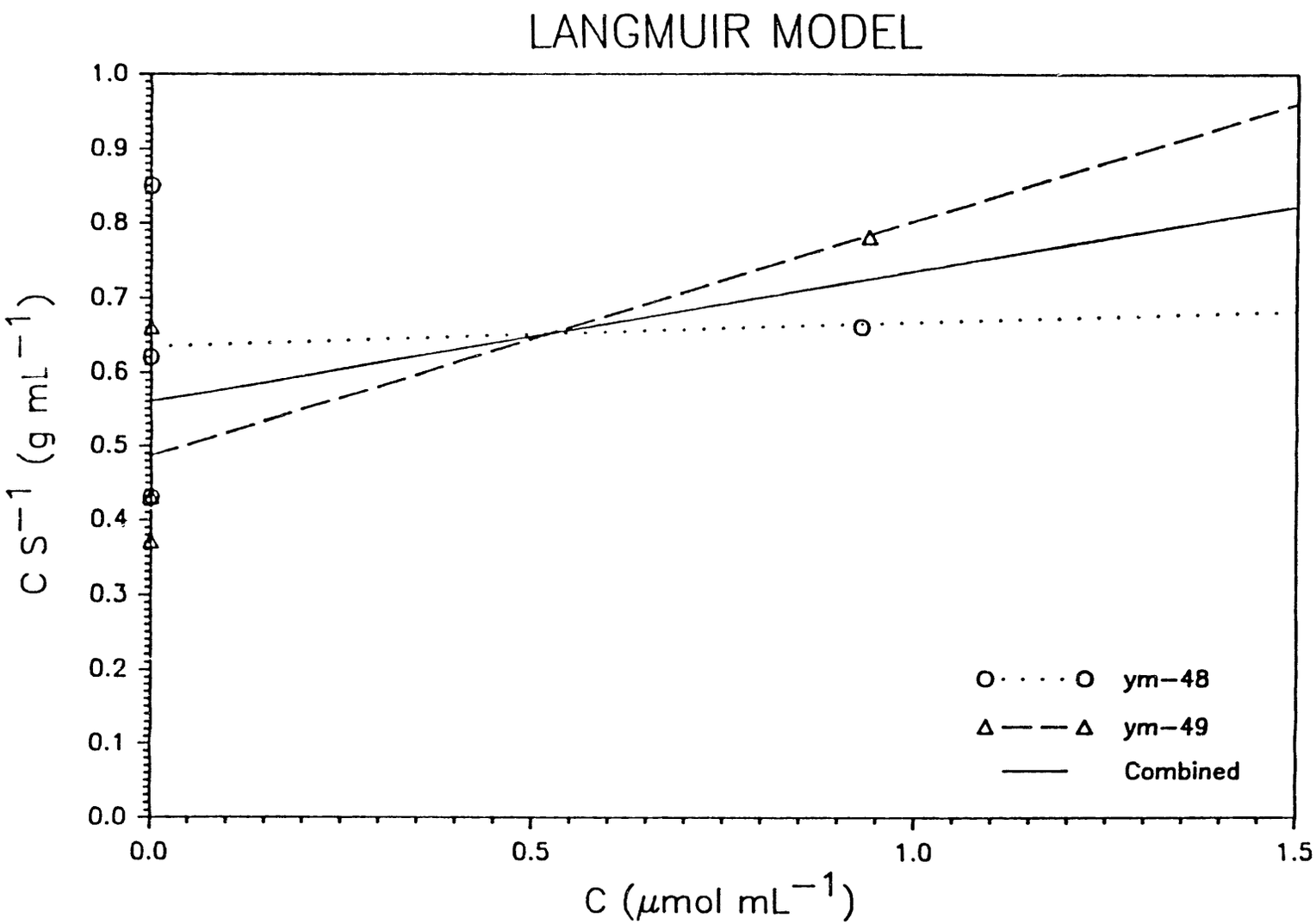

Figure C.75. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-48 Tc 63 air 106-500 amb 484.0 desorption and YM-49 Tc 63 air 106-500 amb 1170.0 desorption; the variable being tested is mineralogy.

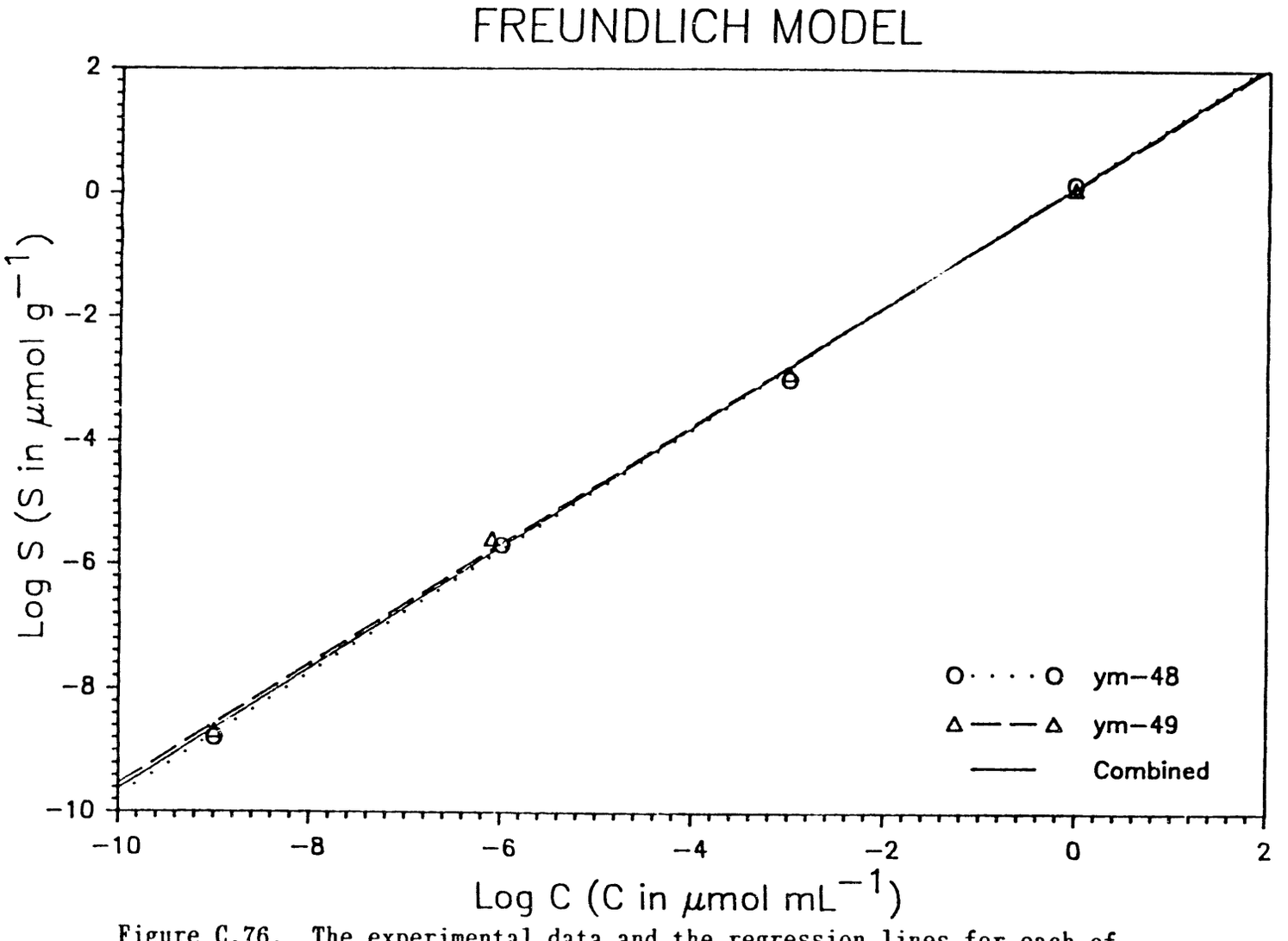

Figure C.76. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-48 Tc 3 air 106-500 amb 484.0 desorption and YM-49 Tc 63 air 106-500 amb 1170.0 desorption; the variable being tested is mineralogy.

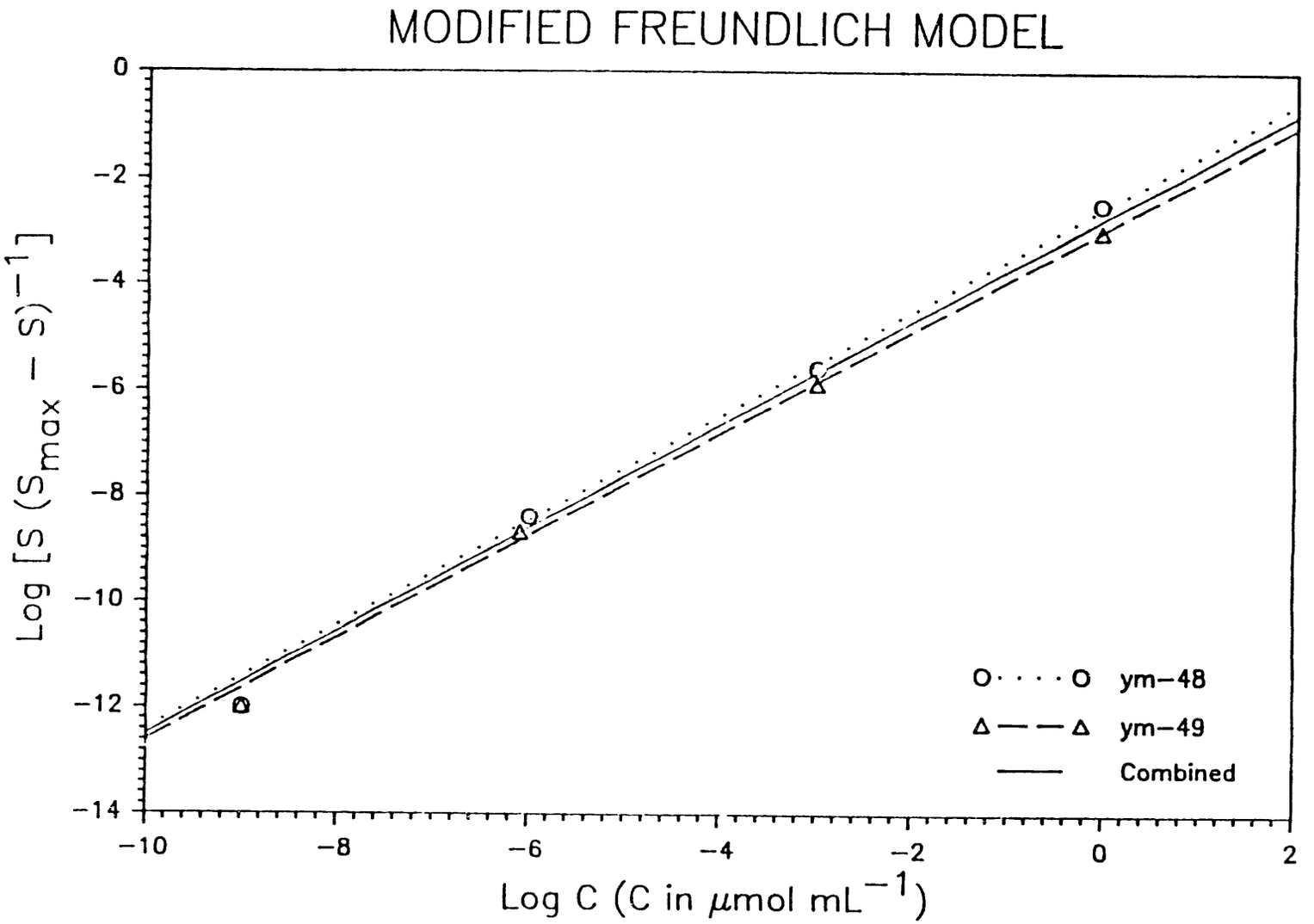

Figure C.77. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-48 Tc 63 air 106-500 amb 484.0 desorption and YM-49 Tc 63 air 106-500 amb 1170.0 desorption; the variable being tested is mineralogy.

TABLE C.III

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION AND DESORPTION

ja-37 U 7 air 355-500 amb n.a. VERSUS ja-37 U 7 air 355-500 amb n.a.

Variable: Hysteresis

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=9.82>Ft=6.94 (Different)	Fc=0.65<Ft=6.94 (Same)	Fc=2.68<Ft=6.94 (Same)	n.a. n.a.
Intercept	n.a. n.a.	Fc=0.41<Ft=6.61 (Same)	Fc=0.04<Ft=6.61 (Same)	n.a. n.a.
Slope	Fc=0.00<Ft=6.61 (Same)	Fc=0.00<Ft=6.61 (Same)	Fc=0.57<Ft=6.61 (Same)	n.a. n.a.

ym-48 Tc 42 air 106-500 amb 484.0 VERSUS ym-48 Tc 63 air 106-500 amb 484.0

Variable: Hysteresis

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=14233734.4>Ft=6.94 (Different)	Fc=11.34>Ft=6.94 (Different)	Fc=33.45>Ft=6.94 (Different)	Fc=33.43>Ft=6.94 (Different)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

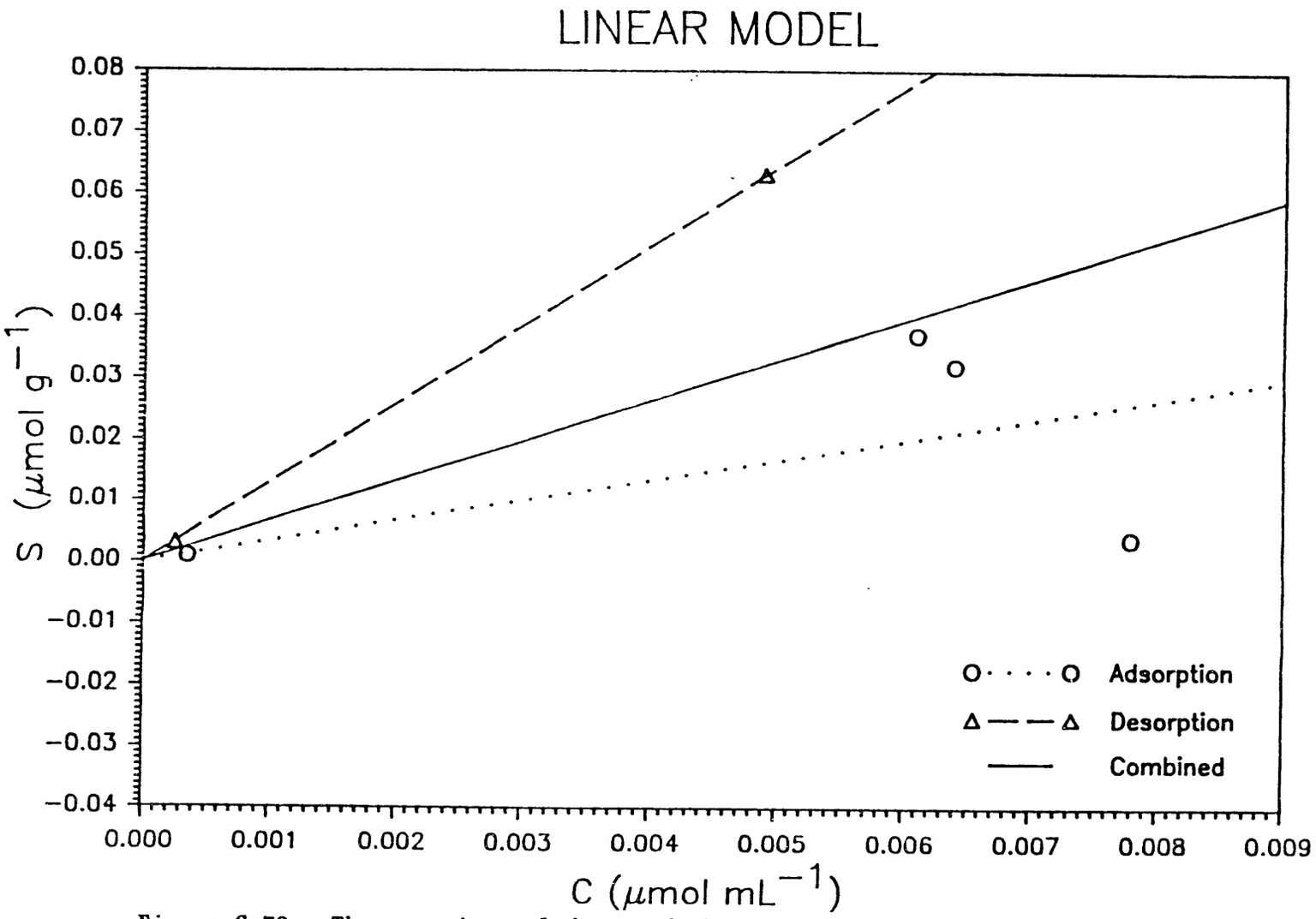

Figure C.78. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are JA-37 U 7 air 355-500 amb n.a. adsorption and JA-37 U 7 air 355-500 amb n.a. desorption; the variable being tested is hysteresis.

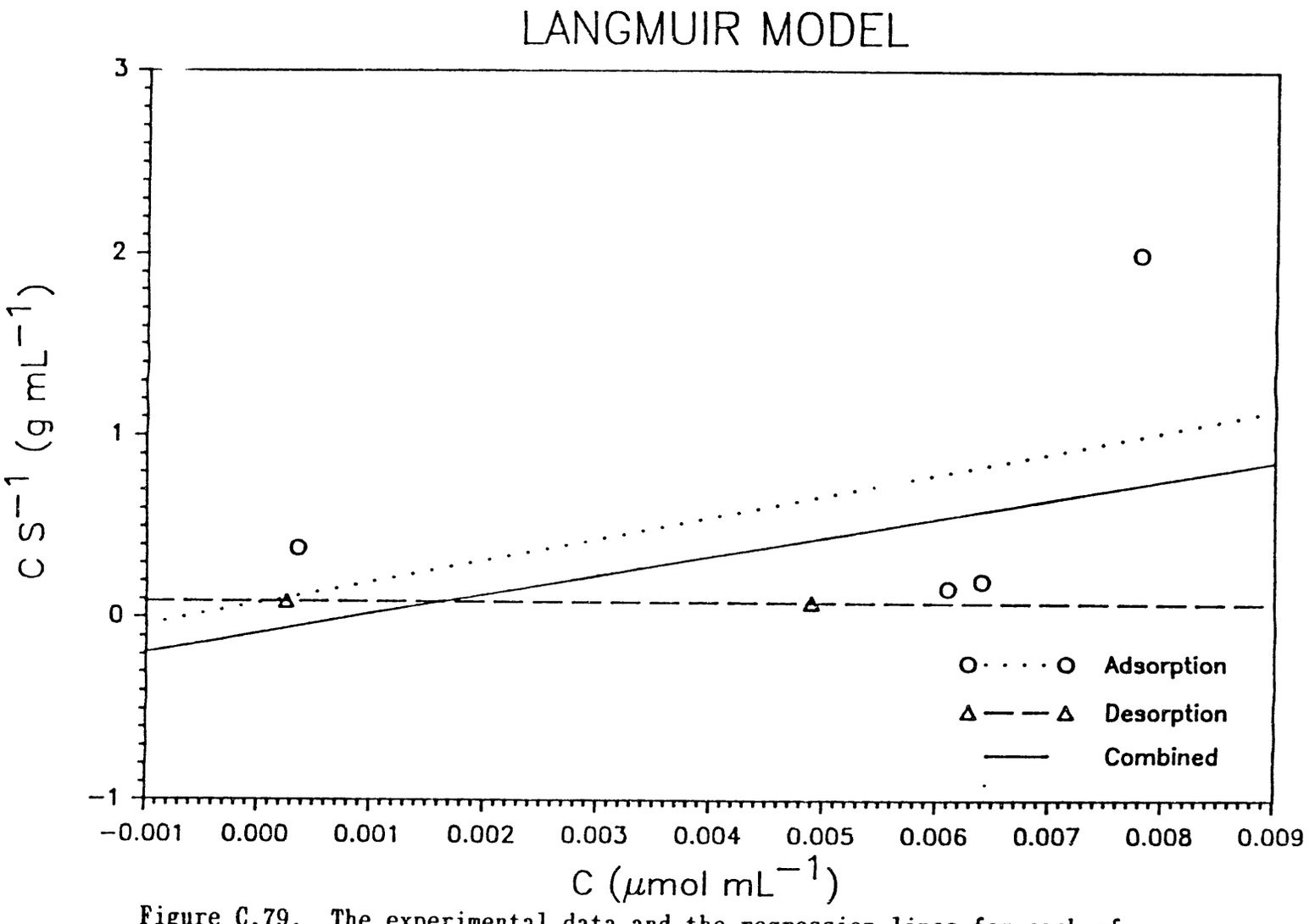

Figure C.79. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are JA-37 U 7 air 355-500 amb n.a. adsorption and JA-37 U 7 air 355-500 amb n.a. desorption; the variable being tested is hysteresis.

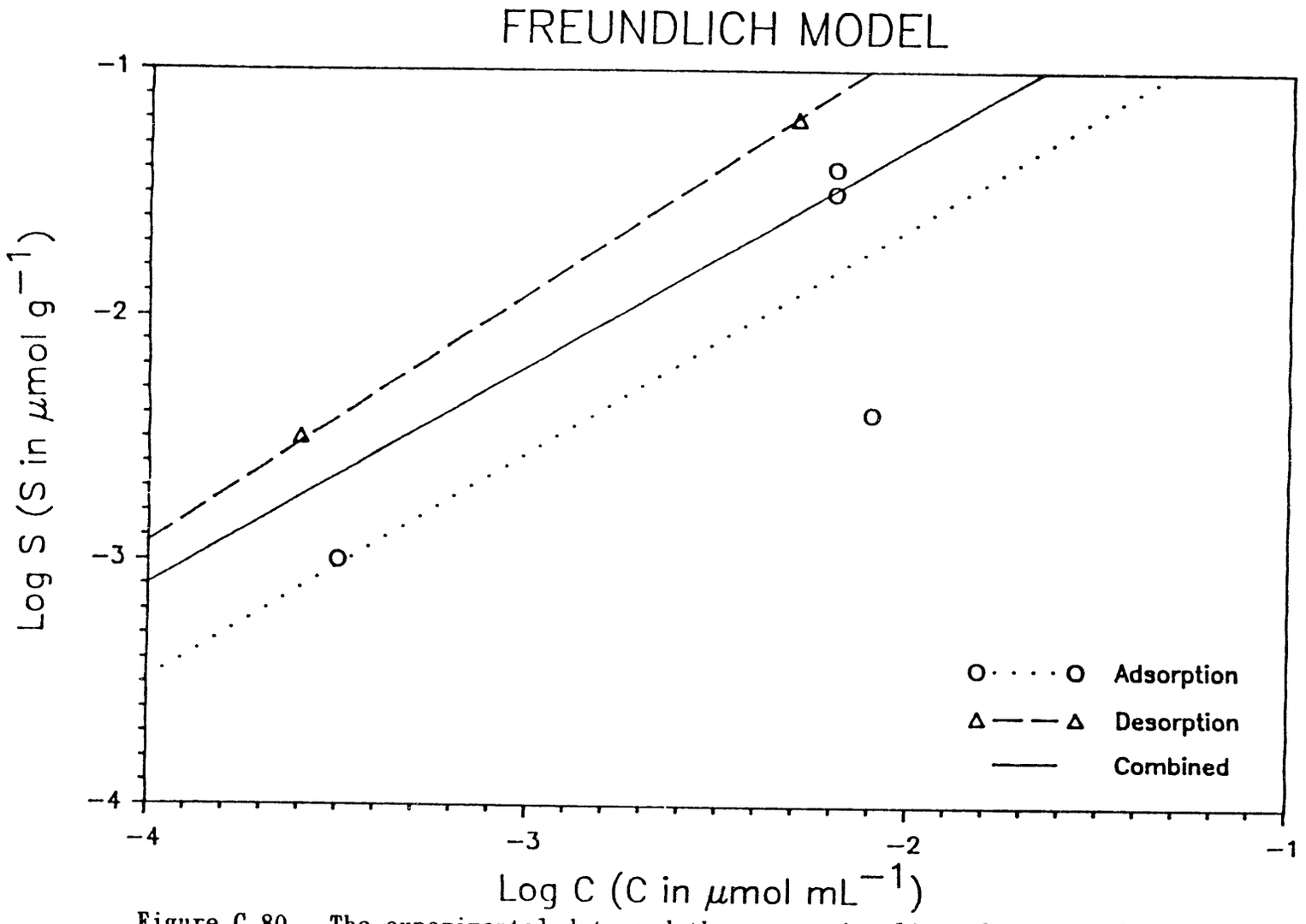

Figure C.80. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are JA-37 U 7 air 355-500 amb n.a. adsorption and JA-37 U 7 air 355-500 amb n.a. desorption; the variable being tested is hysteresis.

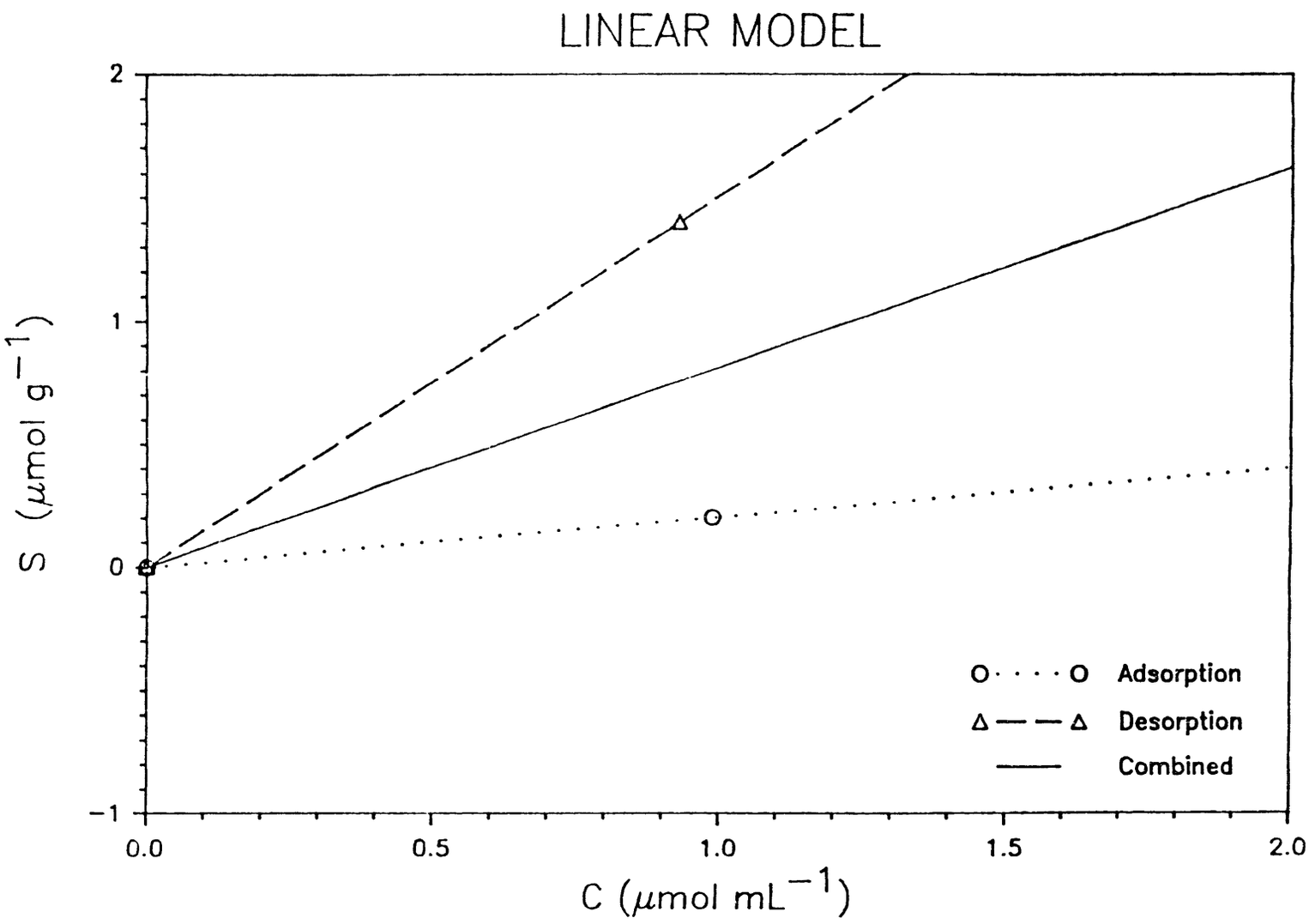

Figure C.81. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 adsorption and YM-48 Tc 42 air 106-500 amb 484.0 desorption; the variable being tested is hysteresis.

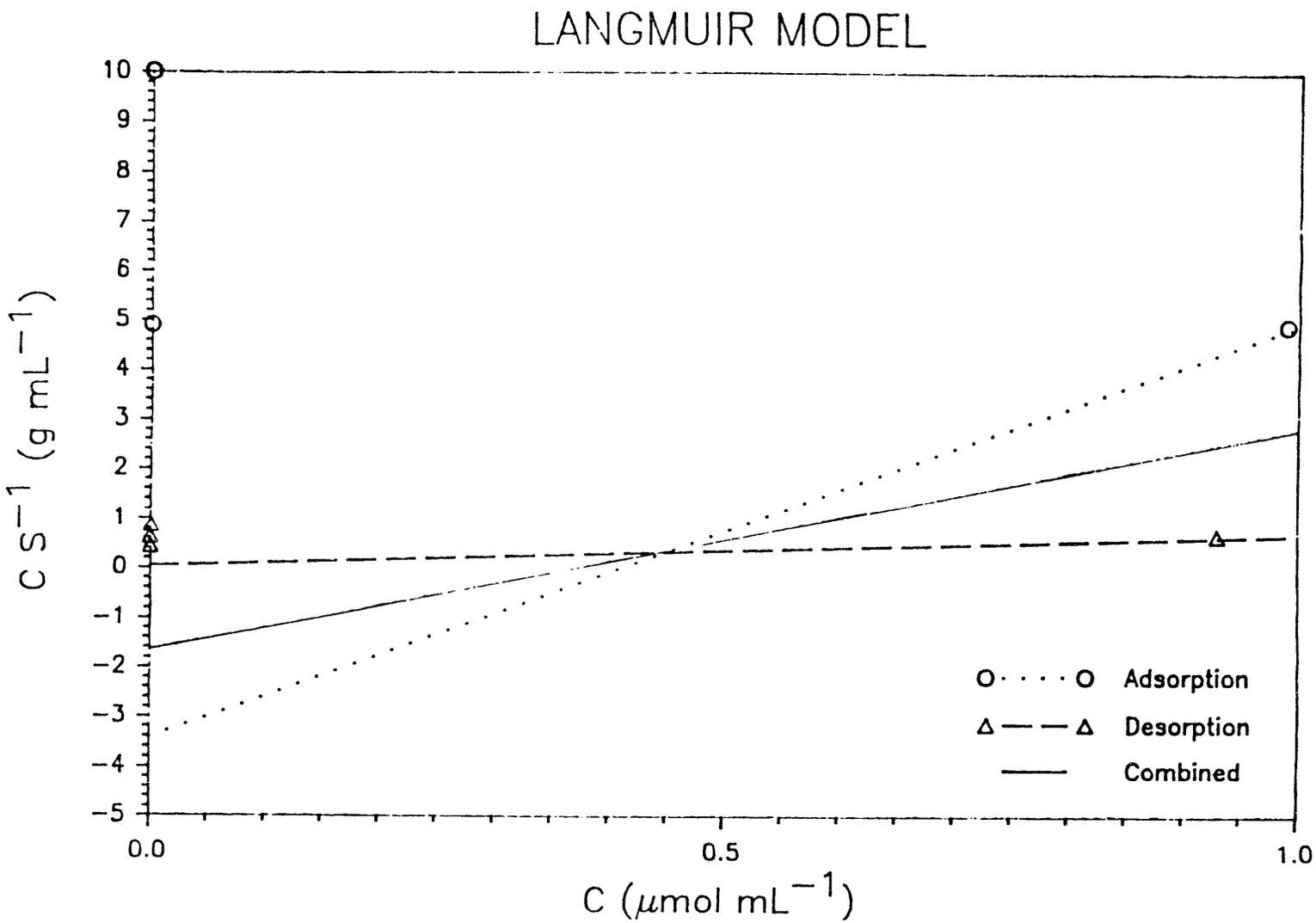

Figure C.82. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 adsorption and YM-48 Tc 42 air 106-500 amb 484.0 desorption; the variable being tested is hysteresis.

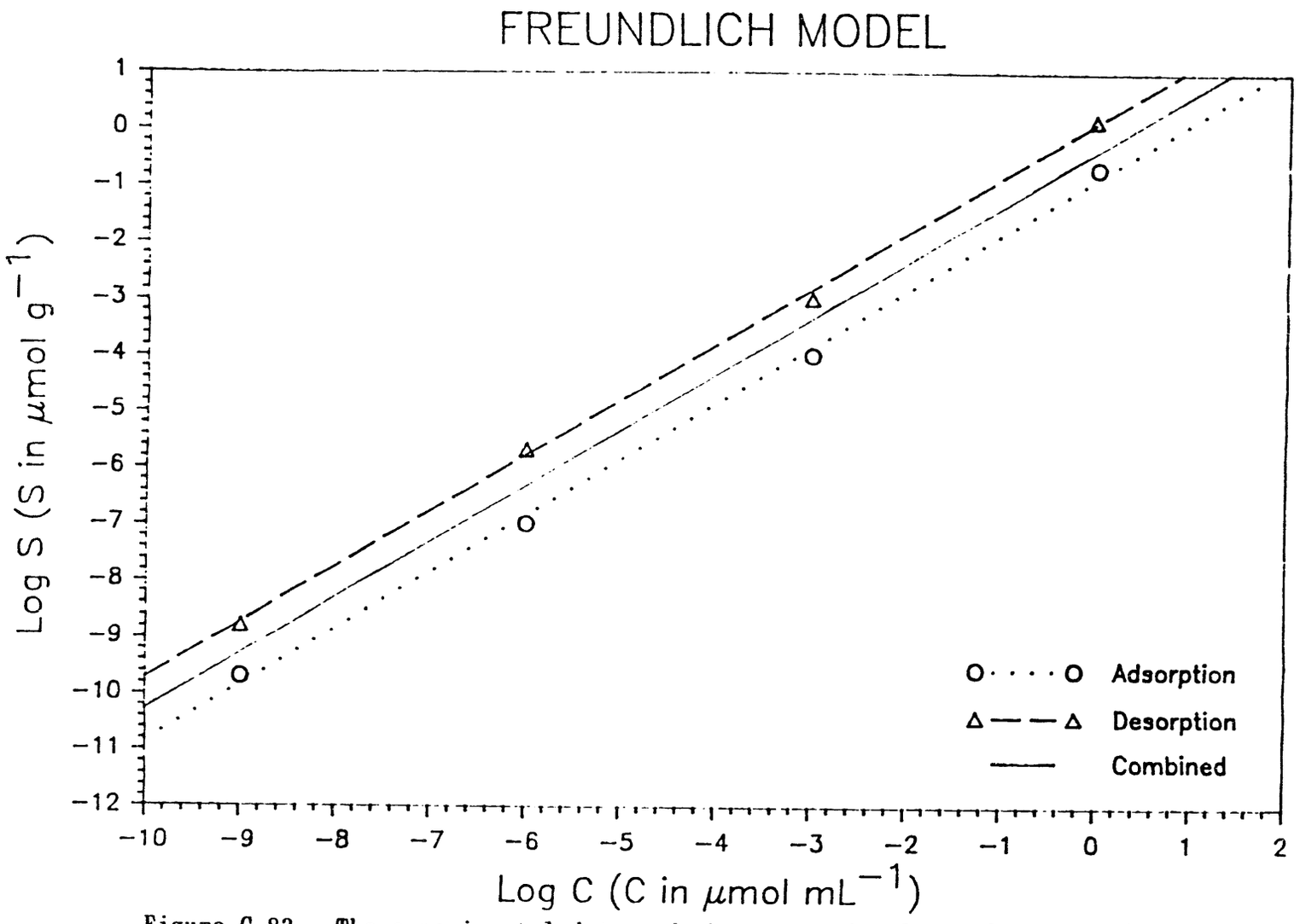

Figure C.83. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 adsorption and YM-48 Tc 42 air 106-500 amb 484.0 desorption; the variable being tested is hysteresis.

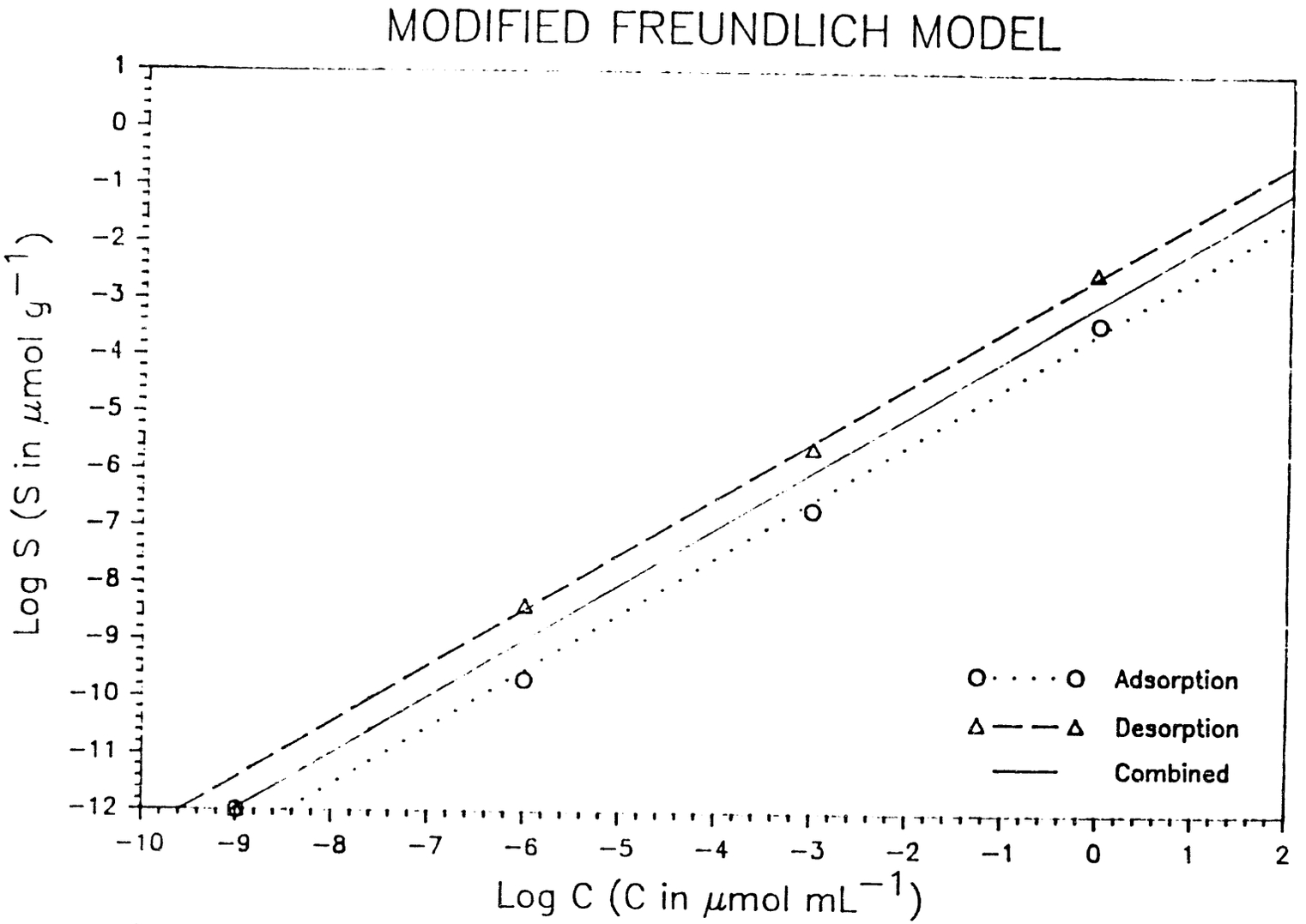

Figure C.84. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-48 Tc 42 air 106-500 amb 484.0 adsorption and YM-48 Tc 42 air 106-500 amb 484.0 desorption; the variable being tested is hysteresis.

TABLE C.III (cont.)

RESULTS FROM TESTS FOR SIGNIFICANT DIFFERENCES AMONG DATA SETS: ADSORPTION AND DESORPTION

ym-49 Tc 42 air 106-500 amb 1170.0 VERSUS ym-49 Tc 63 air 106-500 amb 1170.0

Variable: Hysteresis

F-Test (95% C.L.)	Linear	Langmuir	Freundlich	Modified Freundlich
Regression Line	Fc=23704749.7>Ft=6.94 (Different)	Fc=33.86>Ft=6.94 (Different)	Fc=86.86>Ft=6.94 (Different)	Fc=86.90>Ft=6.94 (Different)
Intercept	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.
Slope	n.a. n.a.	n.a. n.a.	n.a. n.a.	n.a. n.a.

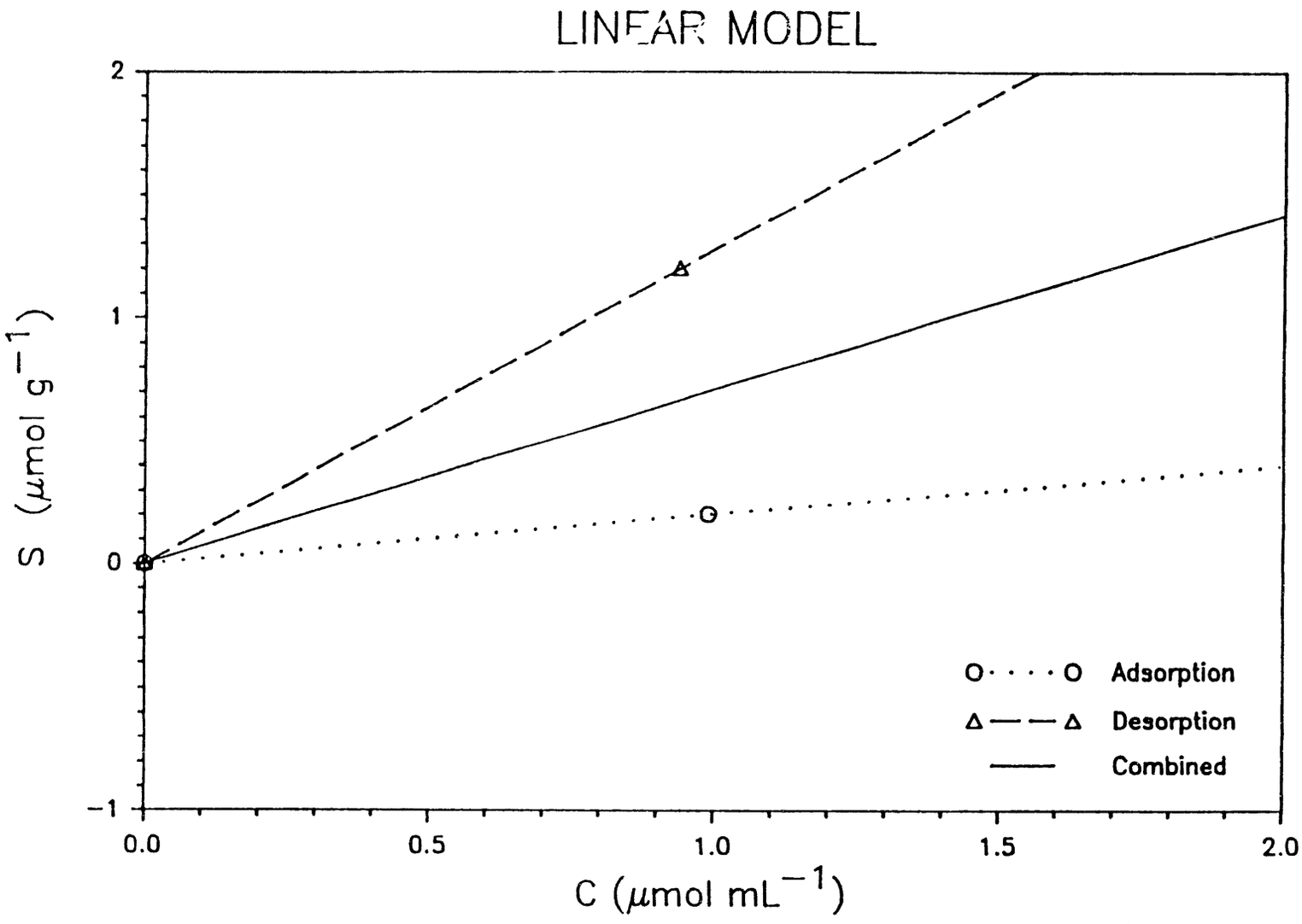

Figure C.85. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Linear isotherm model. The two data sets are YM-49 Tc 42 air 106-500 amb 1170.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 desorption; the variable being tested is hysteresis.

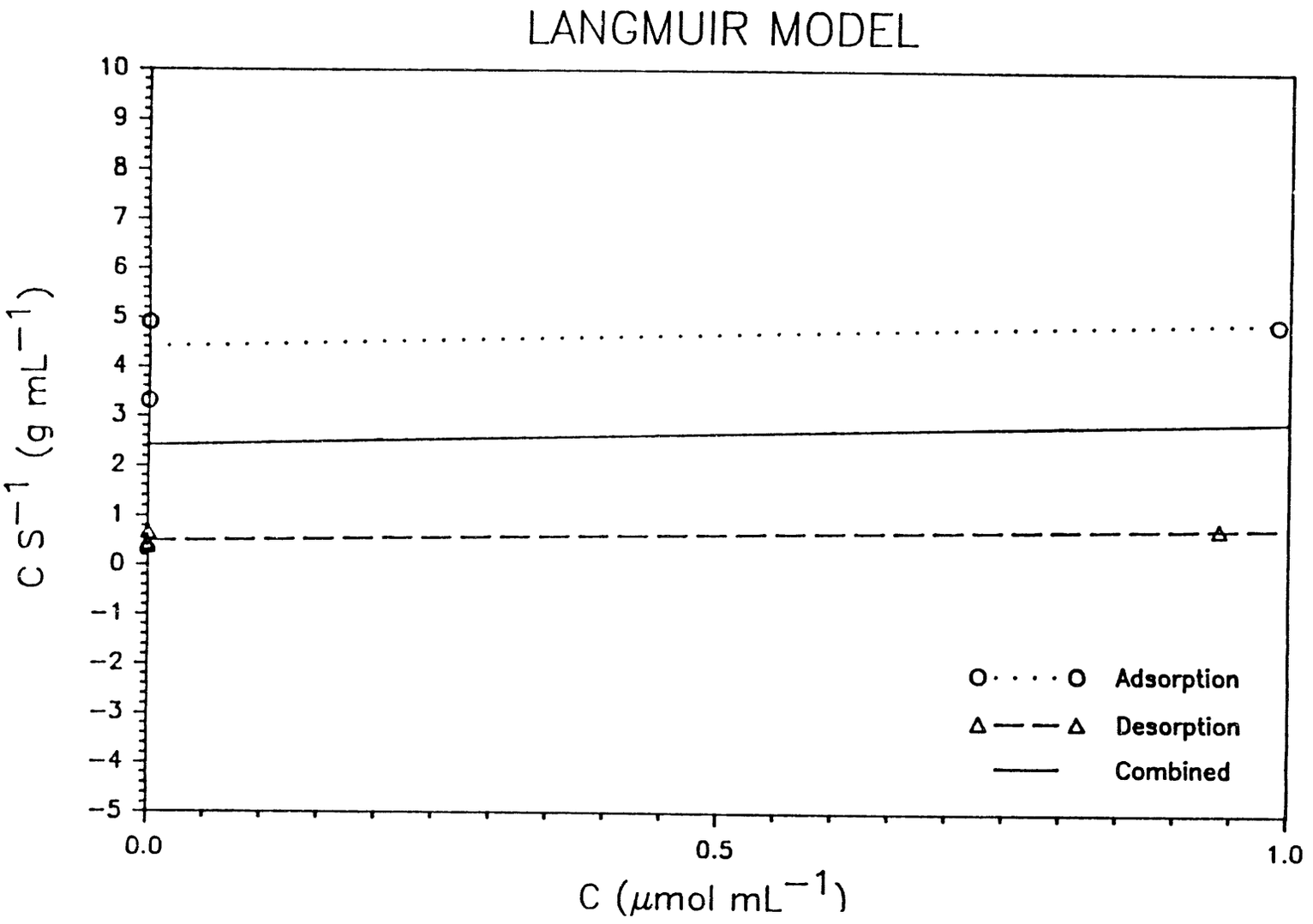

Figure C.86. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Langmuir isotherm model. The two data sets are YM-49 Tc 42 air 106-500 amb 1170.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 desorption; the variable being tested is hysteresis.

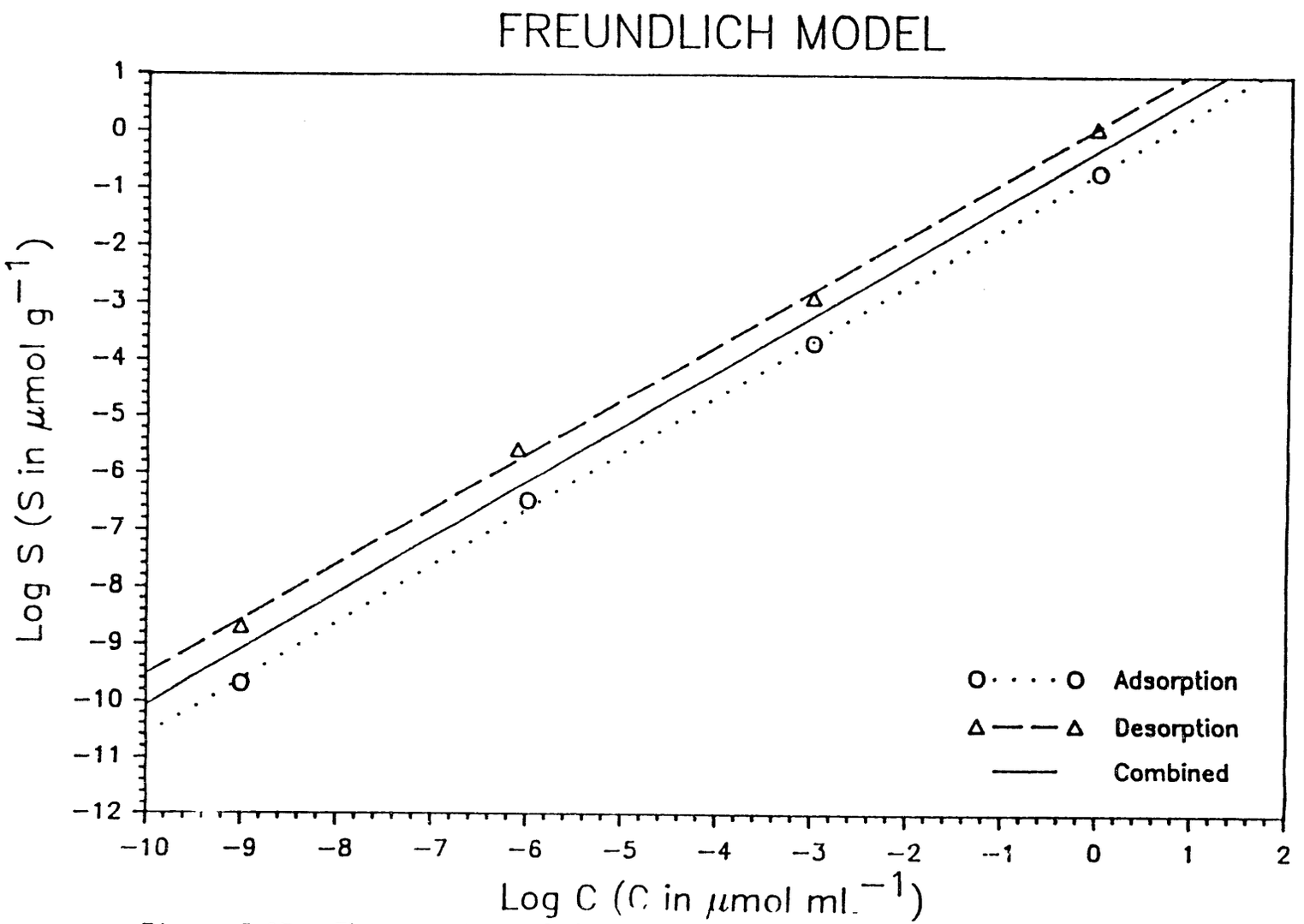

Figure C.87. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Freundlich isotherm model. The two data sets are YM-49 Tc 42 air 106-500 amb 1170.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 desorption; the variable being tested is hysteresis.

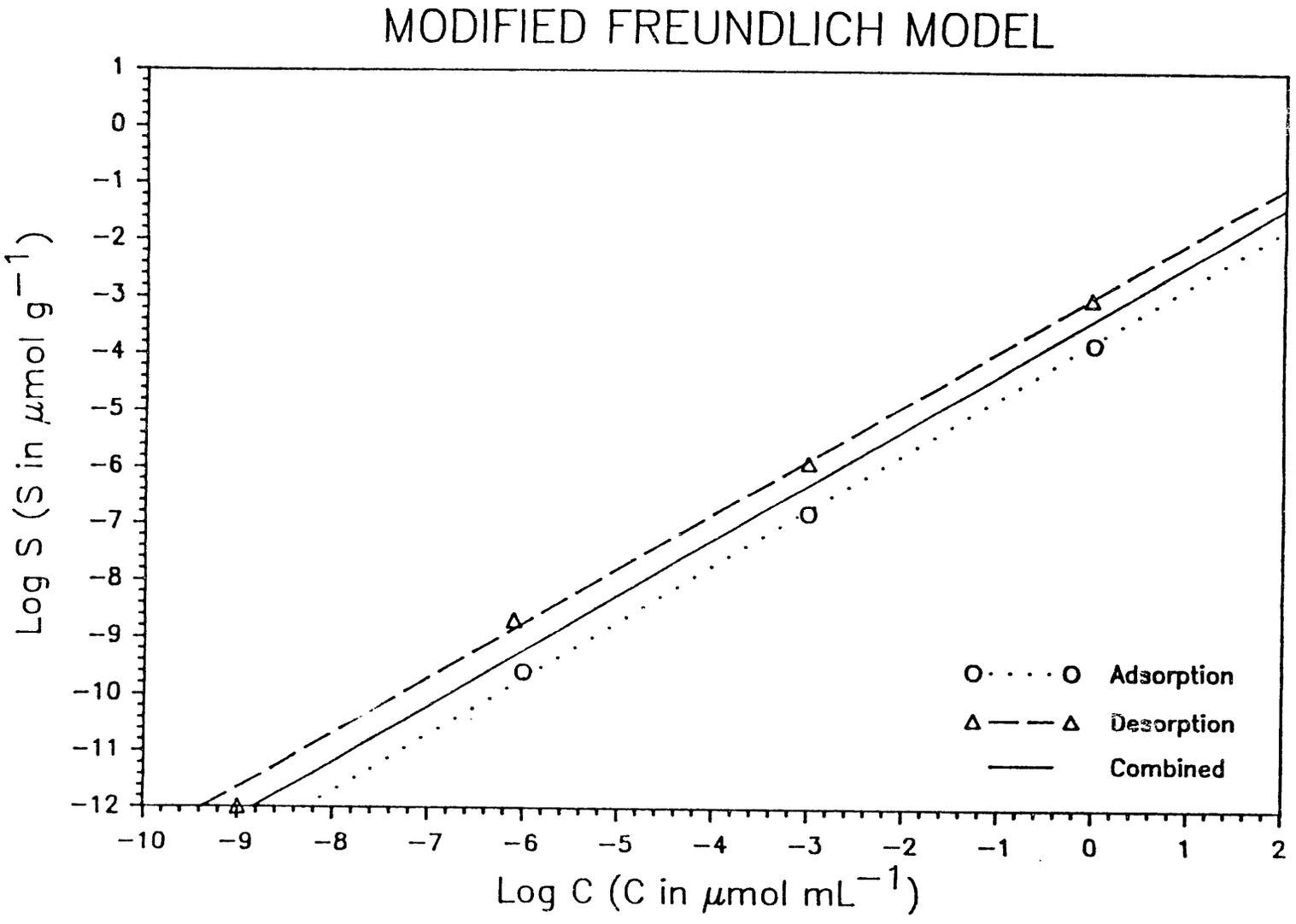

Figure C.88. The experimental data and the regression lines for each of the two data sets and for the combined data sets are presented for the Modified Freundlich isotherm model. The two data sets are YM-49 Tc 42 air 106-500 amb 1170.0 adsorption and YM-49 Tc 42 air 106-500 amb 1170.0 desorption the variable being tested is hysteresis.

END

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