Memorandum

To: Co-worker

From: Johnna Emanuel

Date: September 24, 2013

Re: Estimating Isotherm Parameters

Objective

The objective of this exercise was to fit the data for the sorption of chlordane by GAC with two sorption isotherms – Linear and Freundlich – and select the most appropriate isotherm based on the model fits. The general equations for the Linear and Freundlich isotherm models are displayed as Equations 1 and 2, respectively,

$$q = KC \qquad \text{Eq. 1}$$

$$q = KC^{1/n} \qquad \text{Eq. 2}$$

where q is the mass of the adsorbate adsorbed per mass of adsorbent at equilibrium, C is the concentration of adsorbate in the aqueous phase at equilibrium, K is the Freundlich isotherm soil-water partition coefficient, and 1/n is the Freundlich isotherm intensity parameter.

METHODS

The data set, consisting of the dissolved chlordane concentration, C_{aq} (mg/L) and the adsorbed chlordane concentration, q (mg/[g GAC]), was loaded into KaleidaGraph and displayed on a scatter plot. First, the plot was fit to a Linear isotherm. Before assessing the fit, mathematically, it was necessary to judge the model visually – assessing how well the projected line fit the curve. After visual inspection, KaleidaGraph statistically assessed the goodness of fit by calculating the R^2 value (the coefficient of determination) and K value (the soil-water partition coefficient). The value of R^2 is indicative of the explained variability in the given data set. The closer the value of R^2 is to 1, the better the model fit. Second, the plot was fit to a Freundlich isotherm. The plot was again assessed visually and statistically. Comparing the visual appearance, R^2 values, and K values for the two plots, it was possible to decide which isotherm best fit the given data.

RESULTS AND DISCUSSION

It was found that the Freundlich isotherm, as seen in Figure 1 (with raw data provided in Appendix A), best fit the given data. Visually, the curve is smooth and passes through all of the given data points.

Being that the data naturally displays a concave down curve (1/n < 1 in Eq. 2), it was evident through visual inspection that the Linear isotherm was not going to be a good fit for this data set. The Linear isotherm fell below the data points, and the distance between the data and the projected line increased as the dissolved chlordane concentration increased.

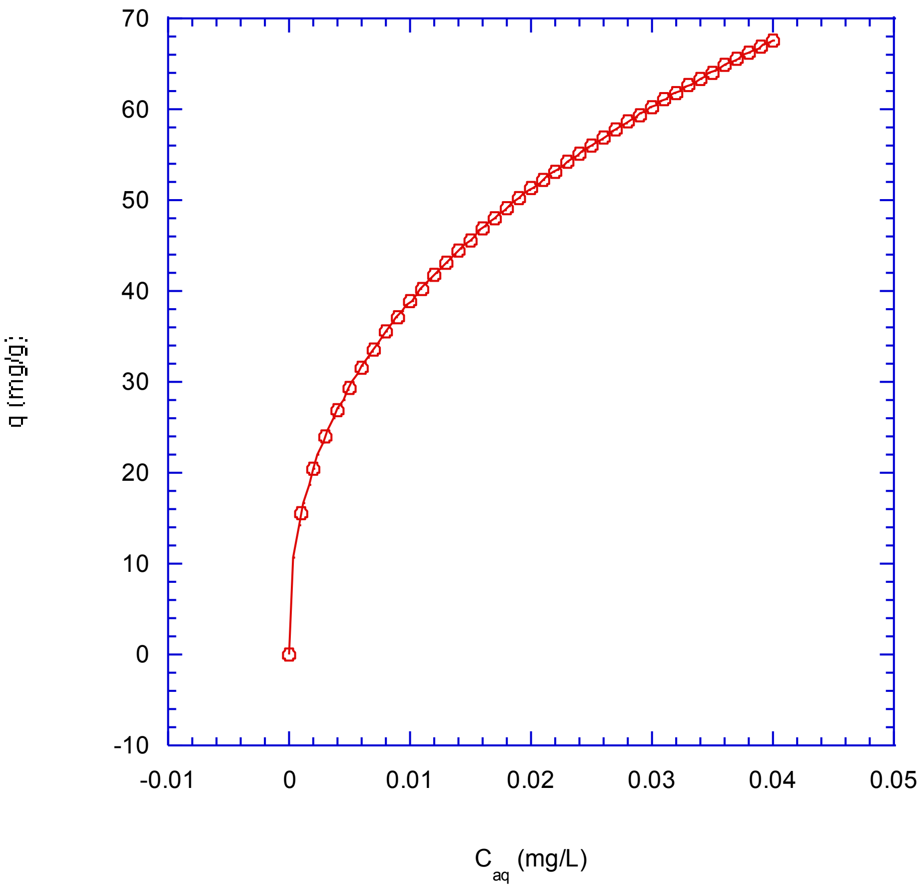

Figure 1. Adsorbed chlordane concentration, q, modeled as a function of dissolved chlordane concentration, C_{aq} – fit to a Freundlich isotherm in which 1/n < 1.

The coefficient of determination, R^2, for the above model is 1 – indicating a good fit. The K value is 245 ((mg/g)(L/mg)). Similarly, it can be inferred from the plot that based on the concavity of the isotherm, concave down (1/n < 1), this reaction is more efficient at higher concentrations of dissolved chlordane – the higher the concentration of dissolved chlordane, the higher the concentration of chlordane that will be adsorbed.

APPENDIX A: RAW DATA

C (mg/L)	q (mg/g)
0.000	0
0.001	15.46
0.002	20.40
0.003	23.99
0.004	26.91
0.005	29.43
0.006	31.65
0.007	33.67
0.008	35.51
0.009	37.23
0.010	38.83
0.011	40.34
0.012	41.77
0.013	43.13
0.014	44.42
0.015	45.67
0.016	46.86
0.017	48.01
0.018	49.12
0.019	50.20
0.020	51.24
0.021	52.25
0.022	53.23
0.023	54.18
0.024	55.11
0.025	56.02
0.026	56.91
0.027	57.77
0.028	58.62
0.029	59.45
0.030	60.26
0.031	61.05
0.032	61.83
0.033	62.60

0.034	63.35
0.035	64.09
0.036	64.82
0.037	65.53
0.038	66.23
0.039	66.93
0.040	67.61