ENGR 340-Introduction to Environmental Engineering

To: Professor Deborah Sills

From: Zwelani Ngwenya

Re: Non-Linear Curve fitting- Sorption

**Objective**

The goal of this analysis is to determine the model parameters for the sorption isotherm of chlordane on Granulated Activated Carbon. Data is going to be fitted to one of the two sorption isotherms – Linear and Freundlich and based on the model fits of the two equations, the most appropriate model will be chosen. The equations to be fitted are Equation and 1 and Equation 2, shown:

Linear Model: q = KC (Eq. 1)

Freundlich Model: q = K (Eq. 2)

Where q = mass of adsorbate adsorbed per mass of adsorbent at equilibrium (mg/g)

C = concentration of adsorbate in the aqueous phase at equilibrium (mg/L)

K = Freundlich isotherm soil – water partition coefficient ((mg/g) (mg/L))

= Freundlich isotherm intensity parameter (unitless)

**Methods**

Graphical analysis of the data was done using KaleidaGraph computer software. The concentration of the adsorbate in the aqueous phase (C) at equilibrium was chosen as the independent variable and the mass of adsorbate adsorbed per mass of adsorbent (q) at equilibrium was the dependent variable. A plot of q against C was made and the Linear and Freundlich models were tried as possible fits for the data, through inputting different mathematical instructions to KaleidaGraph. The model that connected all points smoothly was then chosen as the best fit model. The regression analysis data table that shows up in the plot on the KaleidaGraph software was used to determine the value of Freundlich isotherm soil-water coefficient.

**Results and Discussion**

KaleidaGraph was used to fit the data models to the two isotherm models, Linear and Freundlich. Based on the plotted graphs, the Freundlich model is the best fit model for showing the correlation between dissolved chlordane concentrations against adsorbed chlordane concentration. Figure 1 shows the fitted Freundlich equation on the data sets. By visual inspection, the Freundlich equation is the best model as it produces a perfect curve that connects through all the data points. The linear model did not fit the data points. Figure 1 in Appendix A shows the linear model being tried on the data sets. Of all the data sets analyzed, the linear model only fits two points and hence it is not a good model for showing and analyzing the relationship between mass of adsorbate adsorbed per mass of adsorbent and concentration of adsorbate.

Using the Freundlich model, the Freundlich isotherm soil-water partition coefficient, K was calculated to be 245 ((mg/g)(mg/L)).

Figure 1: Freundlich sorption isotherm Model perfectly fits the data sets with Freundlich isotherm soil-water partition coefficient of K = 245 ((mg/g)(L/mg)).

Appendix A

Figure 4: Linear sorption isotherm model fitted to data, K= 2097((mg/g)(L/mg)).