

# AdDesignS™

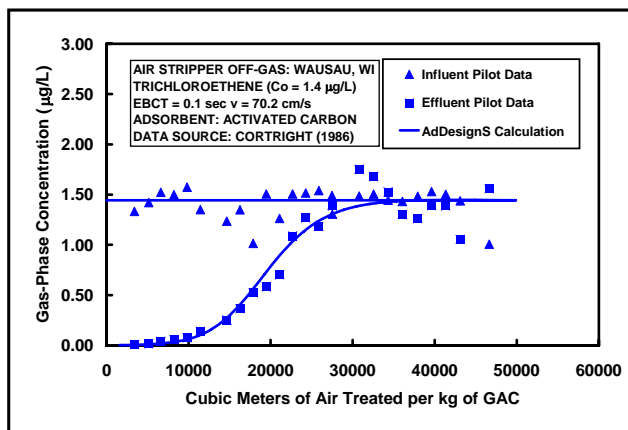
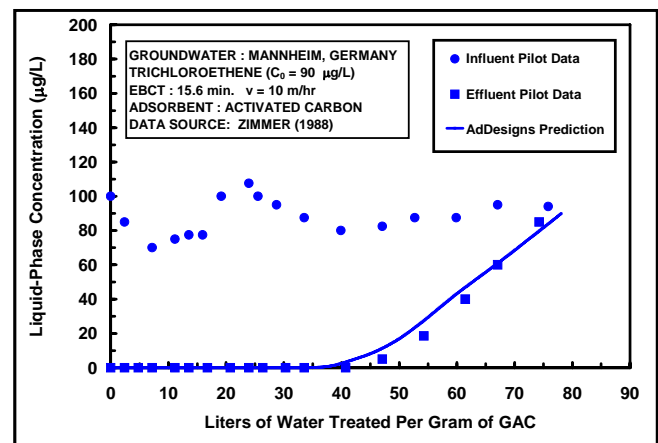
## Adsorption Design Software

An Environmental Technologies Design Option Tool™

*AdDesignS provides design engineers with the capability to evaluate and design fixed-bed adsorption processes for the removal of contaminants from air and water.*

### AdDesignS Features:

- The most comprehensive Adsorption Models developed over the last 19 years at Michigan Technological University
- Extensive Adsorbent Databases
- Commercial Adsorber Databases
- Adsorption Equilibrium Isotherm Parameter Database
- Equilibrium and Kinetic Parameter Estimation Techniques
- Physical and Chemical Properties Database Including Compounds from U.S. EPA's Title III Consolidated Chemical List



### AdDesignS Applications:

- Municipal Water Treatment
- Municipal Wastewater Treatment
- Environmental Remediation
- Air Emissions Treatment
- Pollution Prevention Assessment
- Educational Resource

### AdDesignS Capabilities

Adsorption is one of the most effective processes for removing organic contaminants from air and water. This treatment process can be expensive if it is not designed properly.

The proper design of adsorption processes results from carefully controlled laboratory and/or pilot plant studies that are used to determine important design variables such as the type of adsorbent, empty bed contact time (EBCT) and bed configuration. These studies are very time consuming and expensive if they are not properly planned. The use of mathematical models is a complementary approach to laboratory and pilot plant experimentation because they can simulate the dynamic behavior of an adsorber and can select the optimum process design.

**The mathematical models contained in AdDesignS can be used to:**

- **Assess the Preliminary Design and Feasibility of Using Adsorption Processes**
- **Plan Laboratory and/or Pilot Plant Studies**
- **Interpret Laboratory and Pilot Plant Results**
- **Provide Process Design when Site Specific Model Parameters are Available**

**AdDesignS MODELS**

AdDesignS contains equilibrium and mass transfer models that can be used to evaluate and design gas and liquid phase fixed-bed adsorbers. The models include:

- Equilibrium Column Model (ECM)
- Pore and Surface Diffusion Model (PSDM)
- Constant Pattern Homogeneous Surface Diffusion Model (CPHSDM)

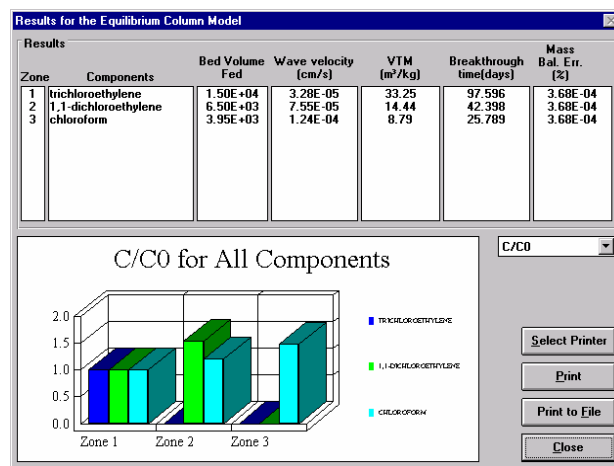
**AdDesignS - ECM**

The ECM is a fixed-bed adsorption model that ignores mass transfer resistance, uses Ideal Adsorbed Solution Theory (IAST) to predict competitive adsorption effects in multi-component mixtures and is designed for a step-up increase in influent concentration (Crittenden, et al., 1987a).

ECM can be used to:

- Determine the elution order of the adsorbing compounds.
- Calculate the highest effluent concentrations due to competitive adsorption.
- Determine the highest possible adsorbent usage rate that can be obtained for a given compound in a multi-component mixture in the absence of mass transfer.
- Reduce the number of compounds to be specified in mass transfer model calculations.

The ECM can be used for both gas and liquid phase calculations.



Sample AdDesignS Output Screen for a Three Component ECM Calculation

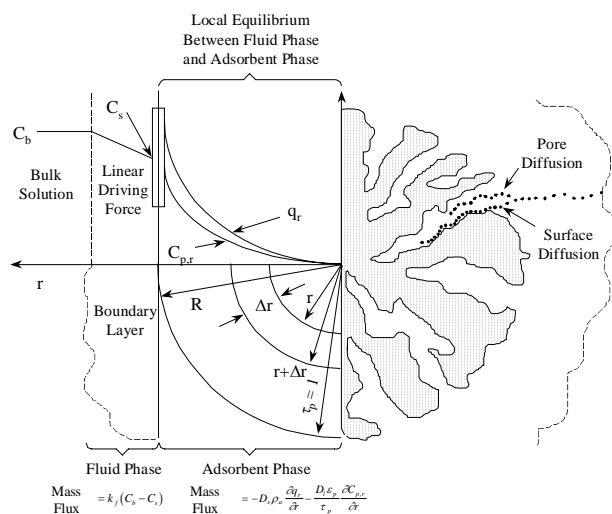
**AdDesignS PSDM**

The PSDM is a dynamic fixed-bed model that incorporates the following mechanisms and assumptions (Crittenden, et al., 1986, 1987b, 1988; and Hand, et al., 1989, 1998):

- Constant flow rate.
- Plug-Flow conditions exist in the bed.
- Linear driving force describes the local bulk phase mass flux at the exterior surface of the adsorbent particle.
- Local adsorption equilibrium exists between the solute adsorbed onto the adsorbent particle and the intra-aggregate stagnant fluid.
- Intraparticle mass flux is described by surface and pore diffusion.
- Adsorption equilibrium of individual compounds is represented by the Freundlich isotherm equation

and IAST describes the competition between the compounds.

- There are no interactions between adsorbing compounds during the diffusion process.

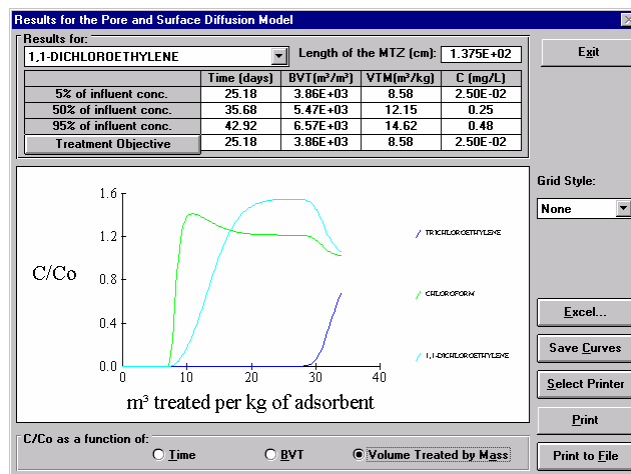


Schematic of the PSDM Mechanisms

Incorporating these mechanisms and assumptions into mass balances on both the bulk and adsorbent phase results in two partial differential equations for each adsorbing compound. A coupling equation between the bulk and the adsorbent phase is obtained from assuming local equilibrium at the exterior of the adsorbent particle.

In cases where pore and surface diffusion are present, local equilibrium is assumed along the pore walls. These equations are non-dimensionalized and solved by numerical methods. Orthogonal collocation is used to convert the set of partial differential equations into ordinary differential equations. The set of ordinary differential equations are solved using a backward differentiation method formula, also known as Gear's stiff method.

The PSDM can be used for both gas and liquid phase calculations.



Sample AdDesignS Output Screen for a Three Component PSDM Calculation

### AdDesignS – CPHSDM

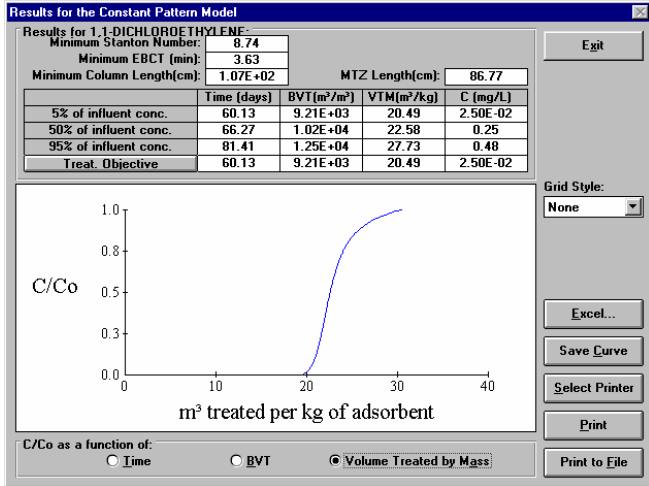
The CPHSDM is a fixed-bed adsorption model for a single compound that incorporates the following assumptions and mechanisms (Hand, et al., 1984):

- Constant flow rate.
- Plug-flow conditions exist in the bed.
- Linear driving force describes the local bulk phase mass flux at the exterior surface of the adsorbent particle.
- Surface diffusion is the predominant intraparticle mass transfer mechanism and is not a function of concentration.
- Local adsorption equilibrium exists between the solute adsorbed onto the adsorbent surface and the solute in the adsorbent pores.
- Adsorption equilibrium is represented by the Freundlich isotherm equation.

Simple empirical expressions are used to describe the CPHSDM solutions. The CPHSDM solutions are valid for these conditions:

- The influent concentration should be nearly constant and does not fluctuate by more than 10 – 30 %.
- The bed length should be long enough such that there is enough time for the mass transfer wave to develop within 10% of constant pattern conditions. This is only possible when the Freundlich 1/n is less than 1.0.

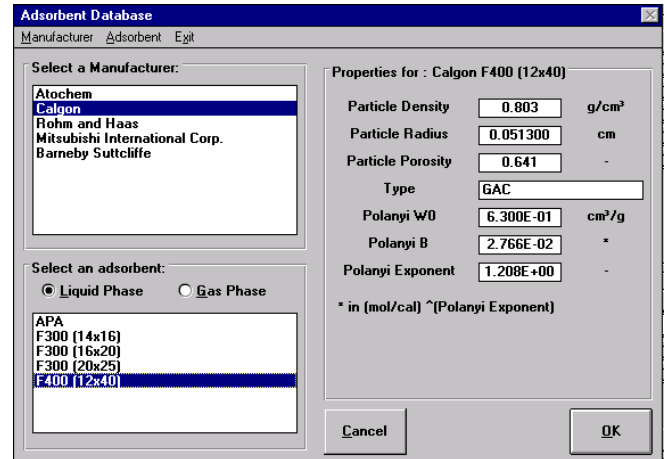
The advantage of the CPHSDM is that a simple empirical expression is used calculate the entire effluent concentration history profile, eliminating the need to solve the complex set of differential equations that describe adsorber dynamics.



Sample AdDesignS Output Screen for a Single Component CPHSDM Calculation

## Adsorbent Database

AdDesignS contains a database of adsorbent physical properties for several commercially available gas and liquid phase adsorbents. These properties are needed to perform model calculations. New or updated adsorbent information can easily be inserted into the adsorbent database.



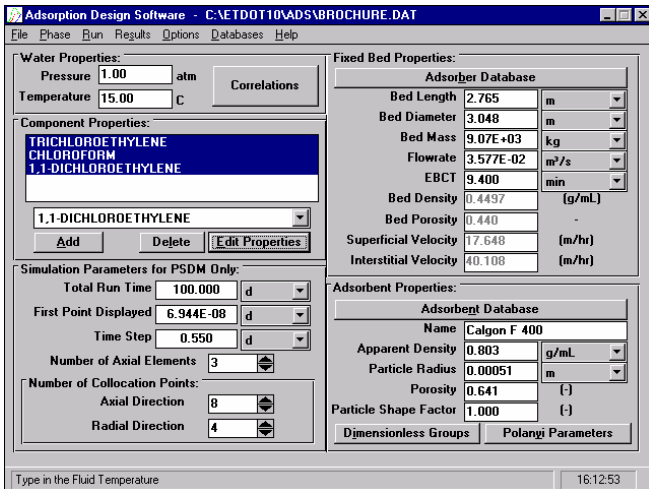
AdDesignS Adsorbent Database Window

## AdDesignS Databases and Parameter Estimation Techniques

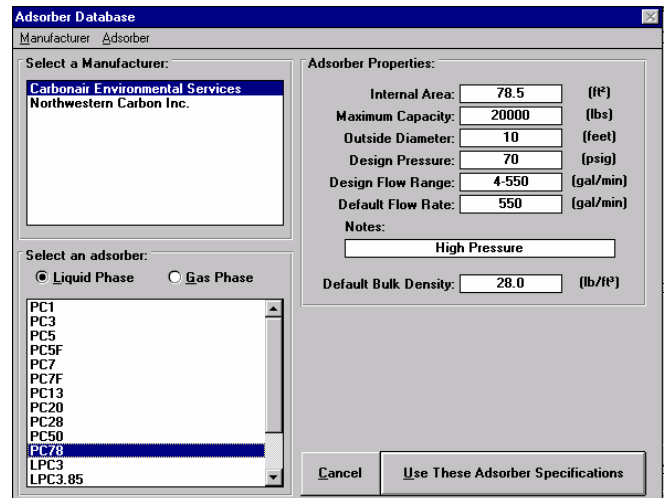
Adsorption calculations using the above models require fixed-bed and adsorbent physical properties, equilibrium and kinetic parameters combined with several physical properties of the adsorbing compound(s) and the adsorbent. These parameters and physical properties are easily obtained using the databases provided by AdDesignS.

## Adsorbent Database

AdDesignS provides a database of commercially available packaged adsorber systems that are readily available for various user applications.



Sample AdDesignS Main Window



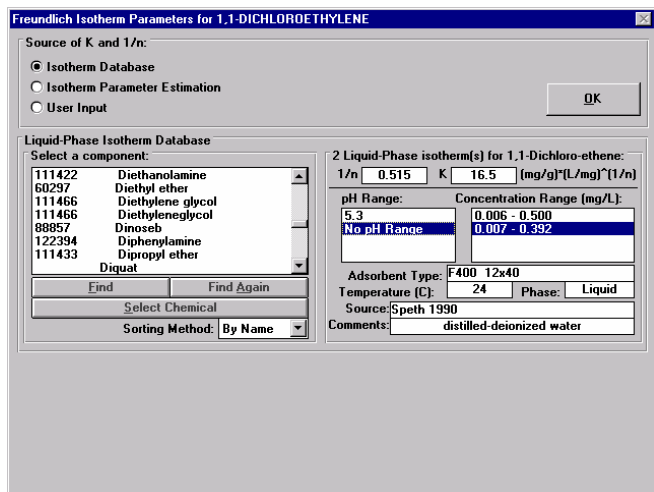
AdDesignS Adsorbent Database Window

## Adsorption Equilibrium Isotherm Parameter Database

The AdDesignS contains an equilibrium isotherm database of over 650 determined aqueous phase Freundlich isotherms for more than 300

compounds on 15 adsorbents. These single solute isotherms are referenced and display the conditions in which they were experimentally determined (e.g. concentration range, pH, temperature, adsorbent type).

AdDesignS also contains gas-phase Freundlich isotherm parameters for more than 300 compounds on two adsorbents. New or updated isotherm information obtained from the manufacturers or literature reported values are easily inserted into the AdDesignS isotherm database.



AdDesignS Isotherm Database Window

### Adsorption Equilibrium Parameter Estimation Techniques

AdDesignS contains Isotherm Parameter Estimation Software (IPES) for calculating gas and liquid phase equilibrium adsorption of organic compounds. IPES uses Polanyi potential theory to estimate single solute Freundlich isotherm parameters for compounds that are not readily available in the AdDesignS adsorption equilibrium isotherm database.

For liquid-phase applications the 3-parameter Polanyi isotherm correlation is used and for gas phase applications, the Dubinin-Radushkevich (D-R) correlation based on spreading pressure evaluation is used.

### Correlations for Natural Organic Matter (NOM) Fouling of Adsorbents

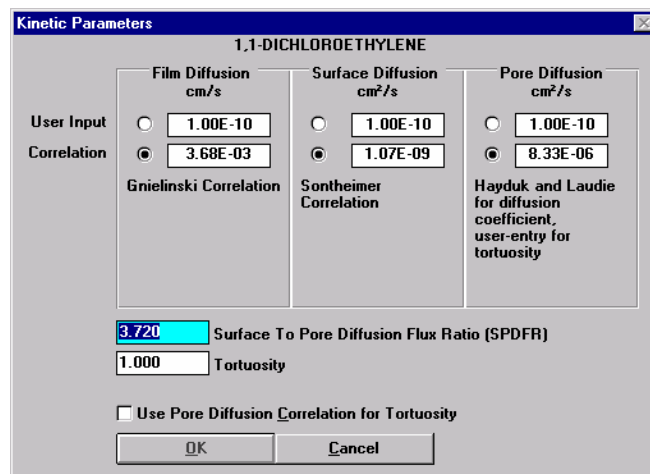
The adsorption behavior of trace organic compounds is quite different when in the presence of NOM, especially in

fixed-beds. For surface and ground waters containing NOM the adsorption capacity and kinetics can be significantly reduced by competition with and/or fouling of the adsorbent by NOM. AdDesignS provides correlations for adjusting the adsorption capacity and kinetics to account for the impact of NOM fouling (Sontheimer, et al., 1988).

### Kinetic Parameter Estimation Techniques

Mass transfer parameters are required for the CPHSDM and the PSDM. These parameters can be experimentally determined. However, at the design stage of a fixed-bed adsorber, such data is often unavailable and correlations are required.

AdDesignS provides the capability to estimate both external and intraparticle mass transfer parameters for several design situations. AdDesignS also provides the capability to determine kinetic parameters from laboratory and pilot plant data.



AdDesignS Kinetic Parameter Window

### Physical and Chemical Properties Database Based on EPA's List of Priority Pollutants

In the process of performing fixed-bed adsorber calculations, the following chemical properties are usually required for gas and liquid phase simulations: molecular weight, normal boiling point, molar volume at the normal boiling point, liquid density, vapor pressure and refractive index. Consequently, AdDesignS is linked to a program called Software to Estimate Physical Properties (StEPP).

StEPP provides these physical properties at the specified temperature. StEPP contains the physical and chemical properties for over 600 compounds, many of which are on cover EPA's list of priority pollutants.

Component Properties	
1,1-DICHLOROETHYLENE	
Name	1,1-DICHLOROETHYLENE
Molecular Weight	96.940 mg/mmol
Molar Volume @ NBP	8.4000E+01 mL/gmol
Boiling Point	31.600 C
Initial Concentration	5.0000E-01 mg/L
Liquid Density	1.2200E+00 g/mL
Solubility	2.7500E+03 mg/L
Vapor Pressure	5.4400E+04 Pa
Refractive Index	1.4218 (-)
CAS Number	75354 (-)
Freundlich Isotherm Parameters	
Freundlich K	18.820 (mg/g)*(L/mg)^(1/n)
Freundlich 1/n	0.564
Source of K and 1/n: Isotherm Parameter Estimation	

AdDesignS Component Properties Window

## Other AdDesignS Options

- Time-variable Influent Data
- Laboratory and Pilot Plant Data Analysis Capabilities
- Excel Spreadsheet Compatible

## Graphical User Interface

ETDOT is designed for the Microsoft Windows environment with a graphical user interface (GUI) to maximize user-friendliness. Making use of the Microsoft Windows interface, with its built-in file and hardware control features, frees the engineer from concerns over printer drivers and other "machine" issues and allows more attention to the computational algorithms. The GUI consists of a Microsoft Visual Basic front-end shell that calls FORTRAN subroutines to perform the calculations.

## System Requirements

The minimum ETDOT system requirements are as follows:

- English-language version of Microsoft Windows 95, Microsoft Windows 98, or Microsoft Windows

NT 4.0; in the case of Microsoft Windows NT 4.0, Service Pack 3 or more recent is required

- 50 MB of hard disk space
- 32 MB of RAM is recommended
- A Pentium or more recent processor is recommended
- A graphic VGA or more recent video display
- A mouse or other pointing device is recommended

## Product Information

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## References

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