

PREDICTING THE PERFORMANCE OF LIQUID PHASE FIXED-BED GRANULAR ACTIVATED CARBON ADSORBERS

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INTRODUCTION

Granular Activated Carbon (GAC) adsorption is an effective treatment technology for the removal of Synthetic Organic Chemicals (SOCs) from drinking water supplies. This treatment process can be expensive, if not properly designed. Application of mathematical models is an attractive method to evaluate the impact of process variables on process design and performance. The main obstacle in using mathematical models is that they require many model parameters, some of which may be site-specific and can only be obtained through a number of bench-scale experiments. Furthermore, sufficient knowledge of various adsorption model options is required for a designer to select appropriate adsorption models and the sequence of model applications necessary to predict adsorber performance in removing SOCs. Hence, this paper presents an approach that will 1) estimate site-specific adsorption model parameters; and 2) select appropriate models to predict the adsorber performance in removing SOCs under specific field conditions.

MODELING APPROACH AND PARAMETER ESTIMATION METHODS

A modeling approach was developed to predict the effluent concentration profiles for SOCs leaving a fixed-bed adsorber. The ultimate goal is to predict the removal of SOCs from a variety of water matrices containing both SOCs and background natural organic matter (NOM). To date, SOC and NOM interactions in fixed beds have been found to be site-specific and significantly impact adsorber performance [1]. The development of this approach will continue as additional information on SOC and NOM interaction provides better insight into model parameter selection. Accordingly, the practical guidelines described herein may be easily updated as new information on SOC and NOM interaction becomes available. This approach logically assimilates a collection of models that describe adsorption equilibrium (thermodynamic models) and the transport of SOCs in a fixed-bed (column models).

The pore and surface diffusion model (PSDM) is used as the fixed bed model. The model includes external mass transfer as well as intraparticle mass transfer due to both pore and surface diffusion. Mass balances on the mobile fluid and stationary adsorbent phases result in two partial differential equations for each component, one for the liquid-phase mass balance and the other for the intraparticle phase. The development and solution of the equations for the PSDM are given by Crittenden *et al.* [2]. In order to apply the model to predict fixed-bed adsorber performance, site specific equilibrium and mass transfer parameters are required and the following methods have been successfully used.

The thermodynamic models include methods to estimate single solute Freundlich isotherm parameters from physical properties and to predict the competitive equilibrium interactions between SOCs using single solute isotherms. When experimental single solute isotherm parameters for a particular organic compound and GAC type are not available, correlations based on Polanyi potential theory can be used. Improved methods for correlating single solute isotherm data were developed and are to be presented. The competitive equilibrium interactions between SOCs were estimated using the ideal adsorbed solution theory (IAST) [3]. IAST requires the use of single solute isotherm parameters for each adsorbing compound. Crittenden *et al.* [4] has discussed the use and limitations of the IAST for adsorption equilibrium calculations. Correlations are presented which describe the reduction in GAC capacity as a function of the exposure time to NOM. These correlations are used in conjunction with the single solute Freundlich isotherm parameters to describe the influence of NOM on dynamic column capacity.

The mass transfer parameters required for model calculations are the external mass transfer coefficient and intraparticle mass transfer coefficients. External mass transfer coefficients are estimated from the correlation presented by Gnielinski [5]. This correlation is valid for cases when multiple components are present because dilute solution conditions prevail in the boundary layer surrounding the particle and there are no diffusion interactions. Intraparticle mass transfer can occur by both pore and surface diffusion. Pore diffusion coefficients are

calculated from a correlation relating the liquid phase diffusivity and intraparticle physical properties [1]. Surface diffusion coefficients are calculated from correlations relating the surface diffusion flux to pore diffusion flux [6].

RESULTS AND DISCUSSION

Pilot plant and field scale data from 15 different studies were utilized to investigate the effectiveness of this approach in predicting adsorber performance. In all, fixed-bed data from the 15 studies on 11 different water sources, 10 different compounds and 50 different empty bed contact times (EBCTs) were compared to the PSDM to determine the heuristics for model parameter estimation and verification. Based on these results, it appears at this point that two correlations of capacity as a function of time describe most of the data: (1) Rhine River water, and (2) Karlsruhe groundwater. These correlations tend to span the expected impact of NOM based on data collected for other surface and groundwaters.

Figures 1 and 2 compare PSDM predictions to effluent concentration profiles for two water sources and compounds using the Rhine River and Karlsruhe groundwater capacity correlations. Satisfactory results are obtained in most cases.

CONCLUSIONS

Equilibrium and dynamic column studies have shown that the presence of background NOM, in both ground and surface waters, can significantly reduce both adsorption capacity and mass transfer for SOCs on GAC. Currently, there are no theoretical mass transfer models which have been developed to predict the diffusion and equilibrium interactions between SOCs and NOM that occur in fixed-beds. However, some trends in the manner in which the effective surface and pore diffusivities change with time and bed length can be observed from comparisons of the models with field data. The empirical models which account for the dependence of adsorption capacity and mass transfer upon time and bed length can be used to estimate effective diffusivities with enough precision to make crude design calculations. Accordingly, the practical guidelines described herein may be considered work in progress, and more comparisons of the model and data are needed to develop additional confidence in the model's ability to describe GAC performance in the field.

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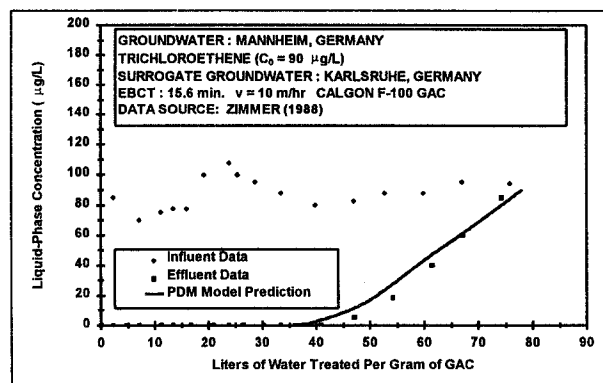


Figure 1. PSDM prediction for trichloroethene using the correlation from Karlsruhe groundwater.

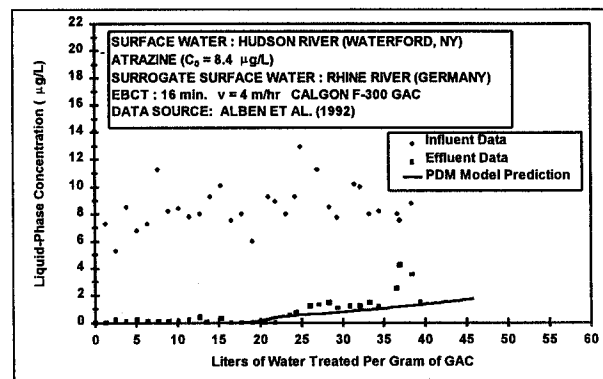


Figure 2. PSDM prediction for atrazine using the correlation from Rhine River water.