



EPA Small Systems Workshop Training

AdDesignS™: Modeling Drinking Water Treatment with Granular Activated Carbon

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US EPA Office of Research and Development

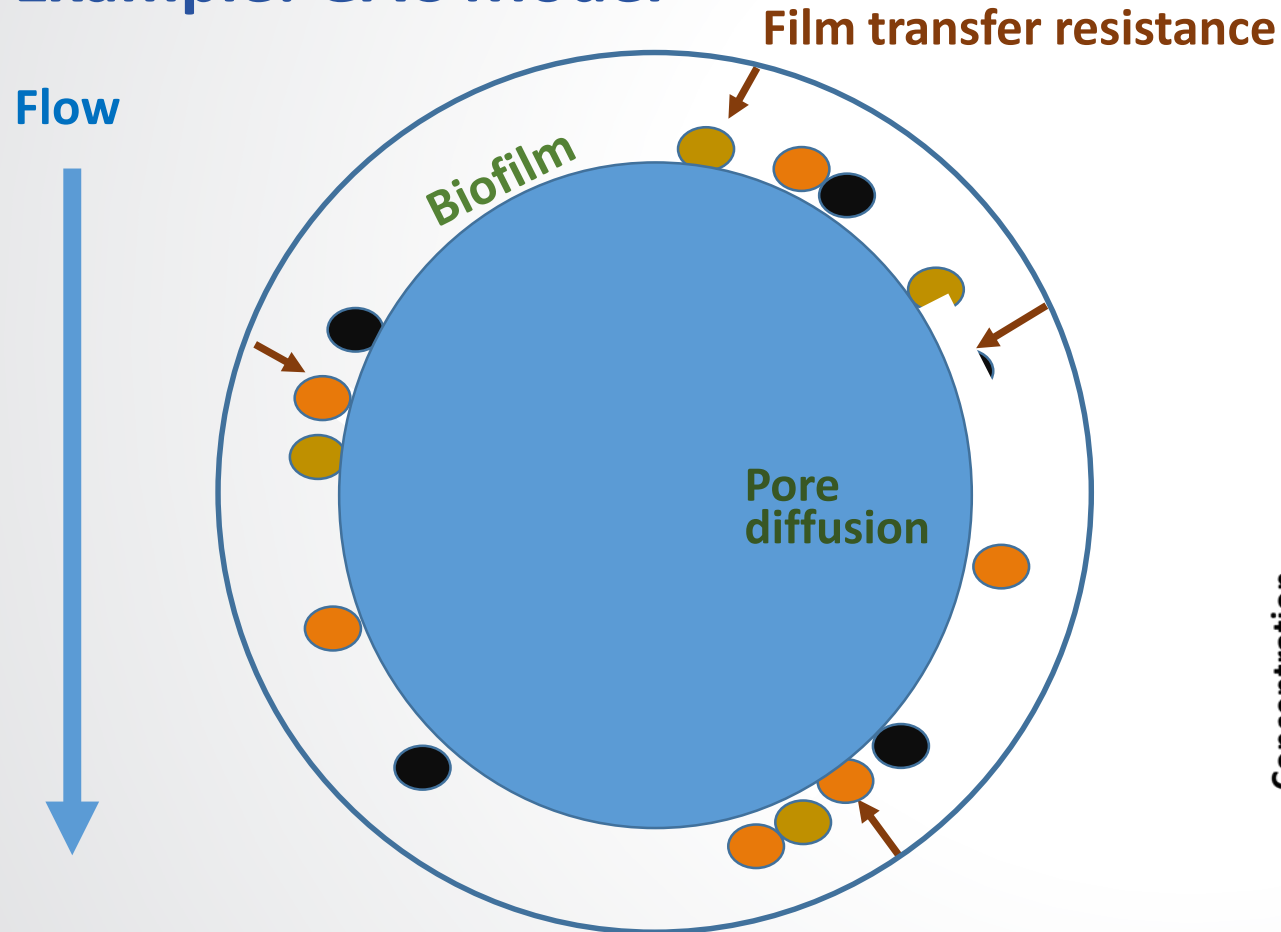
August 31, 2020



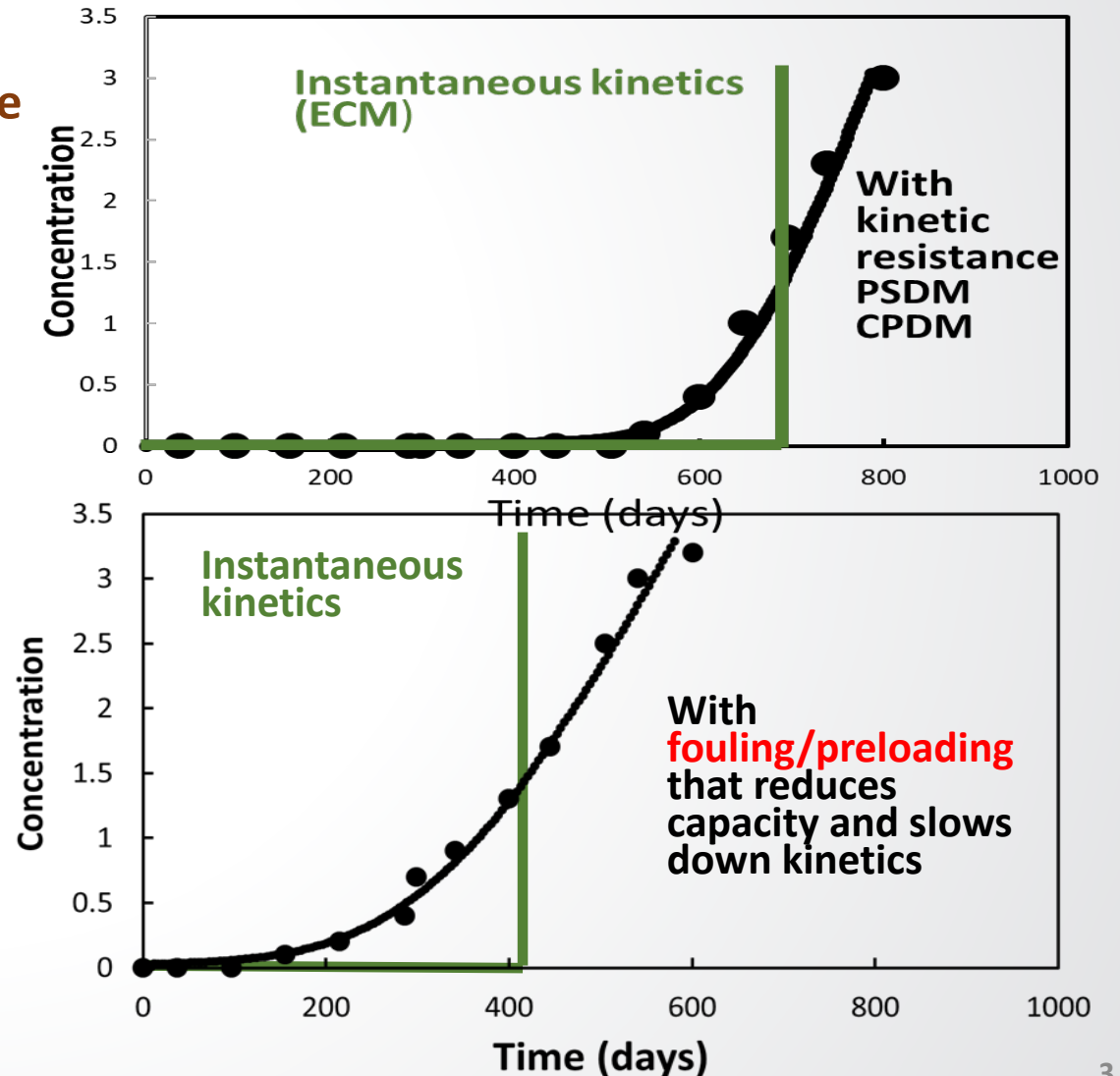
- Background
 - Overview of the models
 - Additional Resources
- Getting Started
 - Downloading Software
- AdDesignS™
 - Basics of the User Interface
 - Dynamic walk through of AdDesignS™ features (not in slides)
- Water Treatment Models
 - Brief introduction to additional tools



Example: GAC Model

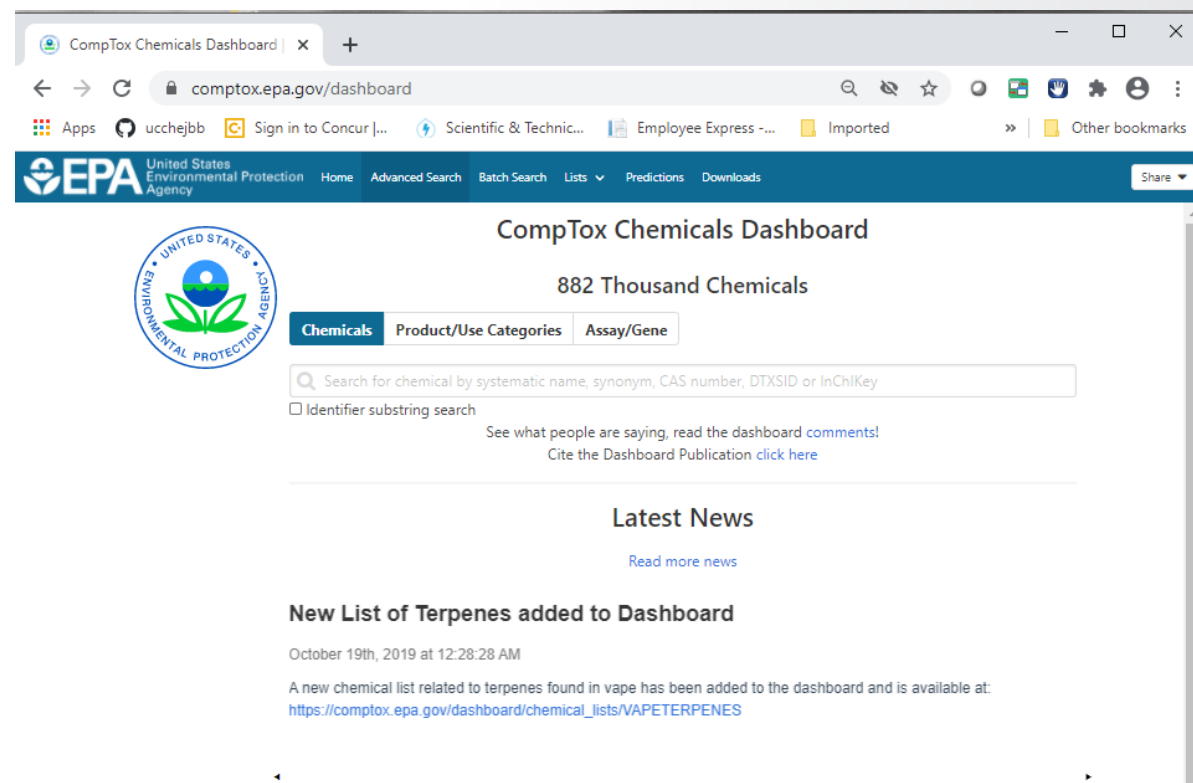


The models range from simple to complex



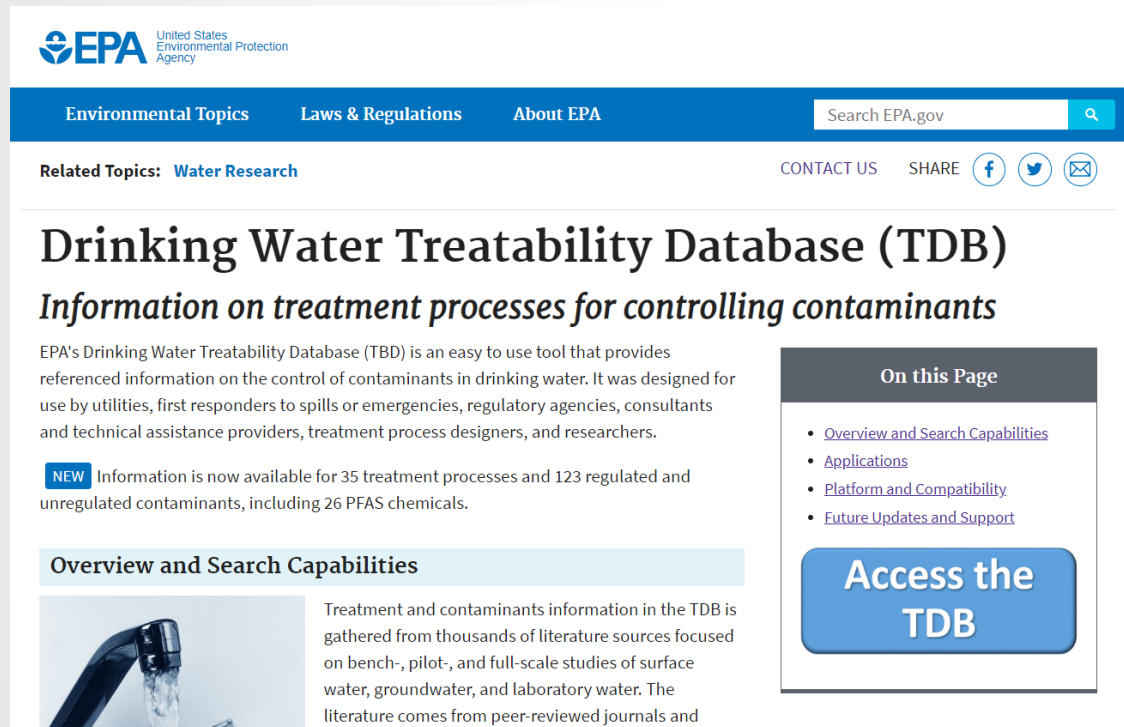
- COMPTOX
 - Searchable
 - Has parameters needed by PSDM
 - Molecular Weight
 - Molar Volume
 - Liquid Density
- General web search may also yield results, but COMPTOX typically has everything in one place

- COMPTOX



<https://comptox.epa.gov/dashboard>
Search: EPA COMPTOX

- Treatability Database



Drinking Water Treatability Database (TDB)
Information on treatment processes for controlling contaminants

EPA's Drinking Water Treatability Database (TDB) is an easy to use tool that provides referenced information on the control of contaminants in drinking water. It was designed for use by utilities, first responders to spills or emergencies, regulatory agencies, consultants and technical assistance providers, treatment process designers, and researchers.

NEW Information is now available for 35 treatment processes and 123 regulated and unregulated contaminants, including 26 PFAS chemicals.

Overview and Search Capabilities

Treatment and contaminants information in the TDB is gathered from thousands of literature sources focused on bench-, pilot-, and full-scale studies of surface water, groundwater, and laboratory water. The literature comes from peer-reviewed journals and

On this Page

- [Overview and Search Capabilities](#)
- [Applications](#)
- [Platform and Compatibility](#)
- [Future Updates and Support](#)

Access the TDB

epa.gov/water-research/drinking-water-treatability-database-tdb

Search: EPA TDB

- Treatability Database

- Has adsorption isotherm information
 - Freundlich Isotherm parameters (K & $1/n$)
- Links to papers where isotherm parameters were reported.



PFAS Treatment: Activated Carbon

Matrix of conditions and results from treatment references that can be downloaded into a spreadsheet

Ref #	Author	Year	Log or Percent Removal	Removal Type	Contaminant Influent	Contaminant Effluent	Contaminant Units	Contaminant	Scale	Design Flow	Water	Location Studied	GAC Type	Manufacturer	Product Name
2441	Dickenson,	2016	-10.5 to 13.7#	Percent	4.4 to 5.1#	5.7 to 6.3#	ng/L	PFHpA	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	-11 to 5#	Percent	3.6 to 5.8#	4.0 to 5.5#	ng/L	PFHxS	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	-13 to 6#	Percent	1.8 to 2.4#	1.7 to 2.7#	ng/L	PFNA	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	-19 to 10#	Percent	6.8 to 7.3#	6.1 to 8.7#	ng/L	PFHxA	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	-26#	Percent	<5.0#	6.3#	ng/L	PFBA	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	-34 to 8#	Percent	0.59 to 0.97#	0.54 to 1.3#	ng/L	PFDA	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	-66 to 70#	Percent	1.23 to 1.81#	0.537 to 2.48#	ng/L	PFBA	F	0.5472 to	GW	Minnesota	B	Calgon	F600
2441	Dickenson,	2016	0 to 19#	Percent	<0.05 to 0.085	<0.05 to 0.069#	ng/L	PFPeA	F	0.5472 to	GW	Minnesota	B	Calgon	F600
2441	Dickenson,	2016	0 to 76#	Percent	<0.05 to 0.210	<0.05#	ng/L	PFHxS	F	0.5472 to	GW	Minnesota	B	Calgon	F600
2441	Dickenson,	2016	33#	Percent	15#	10#	ng/L	PFBA	F	5#	SW	Colorado	B	Norit	GAC 300
2441	Dickenson,	2016	46 to 60#	Percent	0.127 to 0.192	<0.05 to 0.1023	ng/L	PFHxA	F	0.5472 to	GW	Minnesota	B	Calgon	F600
2441	Dickenson,	2016	5 to 6#	Percent	2.1 to 3.6#	2.0 to 3.4#	ng/L	PFBS	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	7.2 to 12.7#	Percent	4.8 to 5.5#	6.4 to 6.9#	ng/L	PFPeA	F	5	SW	New Jersey	B	Calgon	F300
2441	Dickenson,	2016	74#	Percent	17#	4.4#	ng/L	PFPeA	F	5#	SW	Colorado	B	Norit	GAC 300
2441	Dickenson,	2016	91#	Percent	11#	0.97#	ng/L	PFNA	F	5#	SW	Colorado	B	Norit	GAC 300
2441	Dickenson,	2016	>89#	Percent	4.5#	<0.50#	ng/L	PFHpA	F	5#	SW	Colorado	B	Norit	GAC 300
2441	Dickenson,	2016	>96#	Percent	5.8#	<0.25#	ng/L	PFHxS	F	5#	SW	Colorado	B	Norit	GAC 300
2441	Dickenson,	2016	>96#	Percent	6.4#	<0.25#	ng/L	PFBS	F	5#	SW	Colorado	B	Norit	GAC 300
2505	Cummings,	2015	>72 to >93#	Percent	18 to 72	<5	ng/L	PFNA	F		SW	Logan System Birch	B	Calgon	F-400



ETDOT Software

Environmental Technologies Design Option Tool (ETDOT)

United States Environmental Protection Agency

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Environmental Technologies Design Option Tool (ETDOT)

Adsorption treatment modeling for contaminant removal from drinking water and wastewater

The Environmental Technologies Design Option Tool (ETDOT) is a suite of software models that provides engineers with the capability to evaluate and design systems that use granular activated carbon or ion exchange resins for the removal of contaminants, including PFAS, from drinking water and wastewater.

[Suite of Models](#) | [Compatibility](#) | [Applications](#) | [Related EPA Resources](#)

Suite of Models

ETDOT was developed by National Center for Clean Industrial and Treatment Technologies at Michigan Technological University (MTU). In 2019, EPA signed an agreement with MTU to make this suite of adsorption models available to the public at no cost.

Software included in ETDOT:

- Adsorption Design Software for Windows (AdDesignS) Version 1.0
- Advanced Oxidation Process Software (AdOx) Version 1.0.2
- Aeration System Analysis Program (ASAP) Version 1.0

Access ETDOT

Access the ETDOT software, manuals, and more at [ETDOT GitHub site](#). [EXIT](#)

GitHub Site

<https://www.epa.gov/water-research/environmental-technologies-design-option-tool-etdot>

Search: EPA ETDOT



GitHub: ETDOT Software

USEPA / Environmental-Technologies-Design-Option-Tool

Branch: master

ucchejbb committed 4548d46 on Jan 31

File	Commit Message	Time
code	Loading all files	5 months ago
extravb/cpaschk	adding extravb	5 months ago
license/snum	adding license files	5 months ago
manuals	adding manuals folder	5 months ago
programs_vb6	Loading all files	5 months ago
system_vb6	adding system_vb6 files	5 months ago
README.md	correcting readme.md	5 months ago

README.md

ETDOT

The **Environmental Technologies Design Option Tool** (ETDOT) was developed by National Center for Clean Industrial and Treatment Technologies (CenCITT) at Michigan Technological University (MTU).

Version 1.0: Copyright 1994–2005

- David R. Hokanson
- David W. Hand
- John C. Crittenden
- Tony N. Rogers
- Eric J. Oman

Releases 1

ETDOT 1.0 (Latest)
on Mar 23

Packages

No packages published
[Publish your first package](#)

Languages

Language	Percentage
VBA	72.8%
Fortran	18.0%
Rich Text Format	3.7%
C++	1.7%
Makefile	1.5%
Roff	1.1%
Other	1.2%

Current Release

<https://github.com/USEPA/Environmental-Technologies-Design-Option-Tool>



Releases on GitHub: ETDOT Software

USEPA / Environmental-Technologies-Design-Option-Tool

Code Issues 3 Pull requests Actions Projects Wiki Security Insights

Releases Tags

Latest release

ETDOT 1.0

ucchejbb released this on Mar 23 · 1 commit to master since this release

ETDOT suite of software version 1.0. Supplied by MTU.

Assets 3

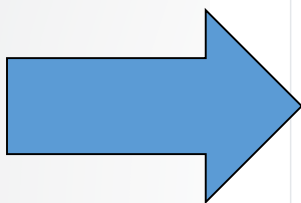
etdot_1-0.zip	70.8 MB
Source code (zip)	
Source code (tar.gz)	

Download 'etdot_1-0.zip'

<https://github.com/USEPA/Environmental-Technologies-Design-Option-Tool/releases/tag/1.0>



Readme.md



Disclaimer:

The United States Environmental Protection Agency (EPA) GitHub project code is provided on an "as is" basis and the user assumes responsibility for its use. EPA has relinquished control of the information and no longer has responsibility to protect the integrity, confidentiality, or availability of the information. Any reference to specific commercial products, processes, or services by service mark, trademark, manufacturer, or otherwise, does not constitute or imply their endorsement, recommendation or favoring by EPA. The EPA seal and logo shall not be used in any manner to imply endorsement of any commercial product or activity by EPA or the United States Government.

Installation Instructions

This software requires *Administrator Rights* to a computer to install and to run. Files are installed directly to a folder X:\ETDOT10... where X is the system main drive.

1. Download zip file in the release tab.
2. Unzip/Unpack zip file
3. Run *setup.exe* and follow prompts
4. When prompted enter license key: CAADV0-R74JM-QXCNP-7EER9-1AT72
5. To run each module in Windows 7 or newer: Edit *properties* of the program to be run and select Compatibility Tab and "run in compatibility mode". Select Windows 98/Me from the Compatibility Mode dropdown menu.

Available Users manuals will be located in the modules subfolder within the help folder.

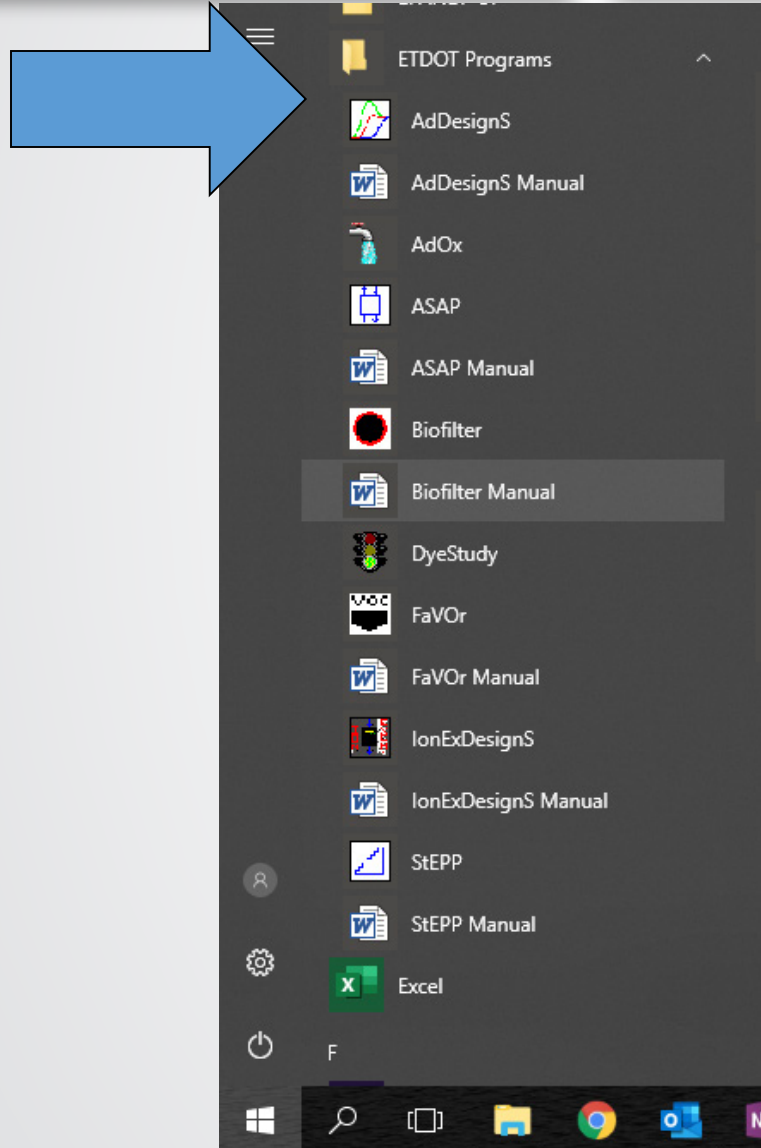
Notes on current software

The ETDOT suite of software packages consists of a FORTRAN engine with a Visual Basic (version 6) graphical user interface. The VB6 portion of the code relies on ActiveX control files which are located in the repository, however, these are an older coding standard and no longer supported with current versions of Visual Studio 20##. Precompiled engine files are included.

<https://github.com/USEPA/Environmental-Technologies-Design-Option-Tool>



Accessing ETDOT Software



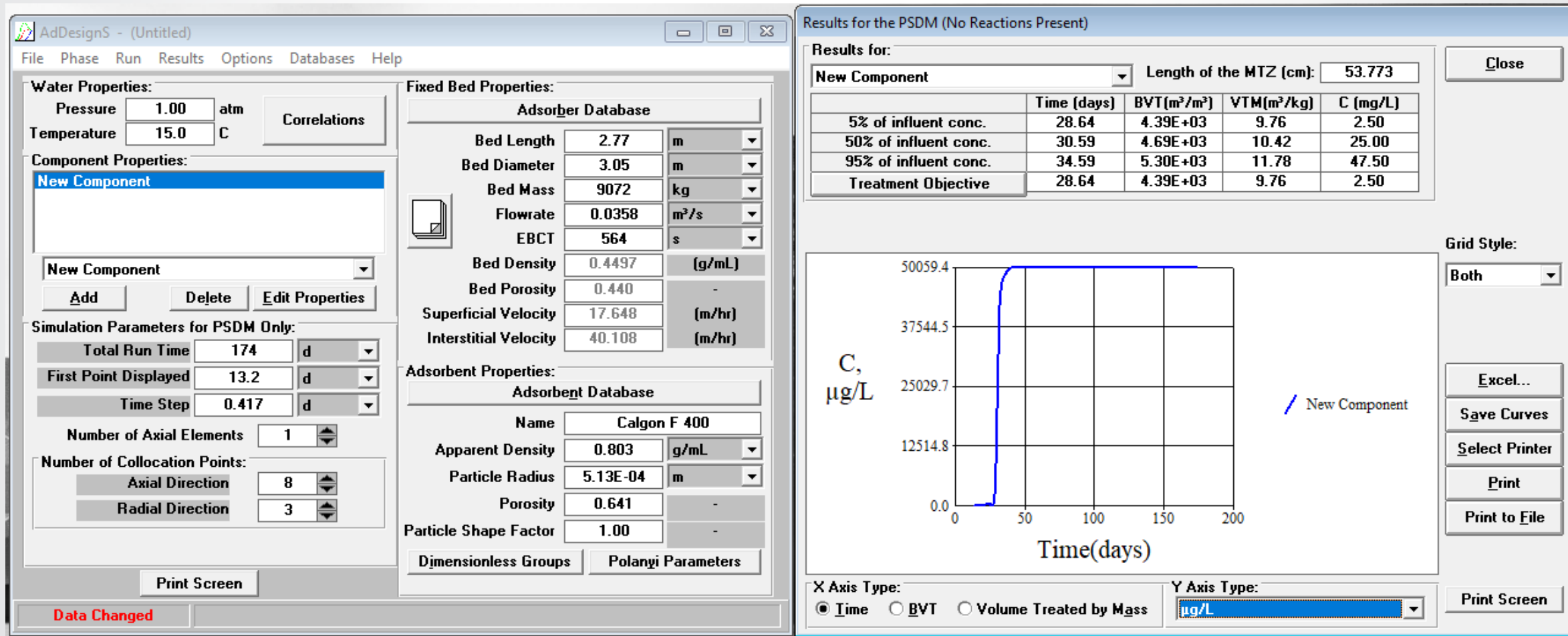
Start Menu:
'ETDOT Programs'

Software & Instruction Manuals are listed





AdDesignS™ Software





Compound Information

Column Information

Duration

AdDesignS - (Untitled)

File Phase Run Results Options Databases Help

Water Properties:

Pressure atm

Temperature C

Component Properties:

Simulation Parameters for PSDM Only:

Total Run Time d

First Point Displayed d

Time Step d

Number of Axial Elements

Number of Collocation Points:

Axial Direction

Radial Direction

Collocation Point Selection

Fixed Bed Properties:

Adsorbent Database

Bed Length m

Bed Diameter m

Bed Mass kg

Flowrate m³/s

EBCT s

Bed Density (g/mL)

Bed Porosity -

Superficial Velocity (m/hr)

Interstitial Velocity (m/hr)

Adsorbent Properties:

Adsorbent Database

Name

Apparent Density g/mL

Particle Radius m

Porosity -

Particle Shape Factor -

Adsorbent Information



Compound Information

- Compound Information
 - Add/Edit Compounds to be modeled

AdDesignS - (Untitled)

File Phase Run Results Options Databases Help

Water Properties:

Pressure atm

Temperature C

Component Properties:

Simulation Parameters for PSDM Only:

Total Run Time d

First Point Displayed d

Time Step d

Number of Axial Elements

Number of Collocation Points:

Axial Direction

Radial Direction

Fixed Bed Properties:

Adsorber Database

Bed Length	<input type="text" value="2.77"/>	m
Bed Diameter	<input type="text" value="3.05"/>	m
Bed Mass	<input type="text" value="9072"/>	kg
Flowrate	<input type="text" value="0.0358"/>	m ³ /s
EBCT	<input type="text" value="564"/>	s
Bed Density	<input type="text" value="0.4497"/>	(g/mL)
Bed Porosity	<input type="text" value="0.440"/>	-
Superficial Velocity	<input type="text" value="17.648"/>	(m/hr)
Interstitial Velocity	<input type="text" value="40.108"/>	(m/hr)

Adsorbent Properties:

Adsorbent Database

Name	<input type="text" value="Calgon F 400"/>	
Apparent Density	<input type="text" value="0.803"/>	g/mL
Particle Radius	<input type="text" value="5.13E-04"/>	m
Porosity	<input type="text" value="0.641"/>	-
Particle Shape Factor	<input type="text" value="1.00"/>	-

Unchanged



- Compound Information
 - Add/Edit Compounds to be modeled

Component Properties

StEPP Link
Obtain properties from StEPP via:

StEPP Export File

Clipboard

Kinetics

Freundlich K and 1/n

Print Screen

Cancel

OK

Unchanged

Type in the component name

Name: New Component

Molecular Weight	131	mg/mmol
Molar Volume @ NBP	102	mL/gmol
Boiling Point	87.0	C
Initial Concentration	50.0	mg/L
Liquid Density	1.53	g/mL
Solubility	1100	mg/L
Vapor Pressure	9830	Pa
Refractive Index	1.48	-
CAS Number	0	-

Freundlich Isotherm Parameters

Freundlich K	98.0	(mg/g)*(L/mg)^(1/n)
Freundlich 1/n	0.430	
Source of K and 1/n	User Entry	

Compound Information

AdDesignS - (Untitled)

File Phase Run Results Options Databases Help

Water Properties:

Pressure	1.00000	atm
Temperature	15.0	C

Correlations

Component Properties:

Add Delete Edit Properties

Simulation Parameters for PSDM Only:

Total Run Time	174	d
First Point Displayed	13.2	d
Time Step	0.417	d
Number of Axial Elements	1	
Number of Collocation Points:		
Axial Direction	8	
Radial Direction	3	

Print Screen

Unchanged

Type in the Fluid Pressure

Fixed Bed Properties:

Adsorbent Database

Bed Length	2.77	m
Bed Diameter	3.05	m
Bed Mass	9072	kg
Flowrate	0.0358	m³/s
EBCT	564	s
Bed Density	0.4497	(g/mL)
Bed Porosity	0.440	-
Superficial Velocity	17.648	(m/hr)
Interstitial Velocity	40.108	(m/hr)

Adsorbent Properties:

Adsorbent Database

Name	Calgon F 400	
Apparent Density	0.803	g/mL
Particle Radius	5.13E-04	m
Porosity	0.641	-
Particle Shape Factor	1.00	-

Dimensionless Groups Polanyi Parameters



- Compound Information
 - Add/Edit Compounds to be modeled

Component Properties

StEPP Link
Obtain properties from StEPP via:

StEPP Export File

Clipboard

Name: New Component

Molecular Weight: 131 mg/mol

Molar Volume @ NBP: 102 mL/gm

Boiling Point: 1100 g/mL

Solubility: 1100 mg/L

Vapor Pressure: 9830 Pa

Refractive Index: 1.48

CAS Number: 0

Freundlich Isotherm Parameters

Freundlich K: 98.0 (mg/g)*(L/mg)^(1/n)

Freundlich 1/n: 0.430

Source of K and 1/n: User Entry

Print Screen

Cancel

OK

Unchanged

Type in the component name

Compound Information

AdDesignS - (Untitled)

Kinetic Parameters for New Component

User Input

Correlation

Film Diffusion cm/s

Surface Diffusion cm²/s

Pore Diffusion cm²/s

Gnielinski Correlation

Sontheimer Correlation

Hayduk and Laudie for diffusion coefficient, user-entry for tortuosity

5.00 Surface To Pore Diffusion Flux Ratio (SPDFR)

1.00 Tortuosity

Use Pore Diffusion Correlation for Tortuosity

OK

Cancel

Print Screen

Unchanged

Type in the user-input film diffusion coefficient



- **Column Information**

- Supply the physical characteristics of the bed
- Supply the flowrate to the system (will recalculate EBCT)
 - Can verify EBCT seems correct
 - Alternatively: adjust EBCT and flowrate will be recalculated (can use for specific throughput analysis)
- Dropdown menus can be adjusted to provide a variety of unit systems

The screenshot shows the AdDesignS software interface with the following sections:

Water Properties:

- Pressure: 1.00000 atm
- Temperature: 15.0 C
- Correlations button

Component Properties:

- Empty box for component name
- Add, Delete, Edit Properties buttons

Simulation Parameters for PSDM Only:

- Total Run Time: 174 d
- First Point Displayed: 13.2 d
- Time Step: 0.417 d
- Number of Axial Elements: 1
- Number of Collocation Points:
 - Axial Direction: 8
 - Radial Direction: 3
- Print Screen button

Fixed Bed Properties:

Adsorber Database

Property	Value	Unit
Bed Length	2.77	m
Bed Diameter	3.05	m
Bed Mass	9072	kg
Flowrate	0.0358	m³/s
EBCT	564	s
Bed Density	0.4497	(g/mL)
Bed Porosity	0.440	-
Superficial Velocity	17.648	(m/hr)
Interstitial Velocity	40.108	(m/hr)

Adsorbent Properties:

Adsorbent Database

Property	Value	Unit
Name	Calgon F 400	
Apparent Density	0.803	g/mL
Particle Radius	5.13E-04	m
Porosity	0.641	-
Particle Shape Factor	1.00	-

Dimensionless Groups | Polanyi Parameters

Unchanged | Type in the Fluid Pressure

Column Information



- Adsorbent Information
 - Defines characteristics of the adsorbent
 - Can access some predefined adsorbents using “Adsorbent Database” Button
 - Apparent density here is not the apparent density typically provided by manufacturer.
 - F400 manufacturer value is 0.55.
 - This value is (AD/packing efficiency of adsorbent)
 $0.803 = 0.55 / \sim 0.685$

AdDesignS - (Untitled)

File Phase Run Results Options Databases Help

Water Properties:

Pressure atm

Temperature C

Component Properties:

Simulation Parameters for PSDM Only:

Total Run Time d

First Point Displayed d

Time Step d

Number of Axial Elements

Number of Collocation Points:

Axial Direction

Radial Direction

Fixed Bed Properties:

Adsorbent Database

Bed Length	<input type="text" value="2.77"/>	m
Bed Diameter	<input type="text" value="3.05"/>	m
Bed Mass	<input type="text" value="9072"/>	kg
Flowrate	<input type="text" value="0.0358"/>	m³/s
EBCT	<input type="text" value="564"/>	s
Bed Density	<input type="text" value="0.4497"/>	(g/mL)
Bed Porosity	<input type="text" value="0.440"/>	-
Superficial Velocity	<input type="text" value="17.648"/>	(m/hr)
Interstitial Velocity	<input type="text" value="40.108"/>	(m/hr)

Adsorbent Properties:

Adsorbent Database

Name	<input type="text" value="Calgon F 400"/>
Apparent Density	<input type="text" value="0.803"/> g/mL
Particle Radius	<input type="text" value="5.13E-04"/> m
Porosity	<input type="text" value="0.641"/> -
Particle Shape Factor	<input type="text" value="1.00"/> -

Type in the Fluid Pressure

Adsorbent Information



- **Collocation Points**

- Defines how many elements are used in the numerical solution
- Increasing these can help smooth PSDM solutions
- Axial Direction ≤ 18
 - If the problem requires more than 18, increase “Number of Axial Elements”
- Radial Direction ≤ 18
 - Typically this value will be less than 10

AdDesignS - (Untitled)

File Phase Run Results Options Databases Help

Water Properties:

Pressure 1.00000 atm

Temperature 15.0 C

Correlations

Component Properties:

Add Delete Edit Properties

Simulation Parameters for PSDM Only:

Total Run Time 174 d

First Point Displayed 13.2 d

Time Step 0.417 d

Collocation Point Selection:

Number of Axial Elements 1

Number of Collocation Points:

Axial Direction 8

Radial Direction 3

Print Screen

Unchanged

Fixed Bed Properties:

Adsorber Database

Bed Length 2.77 m

Bed Diameter 3.05 m

Bed Mass 9072 kg

Flowrate 0.0358 m³/s

EBCT 564 s

Bed Density 0.4497 (g/mL)

Bed Porosity 0.440 -

Superficial Velocity 17.648 (m/hr)

Interstitial Velocity 40.108 (m/hr)

Adsorbent Properties:

Adsorbent Database

Name Calgon F 400

Apparent Density 0.803 g/mL

Particle Radius 5.13E-04 m

Porosity 0.641 -

Particle Shape Factor 1.00 -

Dimensionless Groups Polanyi Parameters

Type in the Fluid Pressure

Collocation Point Selection



- **Duration**

- Defines how long to run the simulation
- Will get an error if more than 400 timesteps will be required
 - Increase “Time Step” and then adjust “Total Run Time”

Duration

AdDesignS - (Untitled)

File Phase Run Results Options Databases Help

Water Properties:

Pressure atm

Temperature C

Component Properties:

Simulation Parameters for PSDM Only:

Total Run Time d

First Point Displayed d

Time Step d

Number of Axial Elements

Number of Collocation Points:

Axial Direction

Radial Direction

Fixed Bed Properties:

Adsorbent Database

Bed Length	<input type="text" value="2.77"/>	m
Bed Diameter	<input type="text" value="3.05"/>	m
Bed Mass	<input type="text" value="9072"/>	kg
Flowrate	<input type="text" value="0.0358"/>	m³/s
EBCT	<input type="text" value="564"/>	s
Bed Density	<input type="text" value="0.4497"/>	(g/mL)
Bed Porosity	<input type="text" value="0.440"/>	-
Superficial Velocity	<input type="text" value="17.648"/>	(m/hr)
Interstitial Velocity	<input type="text" value="40.108"/>	(m/hr)

Adsorbent Properties:

Adsorbent Database

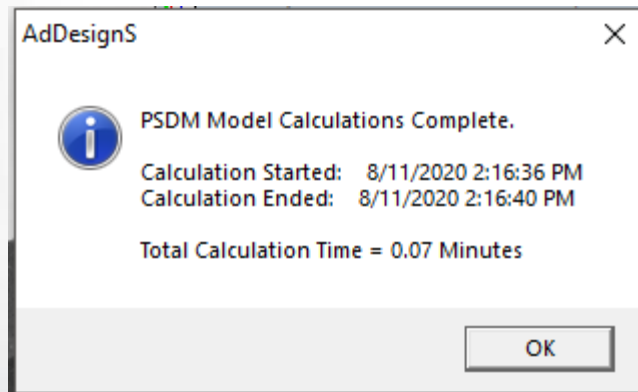
Name	<input type="text" value="Calgon F 400"/>
Apparent Density	<input type="text" value="0.803"/> g/mL
Particle Radius	<input type="text" value="5.13E-04"/> m
Porosity	<input type="text" value="0.641"/> -
Particle Shape Factor	<input type="text" value="1.00"/> -



- **Running a Simulation**

- Liquid.dat, provided with ETDOT installation
- Select individual compounds to consider in the model

- Will get a completion dialog box



AdDesignS - c:\etdot10\ads\examples\liquid.dat

File Phase Run Results Options Databases Help

Water Prop PSDM Shift+F3
Pressur CPHSDM Shift+F4
Temperatur ECM Shift+F5

Component Properties:
TRICHLOROETHYLENE
TETRACHLOROETHYLENE
TOLUENE

TRICHLOROETHYLENE

Add Delete Edit Properties

Simulation Parameters for PSDM Only:

Total Run Time 1000 d
First Point Displayed 10.0 d
Time Step 2.50 d

Number of Axial Elements 2

Number of Collocation Points:
Axial Direction 8
Radial Direction 3

Print Screen

Unchanged Type in the Fluid Pressure

Fixed Bed Properties:

Adsorber Database

Bed Length	1.80	m
Bed Diameter	3.66	m
Bed Mass	8500	kg
Flowrate	500	gpm
EBCT	9.99	min
Bed Density	0.4494	(g/mL)
Bed Porosity	0.440	-
Superficial Velocity	10.808	(m/hr)
Interstitial Velocity	24.546	(m/hr)

Adsorbent Properties:

Adsorbent Database

Name	Calgon F400 (12x40)	
Apparent Density	803	kg/m³
Particle Radius	5.13E-04	m
Porosity	0.641	-
Particle Shape Factor	1.50	-

Dimensionless Groups Polanyi Parameters



- Viewing Results from a Simulation
 - Results -> PSDM

AdDesignS - c:\etdot10\ads\examples\liquid.dat

File Phase Run Results Options Databases Help

Water Properties: Pressure 1 Temperature Component Properties: TRICHLOROETHYLENE TETRACHLOROETHYLENE TOLUENE

PSDM Results F3
CPHSMD Results F4
ECM Results F5
Compare PSDM Results to Data F6
Compare CPHSMD Results to Data F7

Adsorbent Database

Length 1.80 m
Diameter 3.66 m
Bed Mass 8500 kg
Flowrate 500 gpm
EBCT 9.99 min
Bed Density 0.4494 (g/mL)
Bed Porosity 0.440
Superficial Velocity 10.808 (m/hr)
Interstitial Velocity 24.546 (m/hr)

Adsorbent Properties: Adsorbent Database

Name Calgon F400 (12x40)
Apparent Density 803 kg/m³
Particle Radius 5.13E-04 m
Porosity 0.641
Particle Shape Factor 1.50

Dimensionless Groups Polanyi Parameters

Simulation Parameters for PSDM Only:

Total Run Time 1000 d
First Point Displayed 10.0 d
Time Step 2.50 d

Number of Axial Elements 2
Number of Collocation Points: Axial Direction 8 Radial Direction 3

Print Screen

Unchanged Type in the Fluid Pressure

Results for the PSDM (No Reactions Present)

Results for: TRICHLOROETHYLENE Length of the MTZ (cm): 17.416

	Time (days)	BVT(m³/m³)	VTM(m³/kg)	C (mg/L)
5% of influent conc.	2.85E+02	4.10E+04	91.34	1.00E-02
50% of influent conc.	3.01E+02	4.34E+04	96.66	0.10
95% of influent conc.	3.14E+02	4.53E+04	1.01E+02	0.19
Treatment Objective	2.85E+02	4.10E+04	91.34	1.00E-02

Grid Style: Both

C/Co

Time(days)

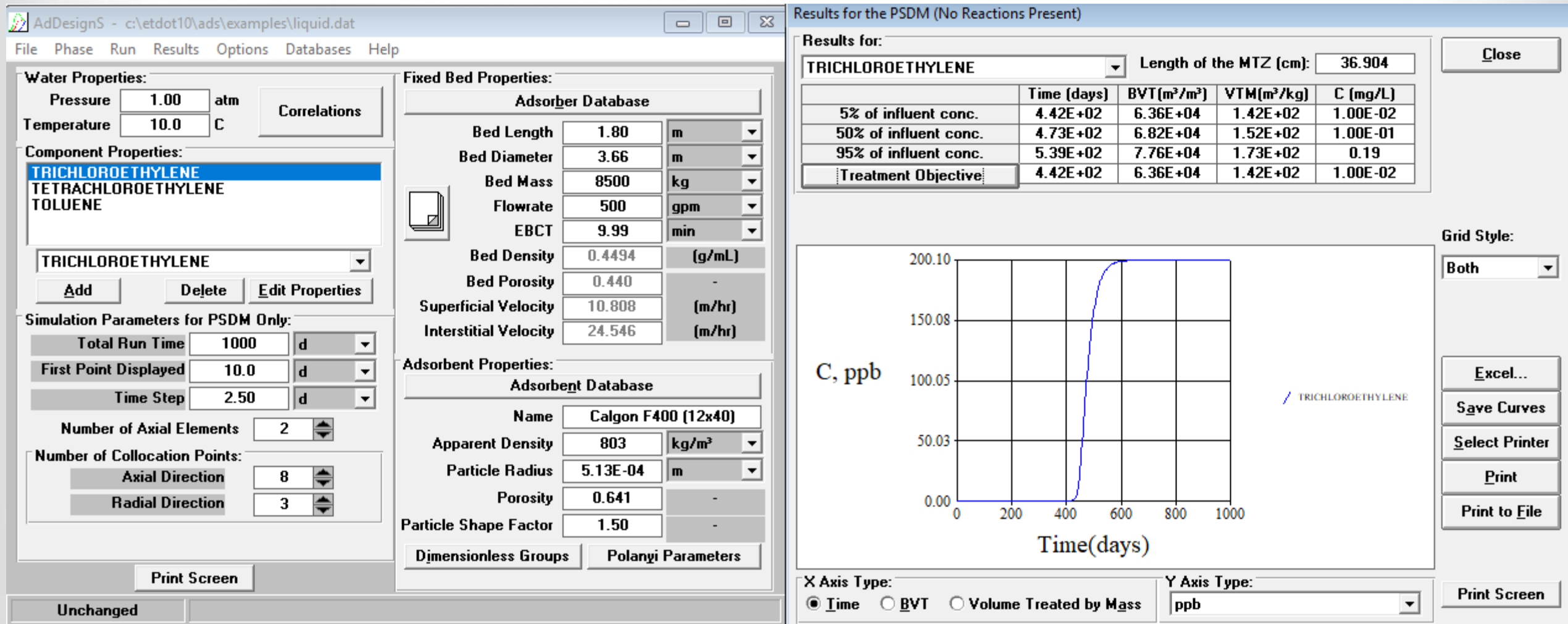
TRICHLOROETHYLENE
TETRACHLOROETHYLENE
TOLUENE

X Axis Type: ☒ Time ☐ BVT ☐ Volume Treated by Mass
Y Axis Type: C/Co

Excel...
Save Curves
Select Printer
Print
Print to File
Print Screen



- Single Compound – No Fouling





- Single Compound – Fouling

AdDesignS - c:\etdot10\ads\examples\liquid.dat

File Phase Run Results Options Databases Help

Water Properties:
Pressure 1.00000
Temperature 10.0

Component Properties:
TRICHLOROETHYLENE
TETRACHLOROETHYLENE
TOLUENE

TRICHLOROETHYLENE

Add Delete Edit Properties

Simulation Parameters for PSDM Only:
Total Run Time 1000 d
First Point Displayed 10.0 d
Time Step 2.50 d
Number of Axial Elements 2
Number of Collocation Points:
Axial Direction 8
Radial Direction 3

Print Screen

Unchanged

Type in the Fluid Pressure

Options menu:
Fouling of GAC
Influent concentrations
Effluent concentrations

Properties:
Adsorbent Database
Bed Length 1.80 m
Bed Diameter 3.66 m
Bed Mass 8500 kg
Flowrate 500 gpm
EBCT 9.99 min
Bed Density 0.4494 (g/mL)
Bed Porosity 0.440
Superficial Velocity 10.808 (m/hr)
Interstitial Velocity 24.546 (m/hr)

Adsorbent Properties:
Adsorbent Database
Name Calgon F400 (12x40)
Apparent Density 803 kg/m³
Particle Radius 5.13E-04 m
Porosity 0.641
Particle Shape Factor 1.50

Dimensionless Groups Polanyi Parameters

Fouling of GAC

Water Type:
Rhine River, Germany, Anthropogenic Input
Edit Water Type Correlations

Chemical Type:
Apply Name Type of correlation used
☒ TRICHLOROETHYLENE Halogenated alkenes
☐ TETRACHLOROETHYLENE
☐ TOLUENE
Edit Chemical Type Correlations

OK Cancel

Under Kinetic Properties For TCE

Kinetic Parameters for TRICHLOROETHYLENE

User Input Correlation

Film Diffusion cm/s	Surface Diffusion cm²/s	Pore Diffusion cm²/s
<input type="radio"/> 5.93E-03	<input type="radio"/> 1.65E-09	<input type="radio"/> 7.42E-06
<input checked="" type="radio"/> 3.61E-03	<input checked="" type="radio"/> 3.33E-41	<input checked="" type="radio"/> 6.42E-06

Gnielinski Correlation Sontheimer Correlation Hayduk and Laudie for diffusion coefficient, user-entry for tortuosity

1.00E-30 Surface To Pore Diffusion Flux Ratio (SPDFR)
For $t \leq 70$ days, tortuosity = 1;
For $t > 70$ days, tortuosity = $0.334 + 0.009518 \cdot (t, \text{days})$

☒ Use Pore Diffusion Correlation for Tortuosity

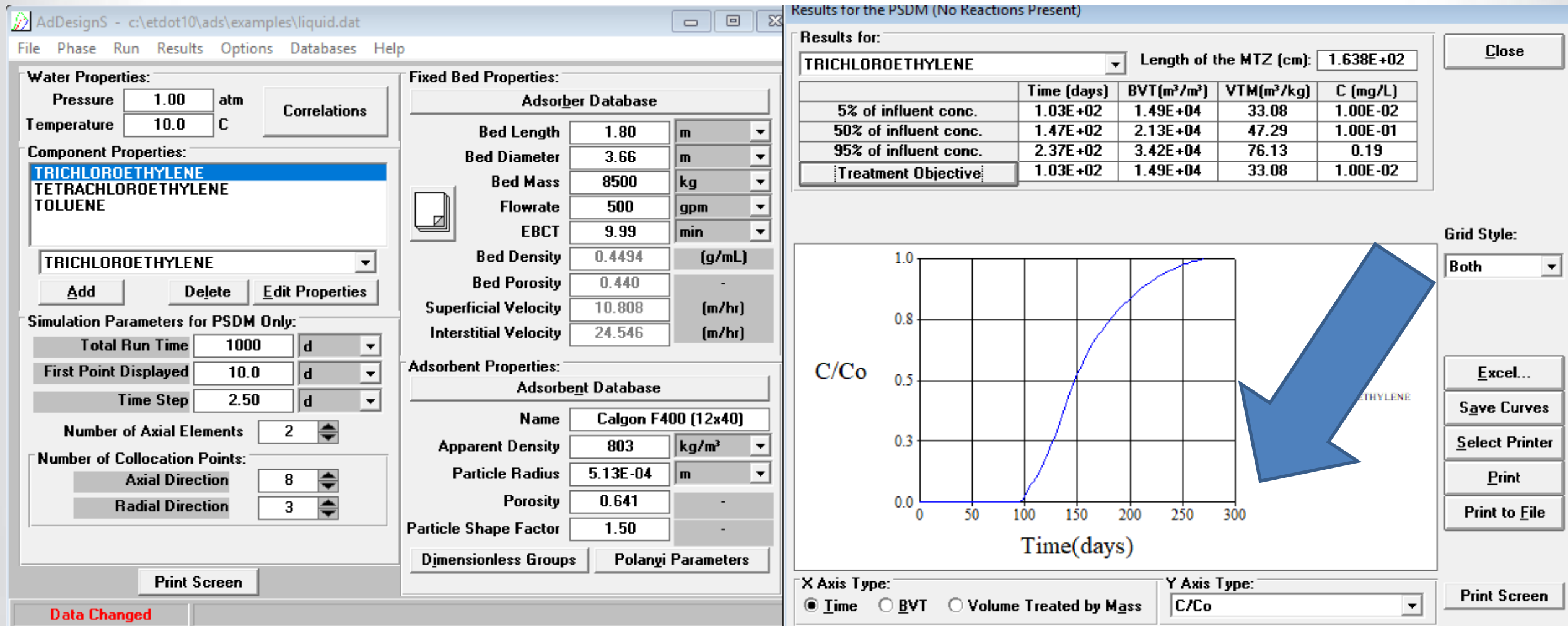
OK Cancel Print Screen

Data Changed



- Single Compound – Rhine River Fouling, halogenated alkene

Note: Time scale is only 300 days, not 1000.
Only plots until $C/C_o = 1$.





Water Treatment Models

Python-Based Tools: Provides a brief overview of capabilities available in a similar tool:

Models were developed to facilitate more automated data fitting and system assessments. Includes PSDM model and updated Ion Exchange Model – (IEX model not discussed here)



Water Treatment Models

Python Tools:
Ion Exchange Model
PSDM – GAC Model

USEPA / Water_Treatment_Models

Code Issues Pull requests Actions Projects Wiki Security Insights

Branch: master Go to file Add file Clone About

ucchejbb committed 4f4f380 2 days ago 48 commits 1 branch 0 tags

File	Commit Message	Time Ago
IonExchangeModel	Clarify Br definition	5 days ago
PSDM	Adding file save to PSDM.run_all_smart	2 days ago
.gitignore	Create .gitignore	26 days ago
LICENSE.md	Adding License.md	27 days ago
Readme.md	Update Readme.md	2 days ago

Readme.md

README for Water Treatment Models

Tools in this repository:

1. Adsorption Model for Granular Activated Carbon (PSDM Folder)
2. Ion Exchange Model (IonExchangeModel Folder)

Both tools are programmed in Python. Additional resources and information associated with either can be found in their respective folders. These tools focus on predicting water treatment unit operation effectiveness, specifically how well treatment technologies (Granular Activated Carbon and Ion Exchange Resin) will work for removing contaminants.

Status

All code in this repository is being provided in a "draft" state and has not been reviewed or cleared by US EPA. This status will be updated as models are reviewed.

Additional Information

Releases: No releases published. Create a new release.

Packages: No packages published. Publish your first package.

Contributors: 3

- LeviHaupt LeviHaupt
- ucchejbb ucchejbb
- datsovb datsovb

Languages: Python 100.0%

https://github.com/USEPA/Water_Treatment_Models



Water Treatment Models

Python Tools:
Ion Exchange Model
PSDM – GAC Model

USEPA / Water_Treatment_Models

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Readme.md

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Clone with HTTPS ? Use SSH

Use Git or checkout with SVN using the web URL.

`https://github.com/USEPA/Water_Treatment_Models`

Open in Desktop Download ZIP

Languages

- Python 100.0%

[https://github.com/USEPA/Water Treatment Models](https://github.com/USEPA/Water_Treatment_Models)



Pore and Surface Diffusion Model (PSDM)

Water_Treatment_Models/PSDM x +

github.com/USEPA/Water_Treatment_Models/tree/master/PSDM

USEPA / Water_Treatment_Models Unwatch

<> Code ! Issues 🔗 Pull requests ⚙ Actions 📁 Projects 📖 Wiki 🛡 Security 📊 Insights

Branch: master Water_Treatment_Models / PSDM / Go to file Add file ▾

ucchejbb committed 4f4f380 2 days ago History

..

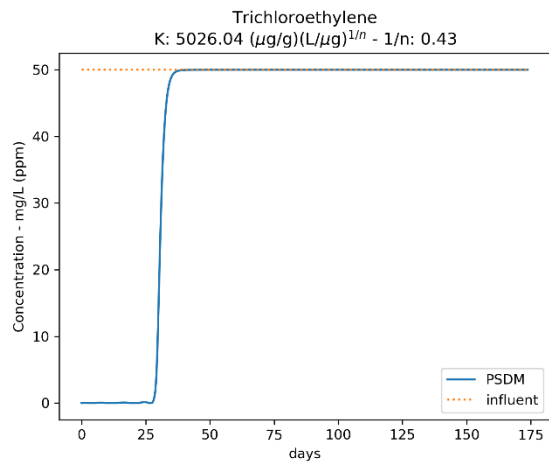
Example_Multi.py	Uploading PSDM code	6 days ago
Example_Multi.xlsx	Uploading PSDM code	6 days ago
Example_TCE.py	Uploading PSDM code	6 days ago
Example_TCE.xlsx	Uploading PSDM code	6 days ago
Example_isotherm.py	Uploading PSDM code	6 days ago
PSDM.py	Adding file save to PSDM.run_all_smart	2 days ago
PSDM_functions.py	Uploading PSDM code	6 days ago
PSDM_tools.py	Uploading PSDM code	6 days ago
Readme.md	Uploading PSDM code	6 days ago
test.xlsx	Uploading PSDM code	6 days ago
test_PSDM.py	Uploading PSDM code	6 days ago

Examples

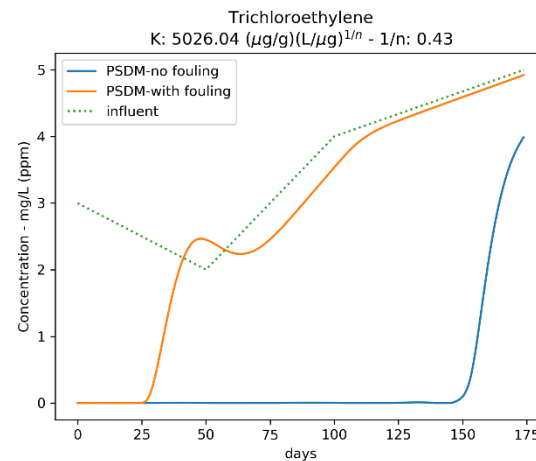
https://github.com/USEPA/Water_Treatment_Models



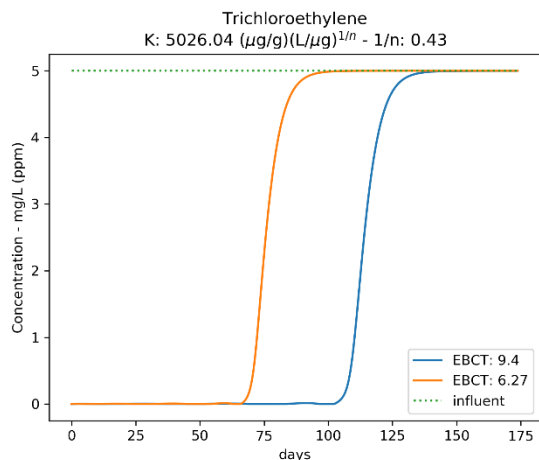
PSDM Model Examples



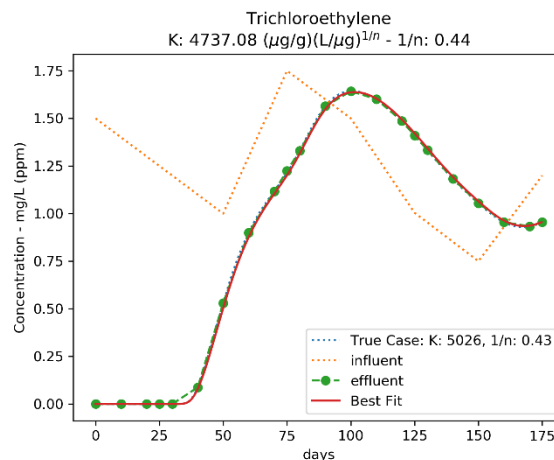
Single Compound



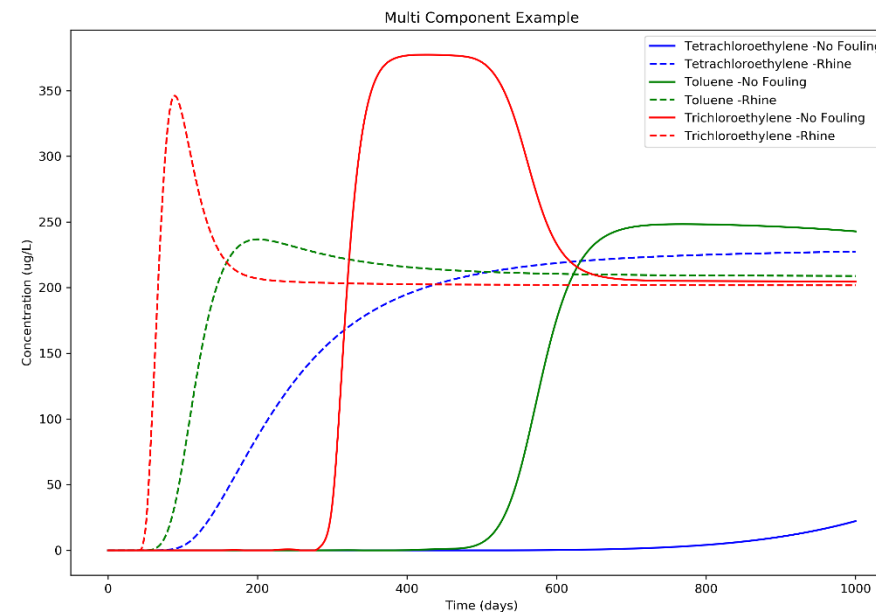
Modeling Fouling



Comparing EBCT



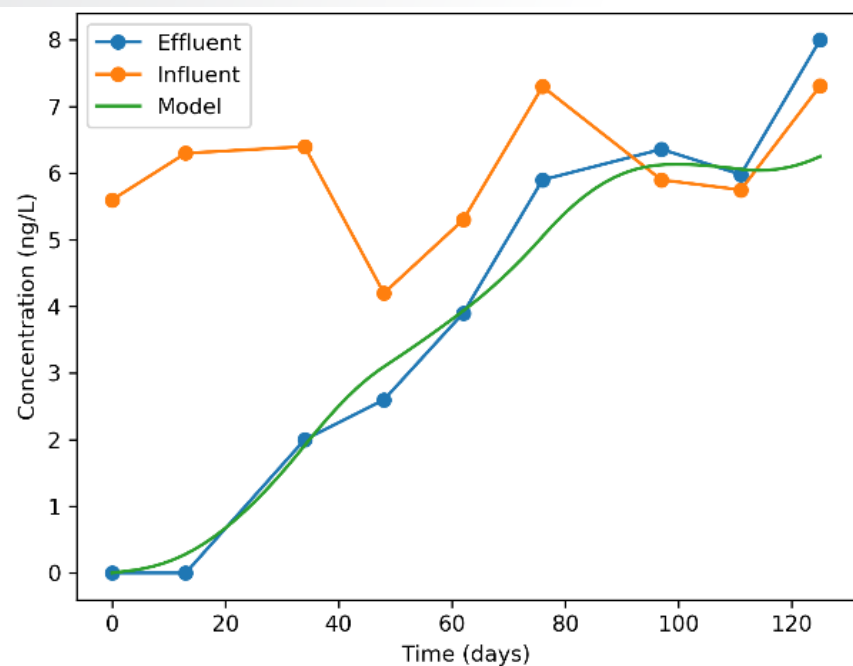
Fitting Pilot Data



Multicomponent competitive modeling

Models can be used to perform a variety of different analyses or applications

Fitting Pilot / Full-scale Data



Predicting Results for Consistent Design

- Allows for comparison across technologies by cost

Allows for Predicting other Scenarios

- Other designs: number of contactors, contactor Empty Bed Contact Times (EBCTs), different treatment goals, etc.
- Other influent conditions: Changing concentrations of modeled species or background constituents, changing demand, etc.



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