EPA Small Systems Workshop Training

AdDesignS™: Modeling Drinking Water Treatment with Granular Activated Carbon

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Progress for a Stronger Future

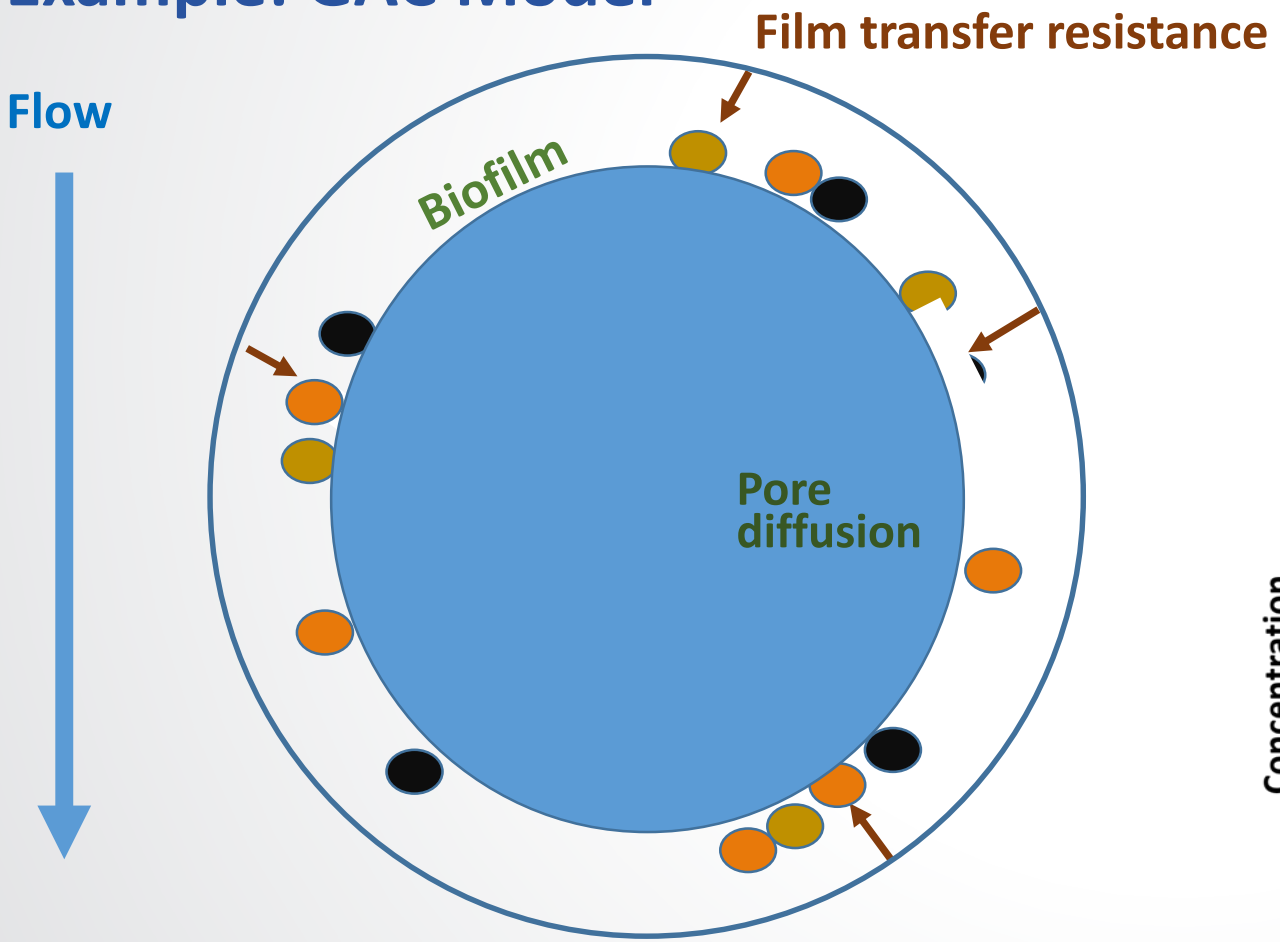
Overview

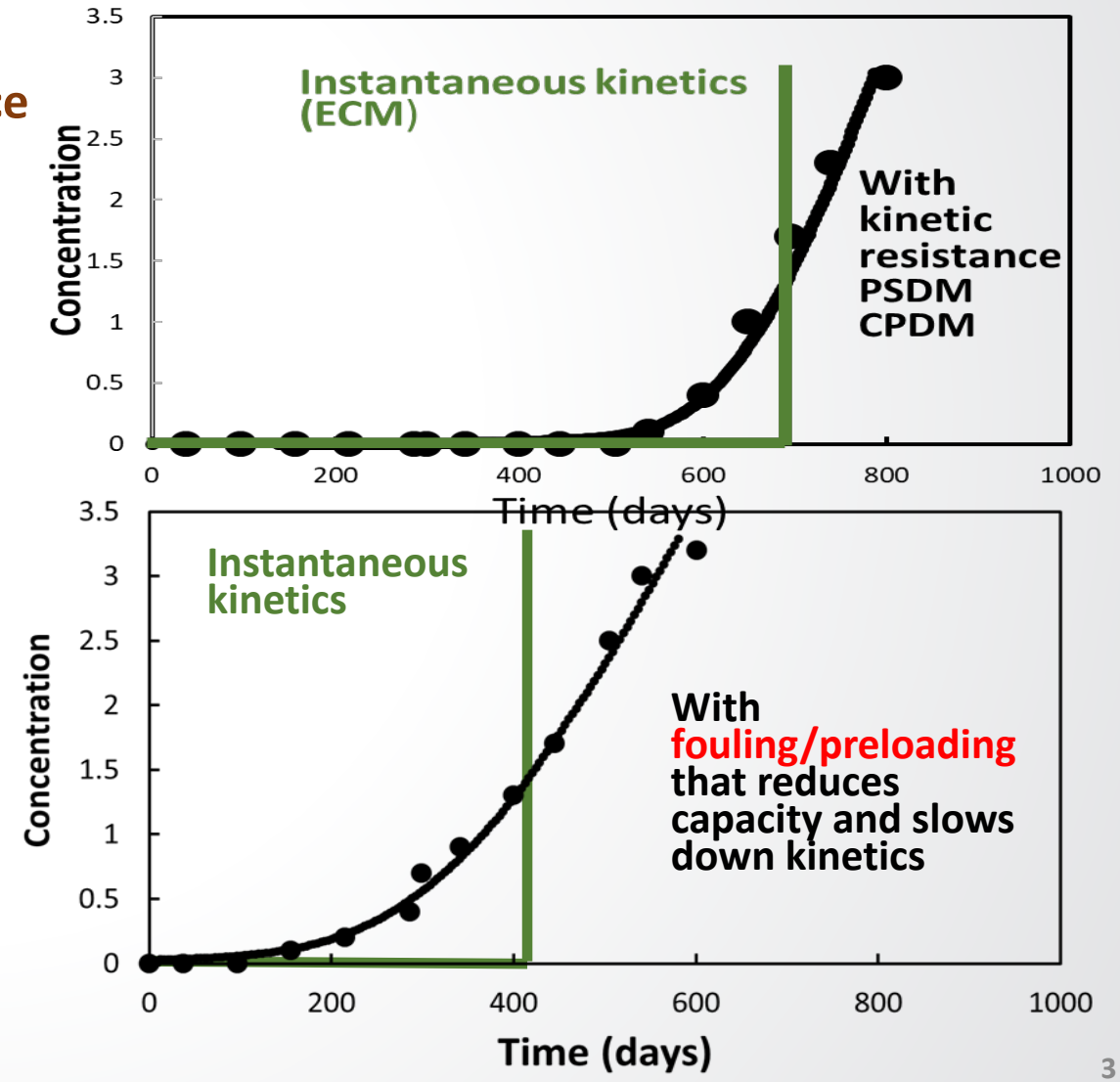
- Background
  - Overview of the models
  - Additional Resources
- Getting Started
  - Downloading Software

- AdDesignS™
  - Basics of the User Interface
  - Dynamic walk through of AdDesignS™ features (not in slides)
- Water Treatment Models
  - Brief introduction to additional tools

Overview of the Models

Example: GAC Model



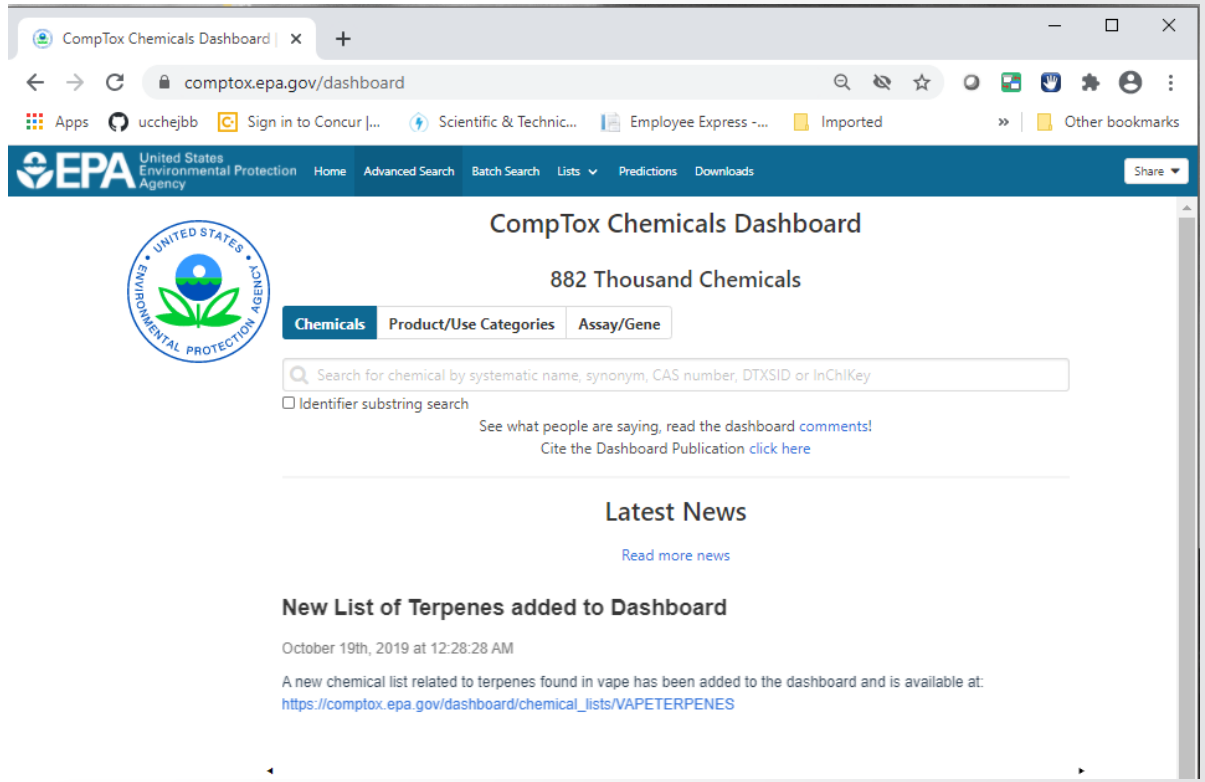


The models range from simple to complex

Additional Useful Resources

- 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

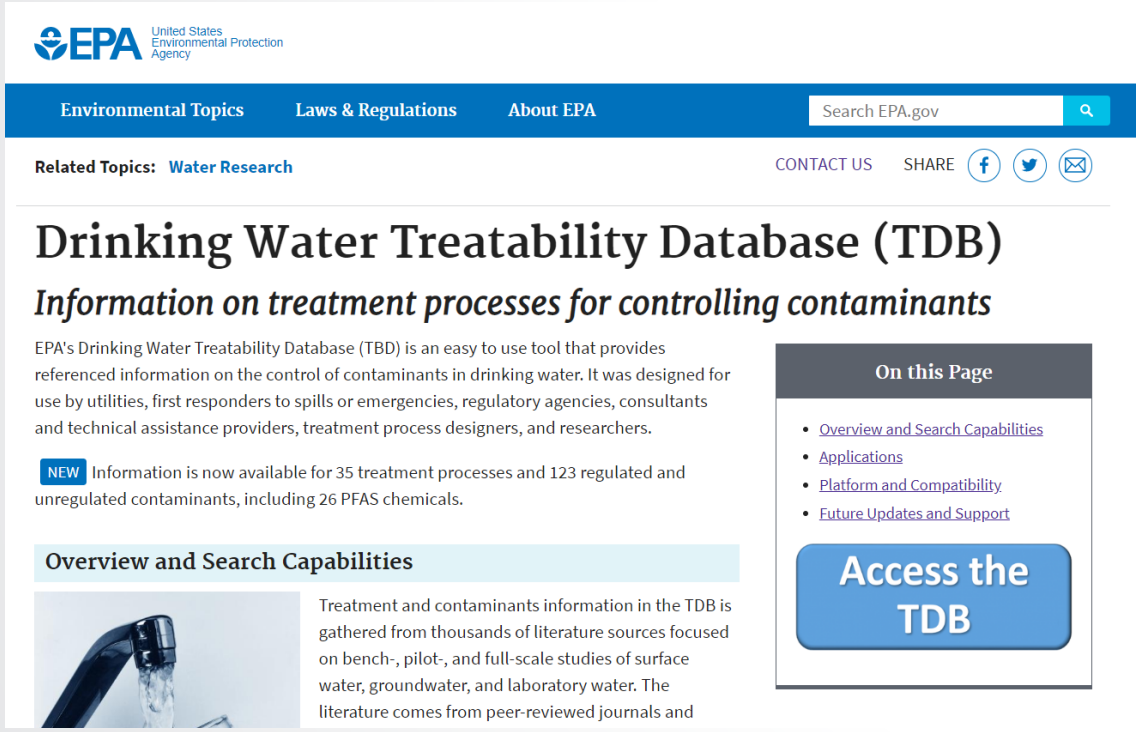


https://comptox.epa.gov/dashboard

Search: EPA COMPTOX

Additional Useful Resources

- Treatability Database



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

Search: EPA TDB

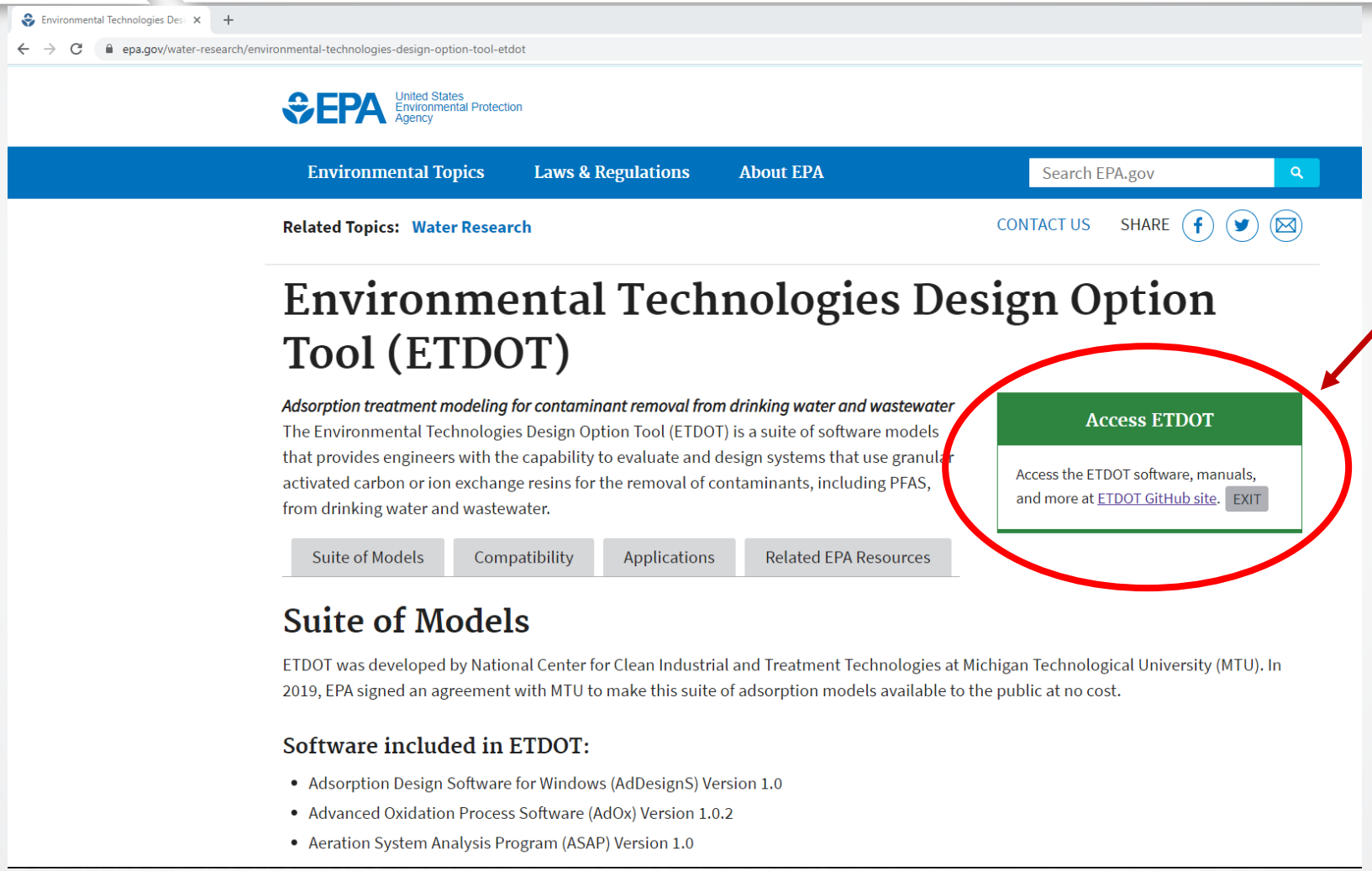
- Treatability Database
  - Has adsorption isotherm information
    - Freundlich Isotherm parameters (K & 1/n)
  - Links to papers where isotherm parameters were reported.

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

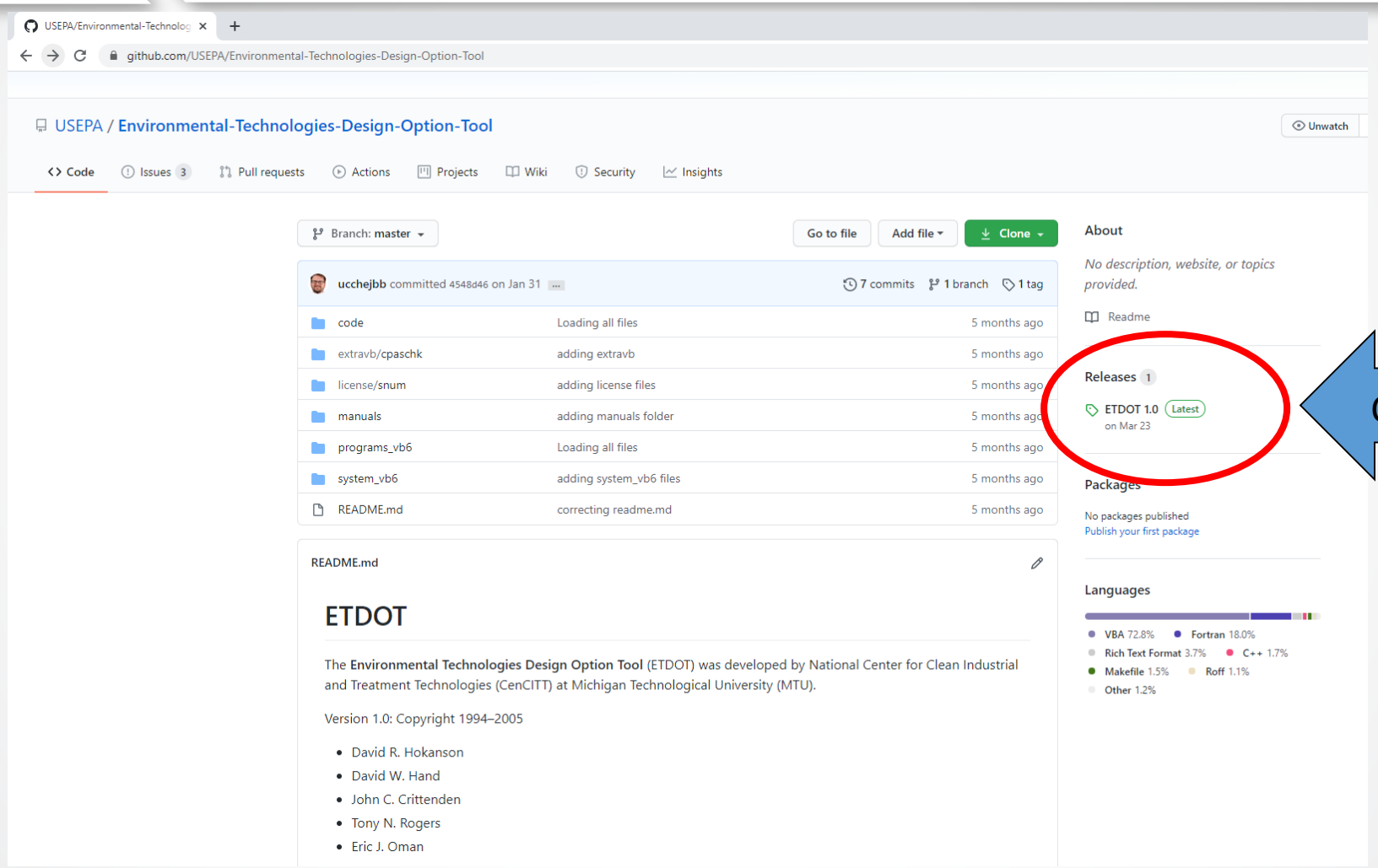


GitHub Site

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

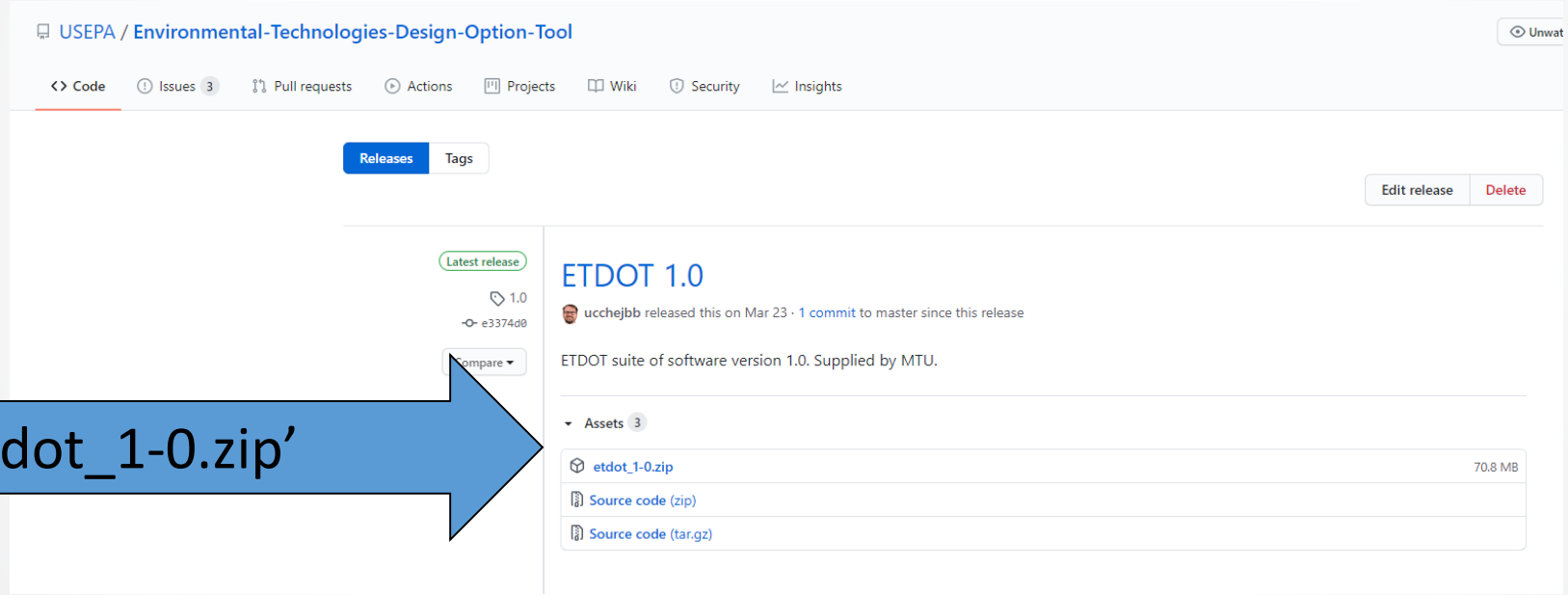
Search: EPA ETDOT

GitHub: ETDOT Software



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

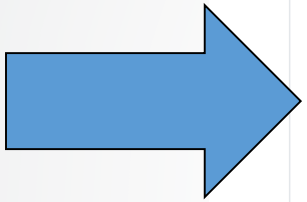
Releases on GitHub: ETDOT Software



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.

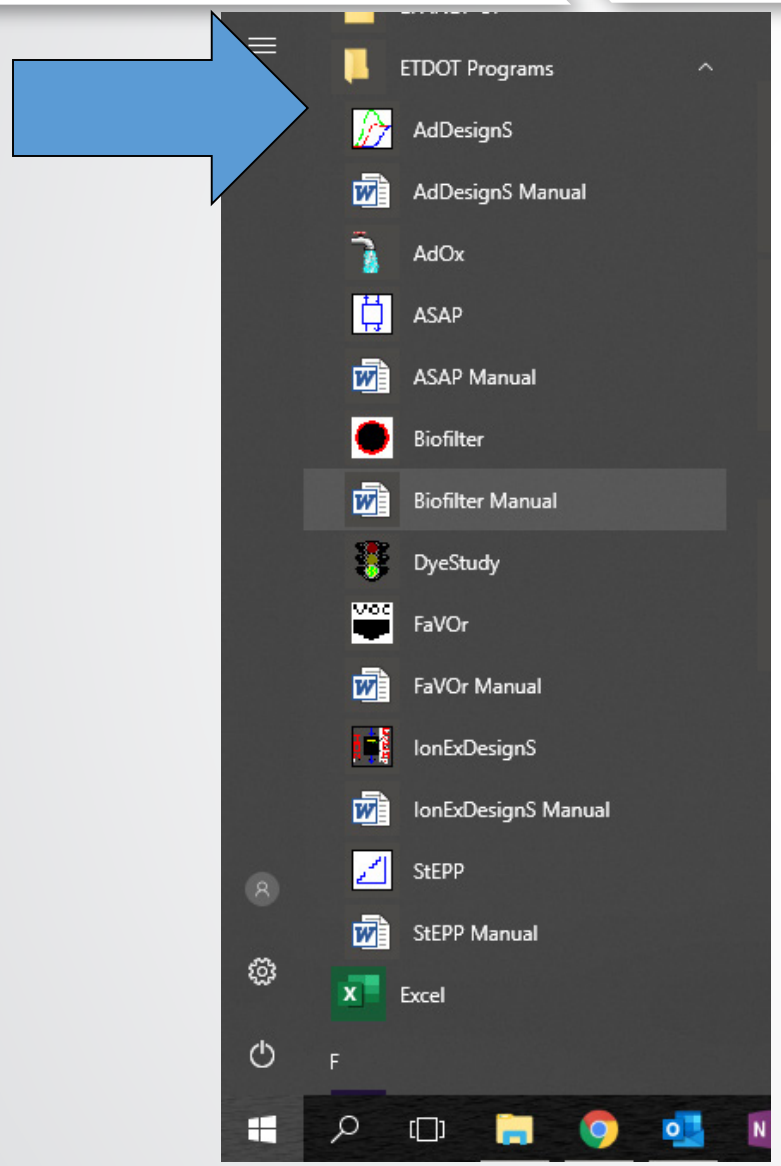
Available Users manuals will be located in the modules subfolder within the help folder.

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.

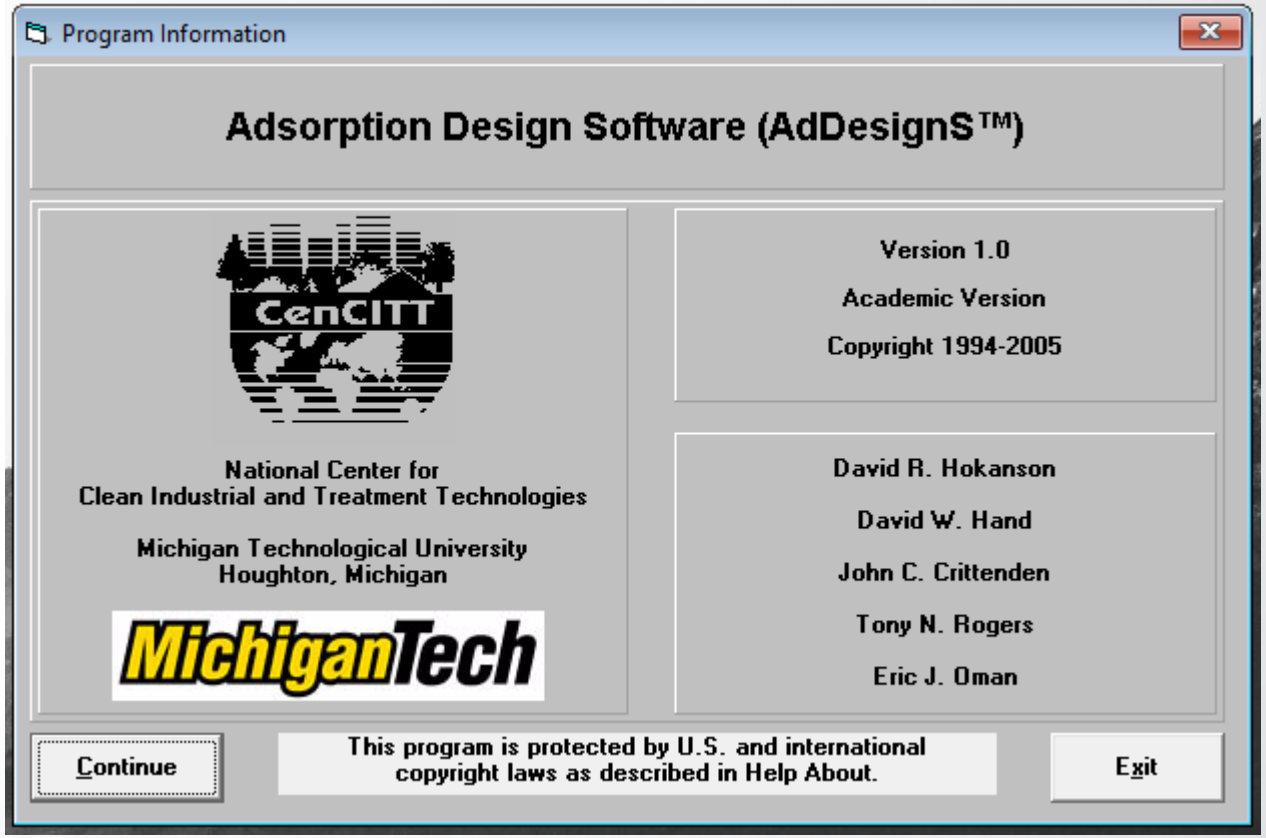
https://github.com/USEPA/Environmental-Technologies-Design-Option-Tool

Accessing ETDOT Software

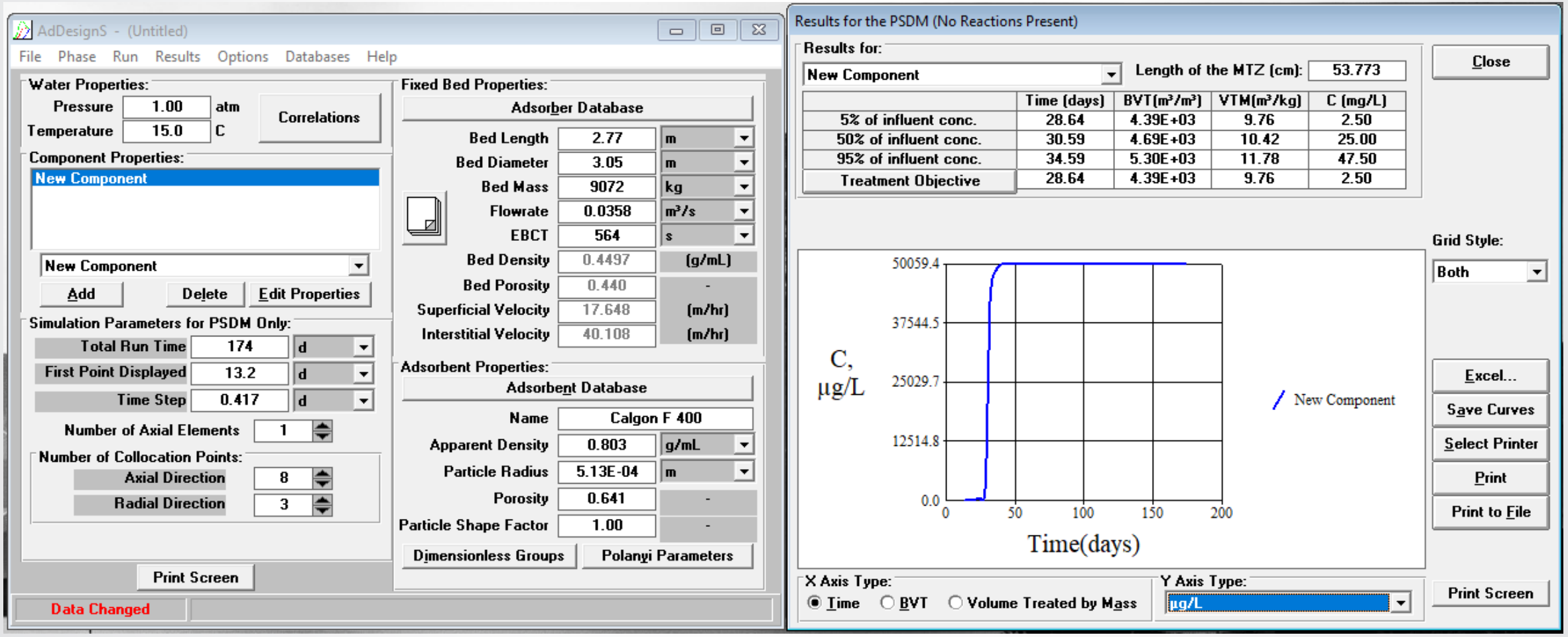


Start Menu:
'ETDOT Programs'

Software & Instruction Manuals are listed

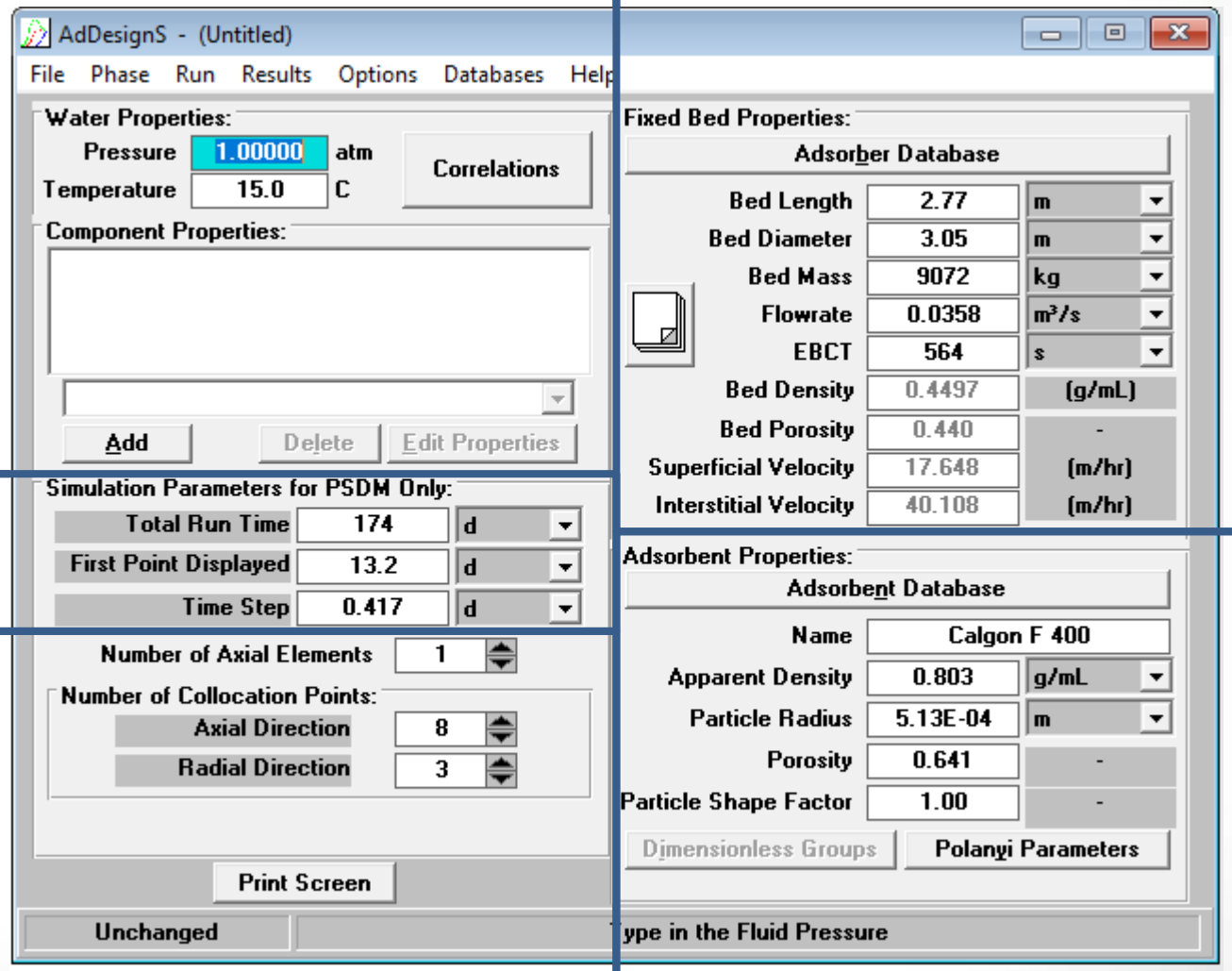


AdDesignS™ Software



Compound Information

Column Information



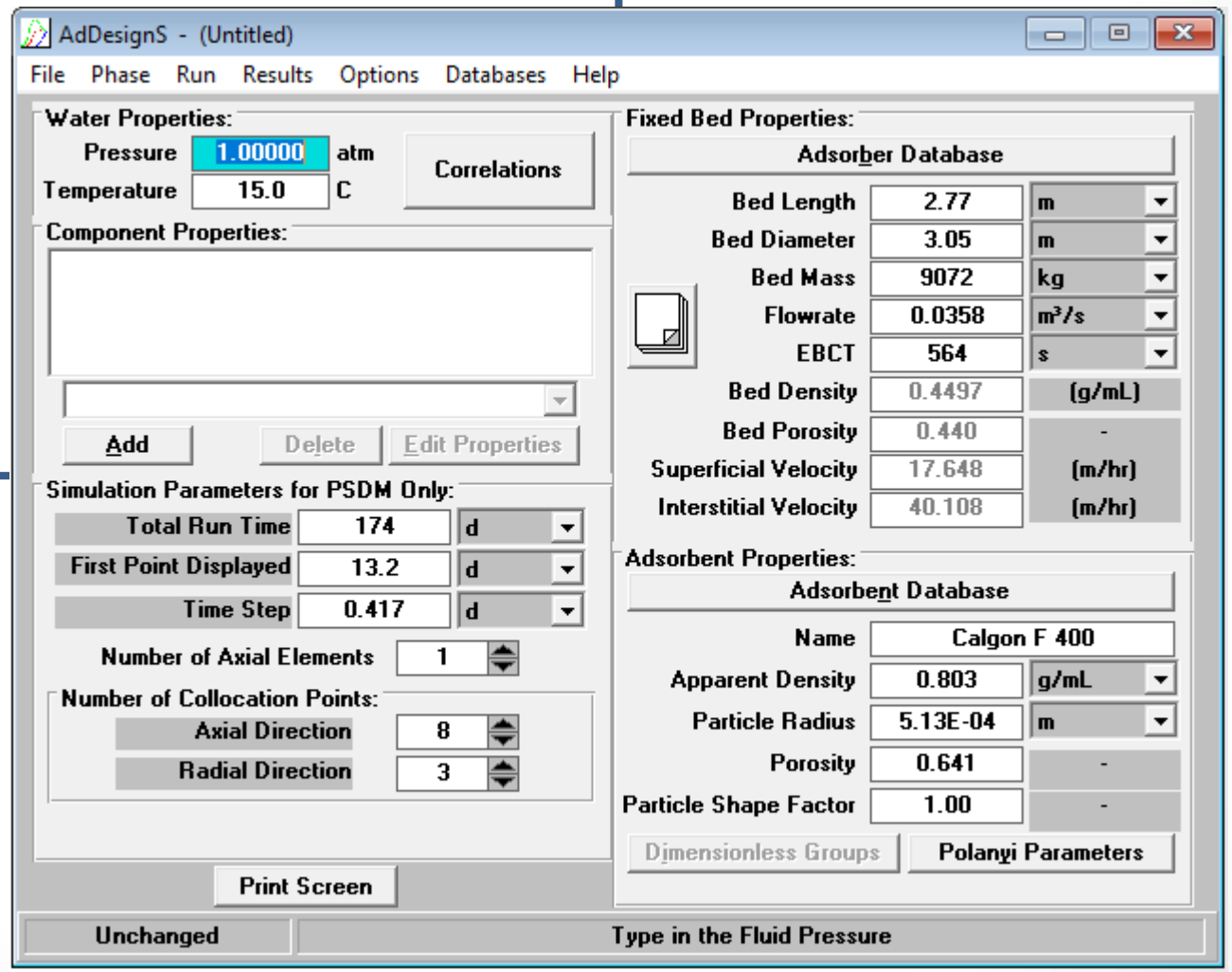
Duration

Collocation Point Selection

Adsorbent Information

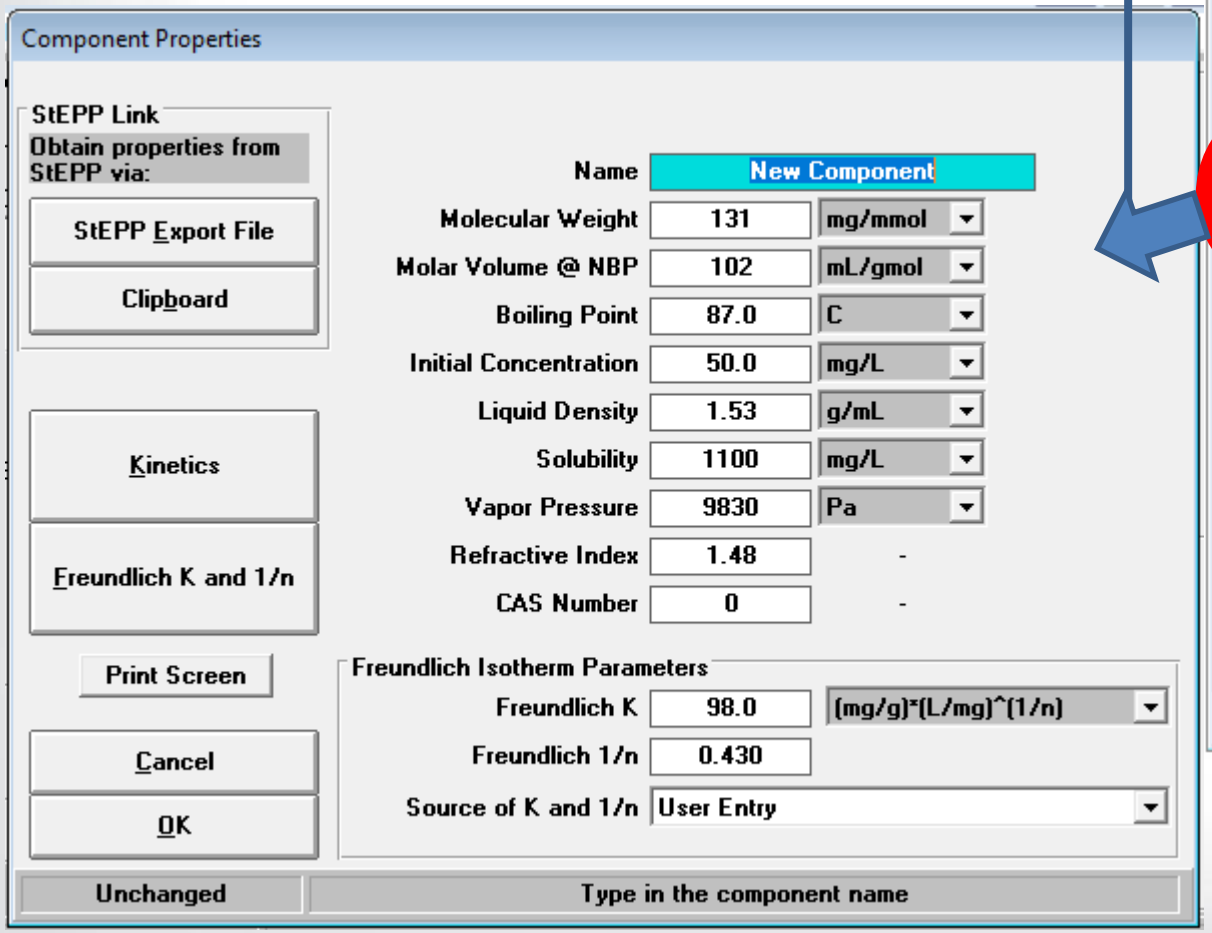
- Compound Information
  - Add/Edit Compounds to be modeled

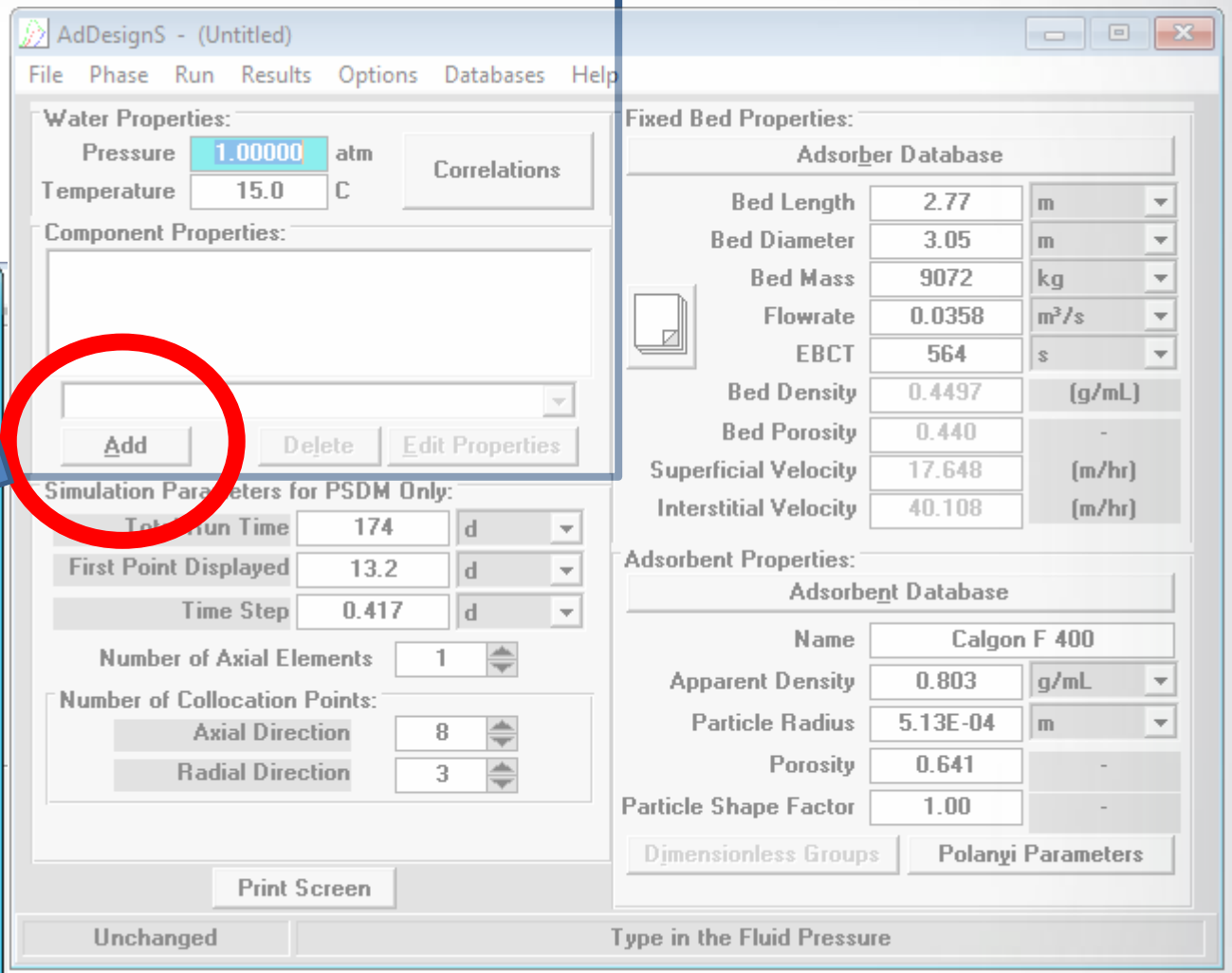
Compound Information



Compound Information

- Compound Information
  - Add/Edit Compounds to be modeled





Compound Information

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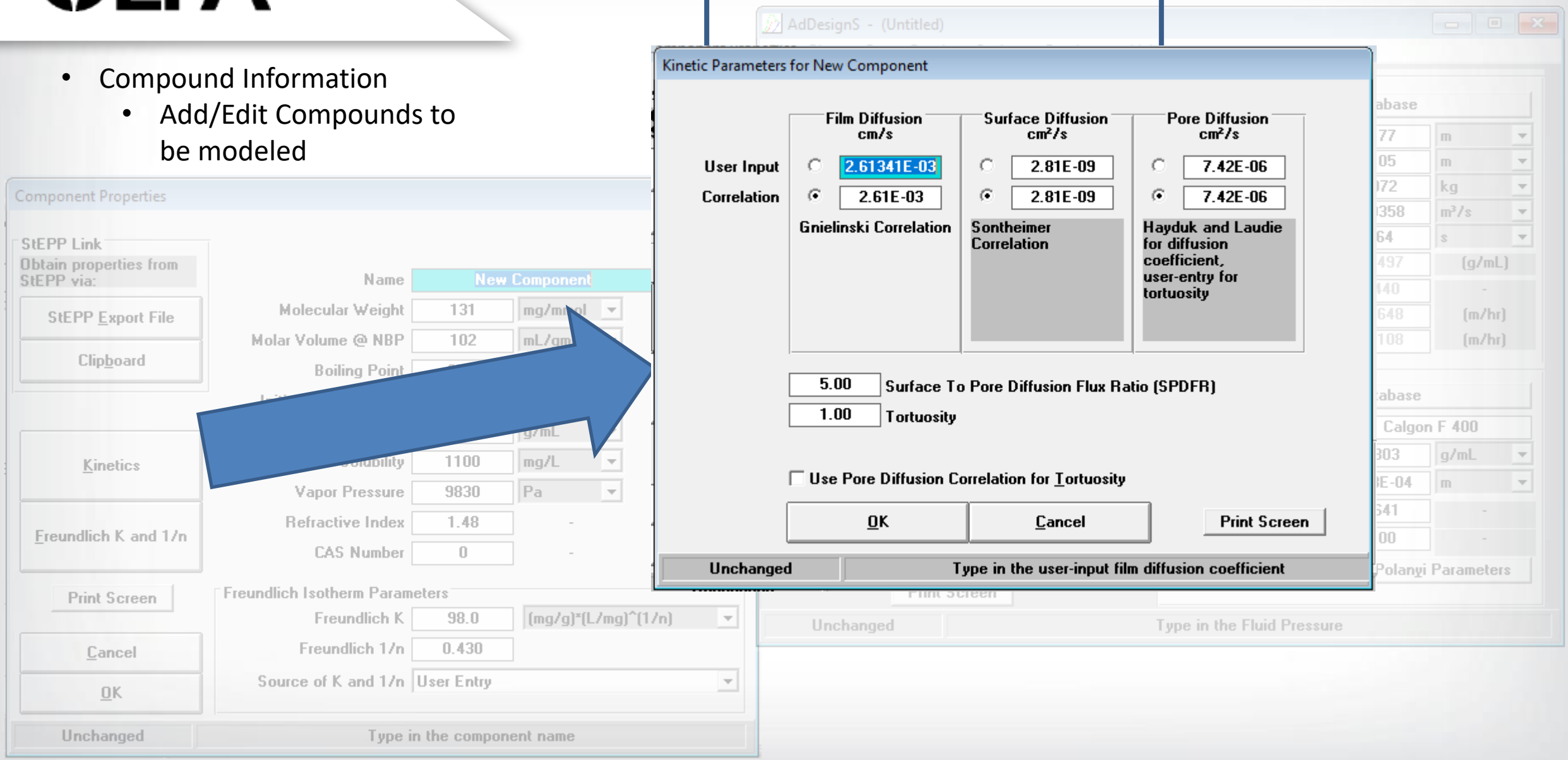
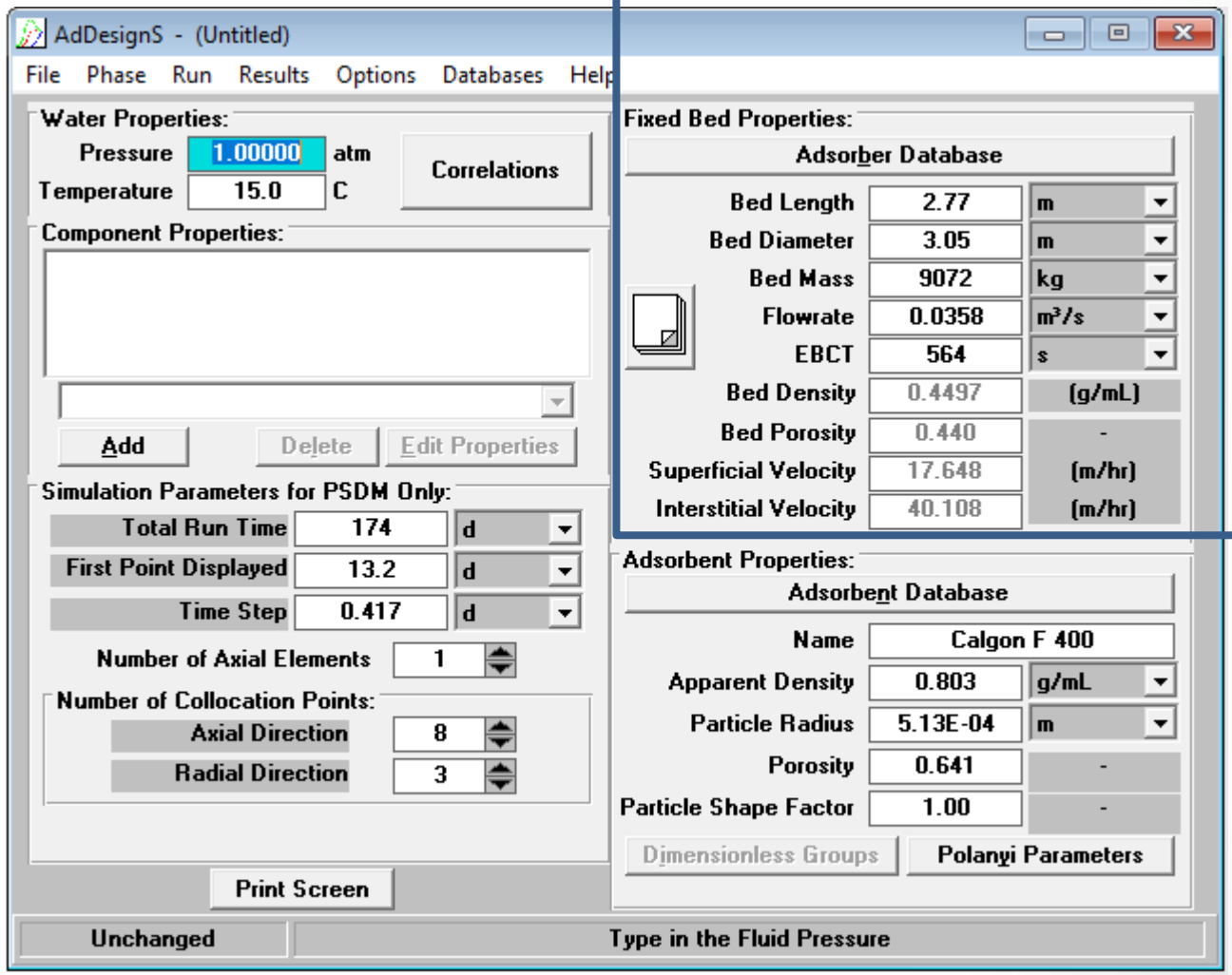
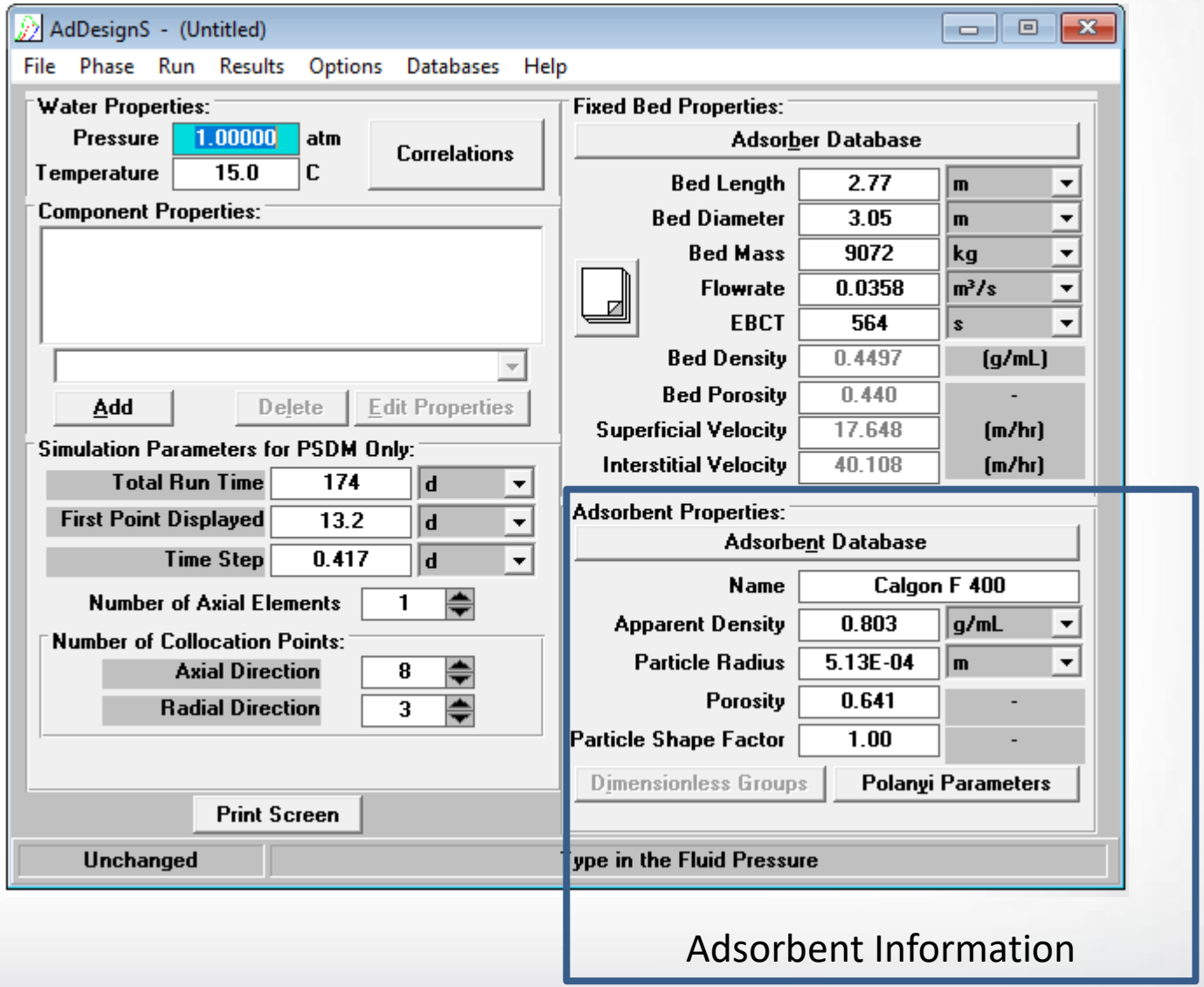
  - Add/Edit Compounds to be modeled



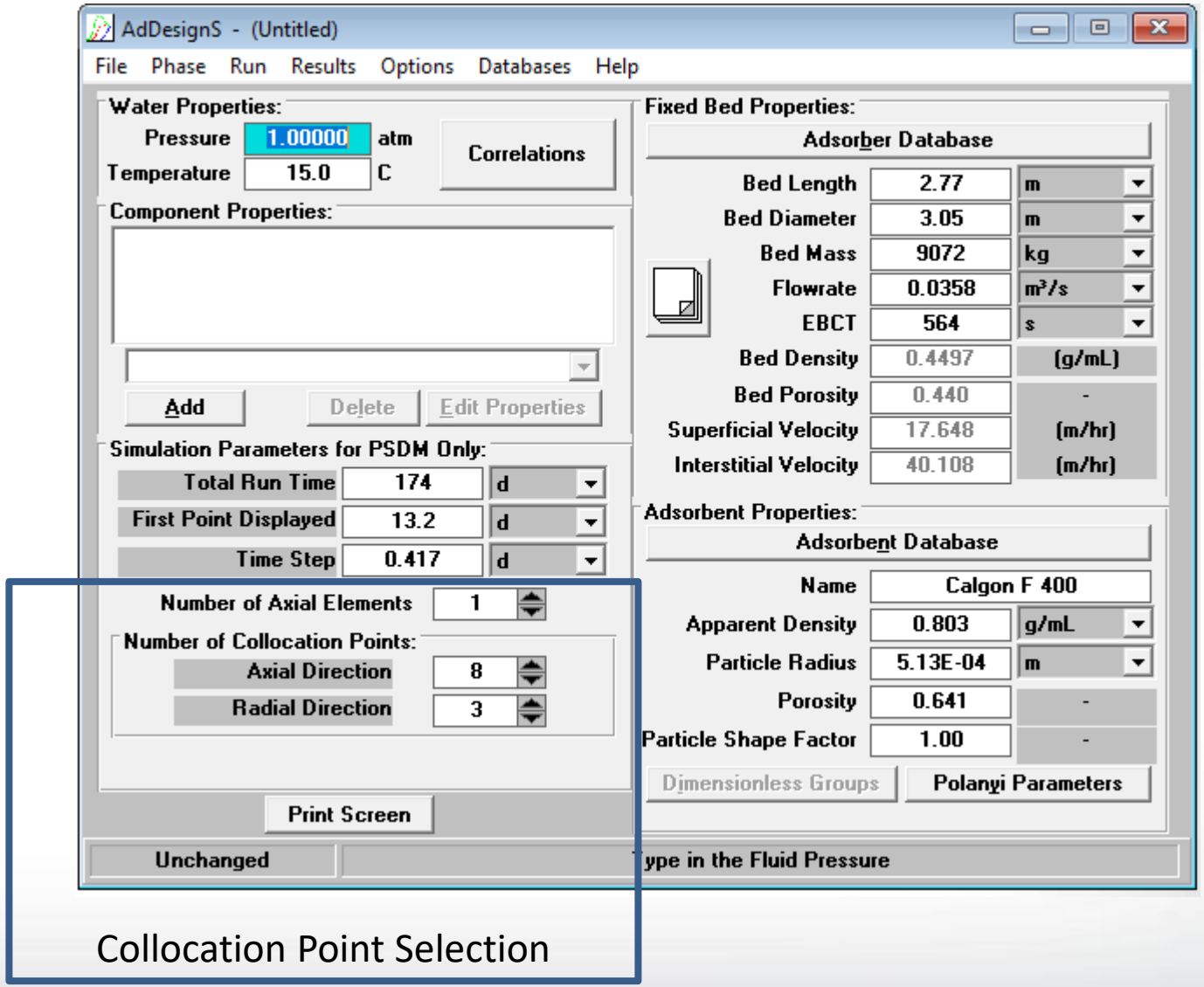
- **Column Information**
  - Supply the physical characteristics of the bed
  - Supply the flowrate to the system (will recalculate EBCT)
    - Can verify EBCT seems correct
    - Alternatively: adjust EBCT and flowrate will be recalculated (can use for specific throughput analysis)
  - Dropdown menus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



- 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/~0.685



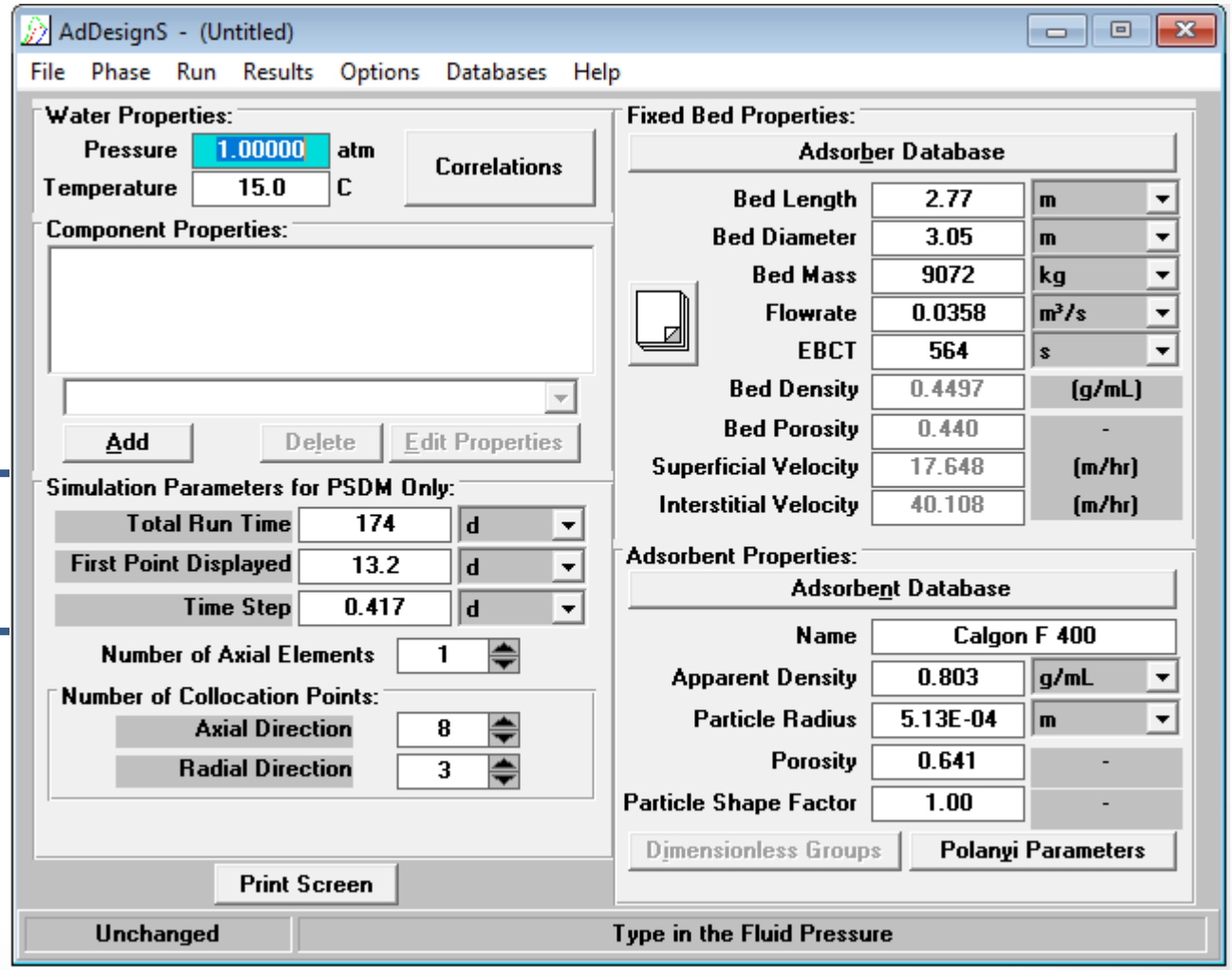
- **Collocation Points**
  - Defines how many elements are used in the numerical solution
  - Increasing these can help smooth PSDM solutions
  - Axial Direction ≤ 18
    - If the problem requires more than 18, increase "Number of Axial Elements"
  - Radial Direction ≤ 18
    - Typically this value will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



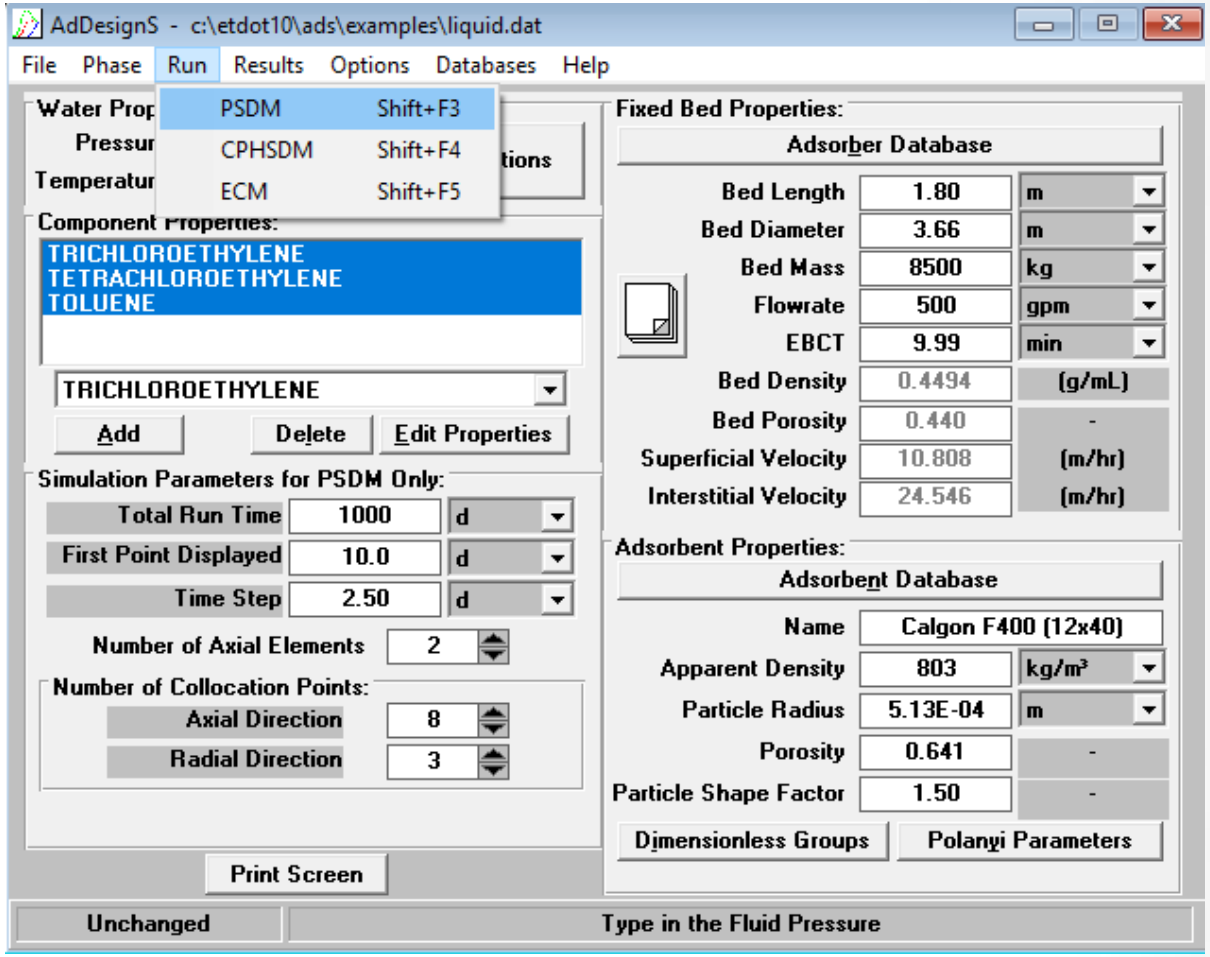
Collocation Point Selection

- **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”

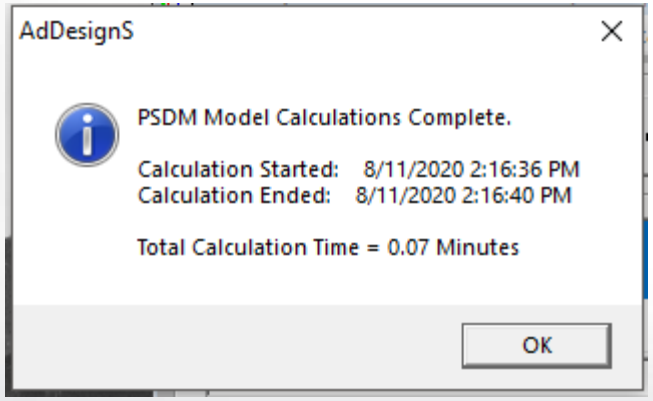
Duration



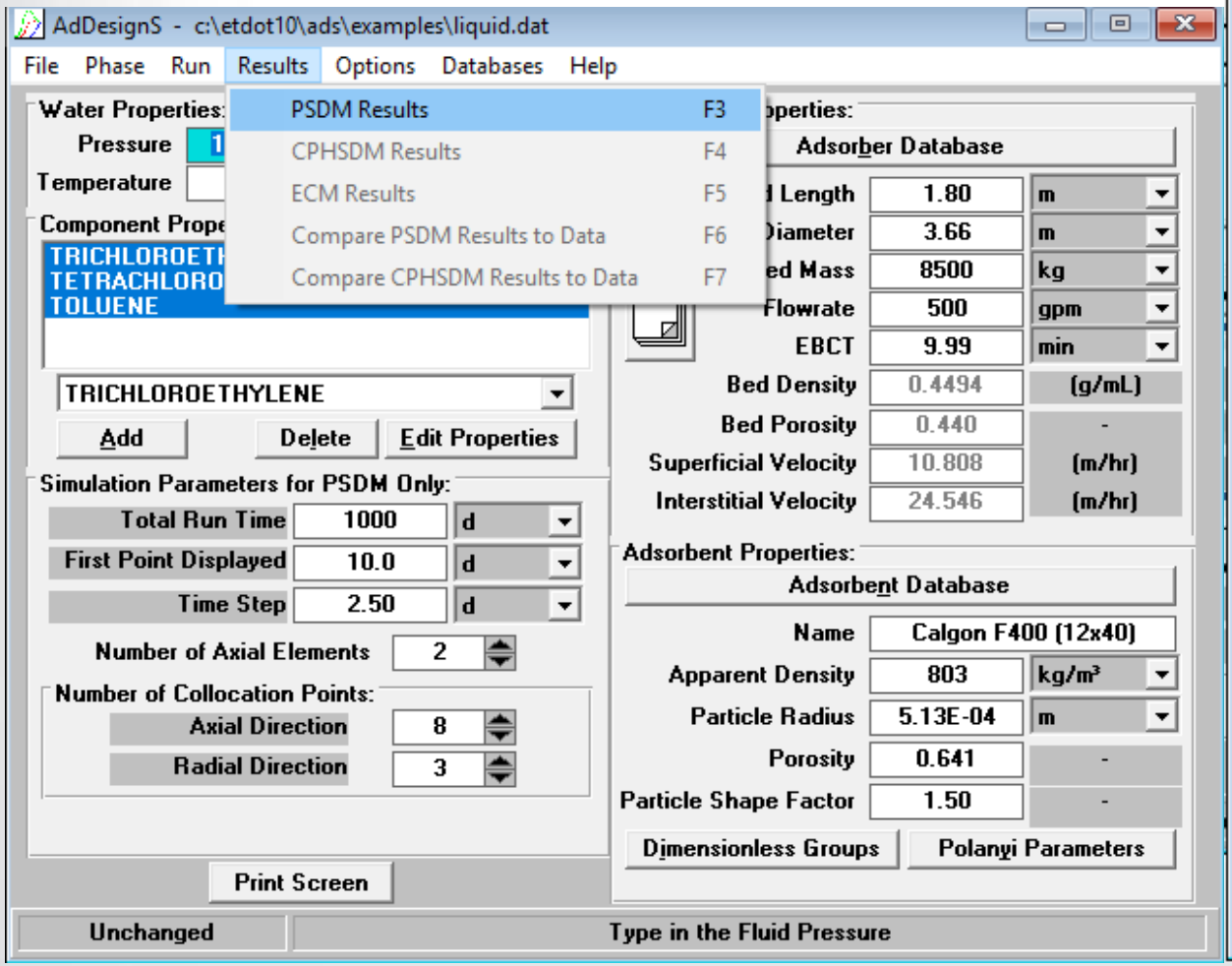
- **Running a Simulation**
  - Liquid.dat, provided with ETDOT installation
  - Select individual compounds to consider in the model

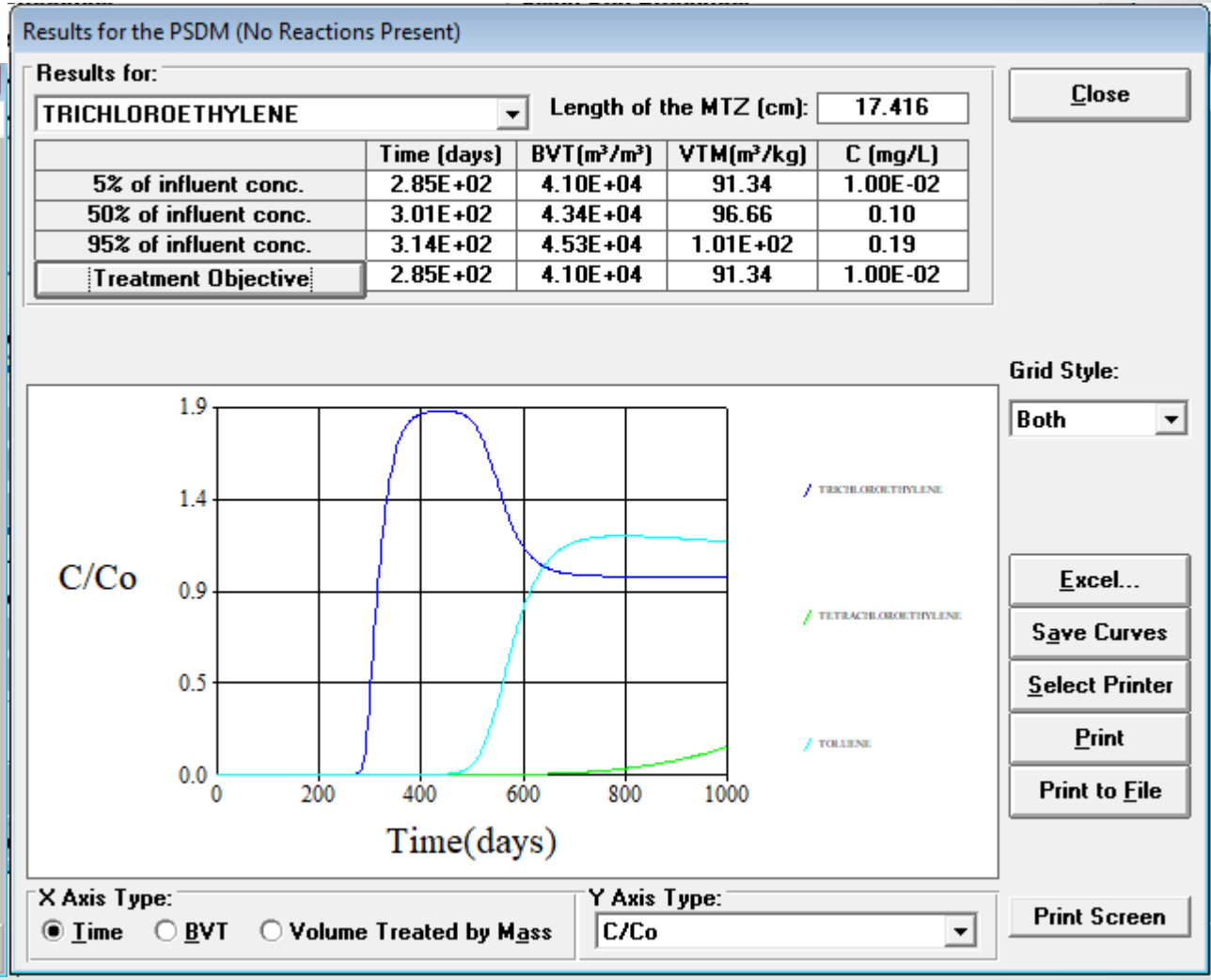


- Will get a completion dialog box

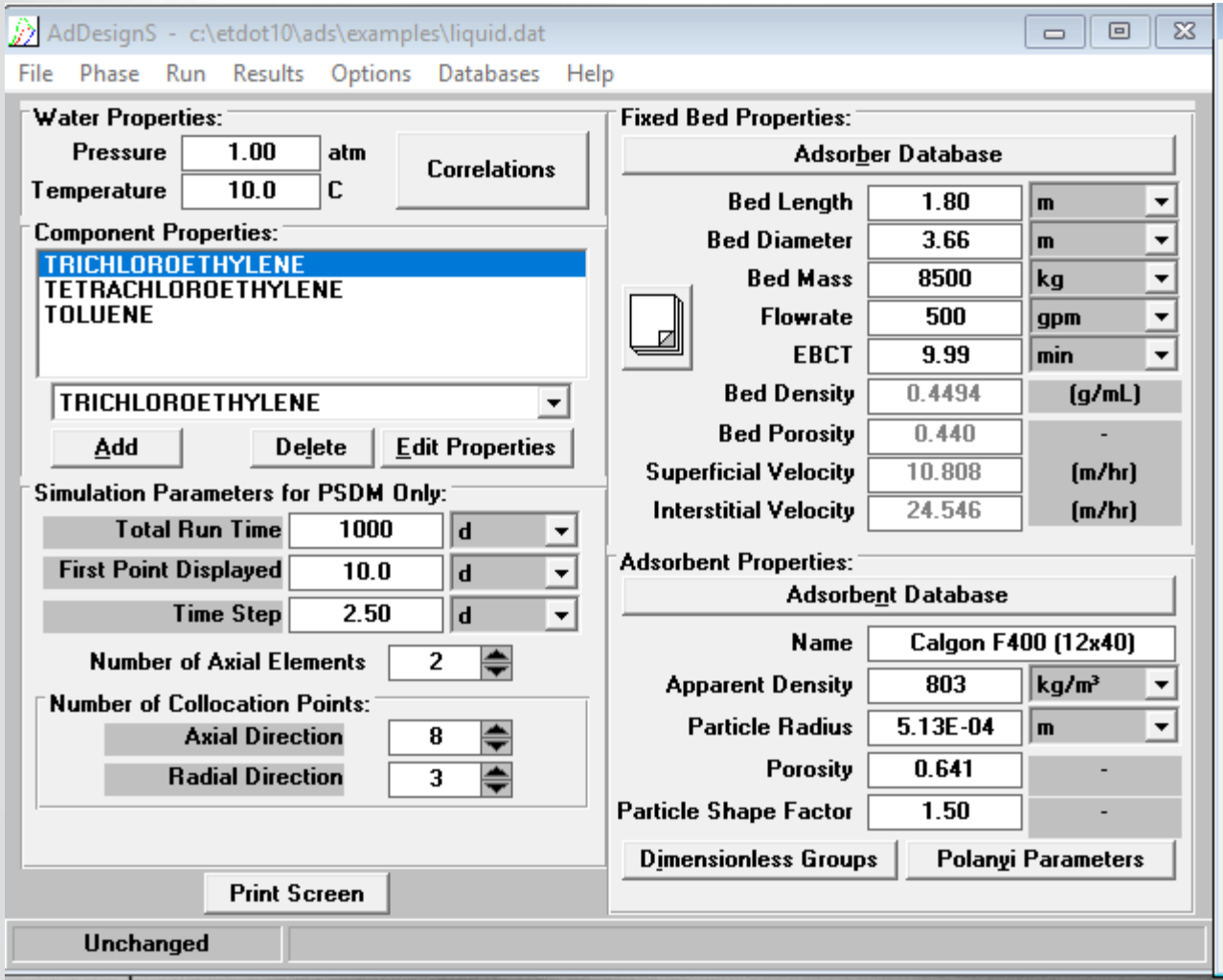


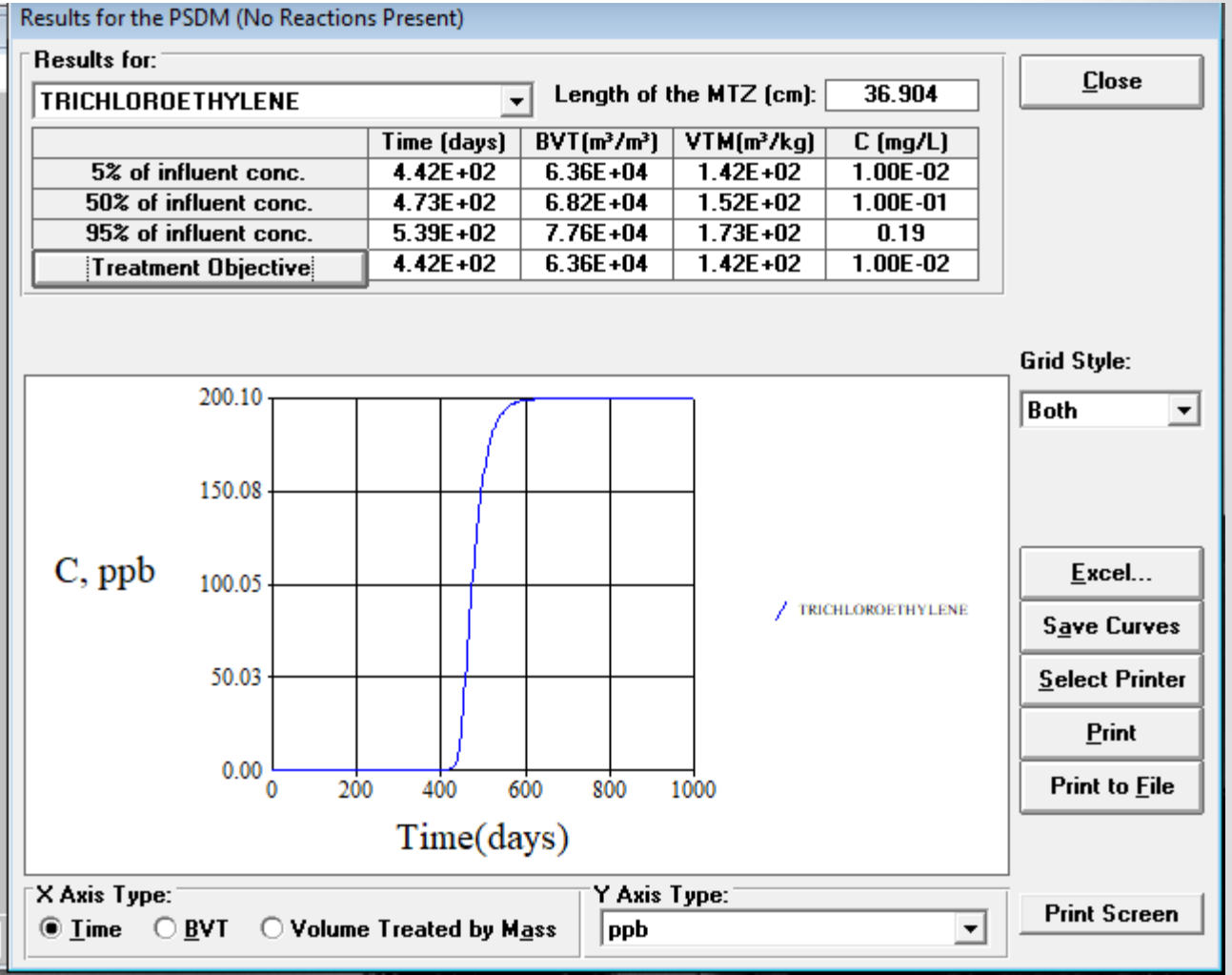
- **Viewing Results from a Simulation**
  - Results -> PSDM



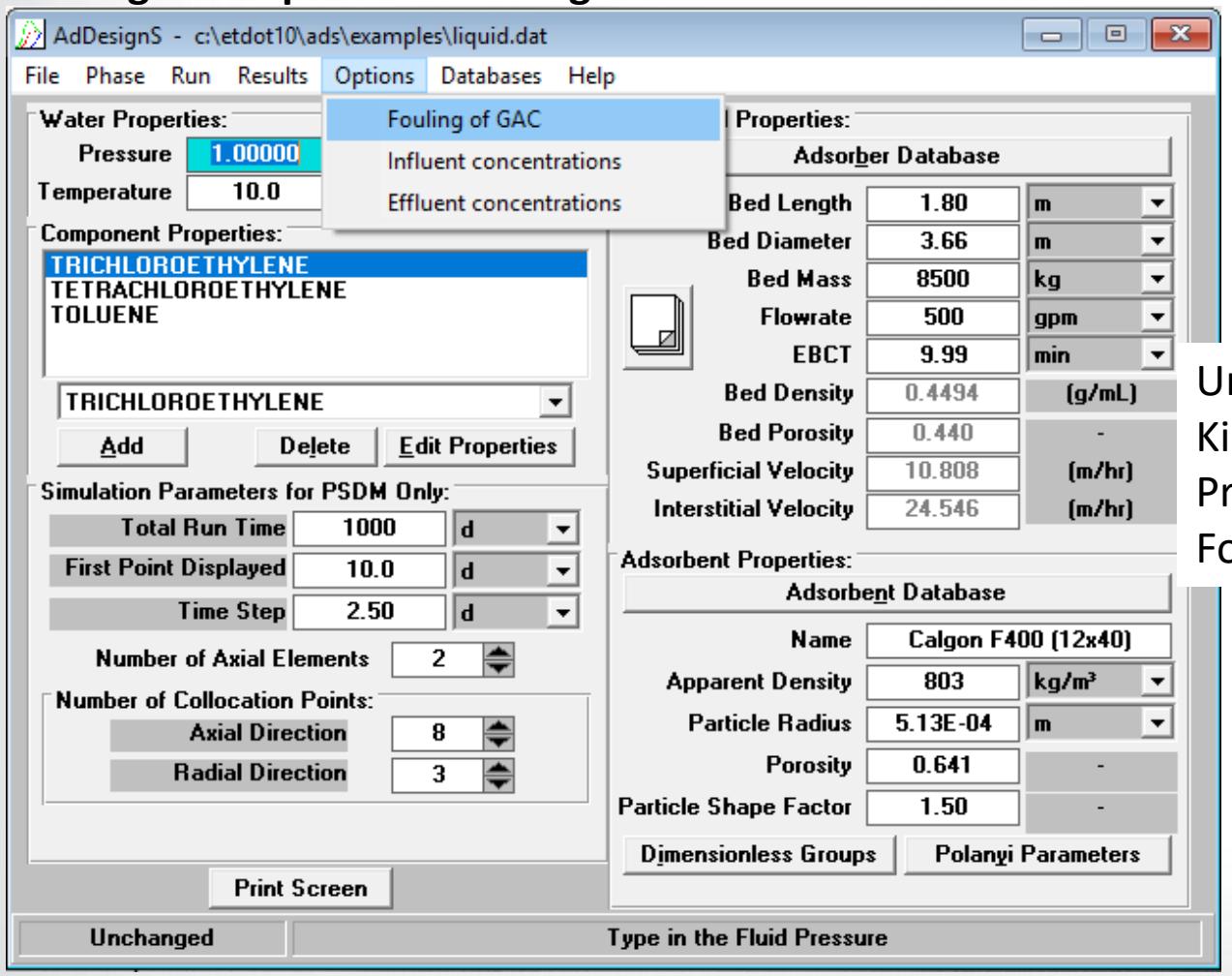


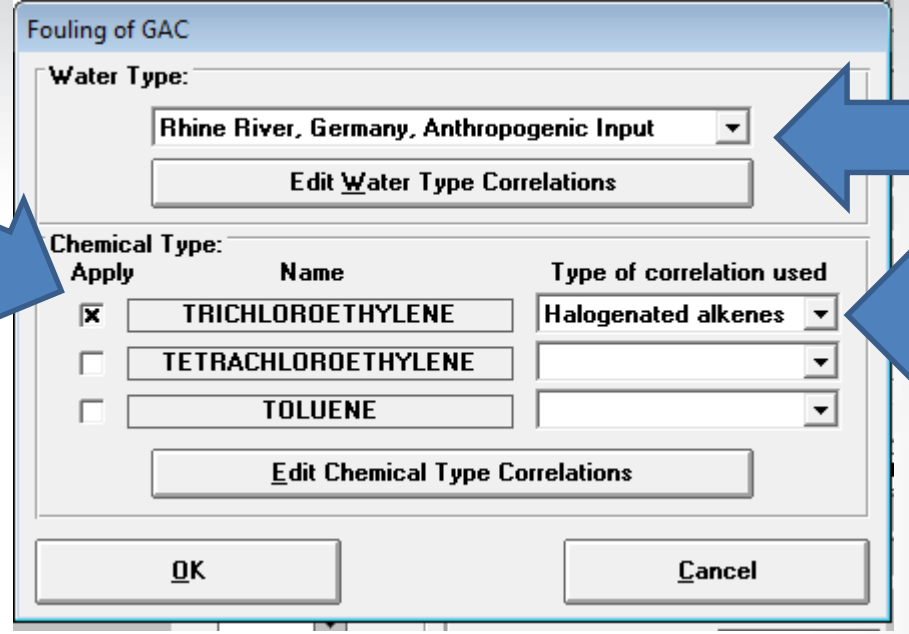
- **Single Compound – No Fouling**



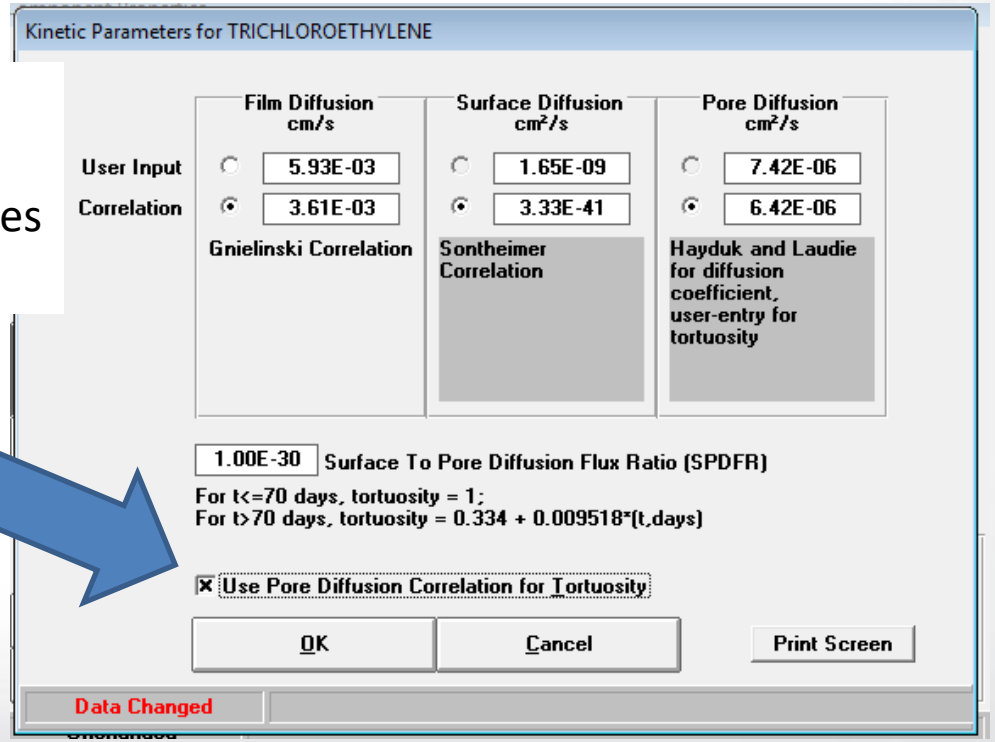


- **Single Compound – Fouling**



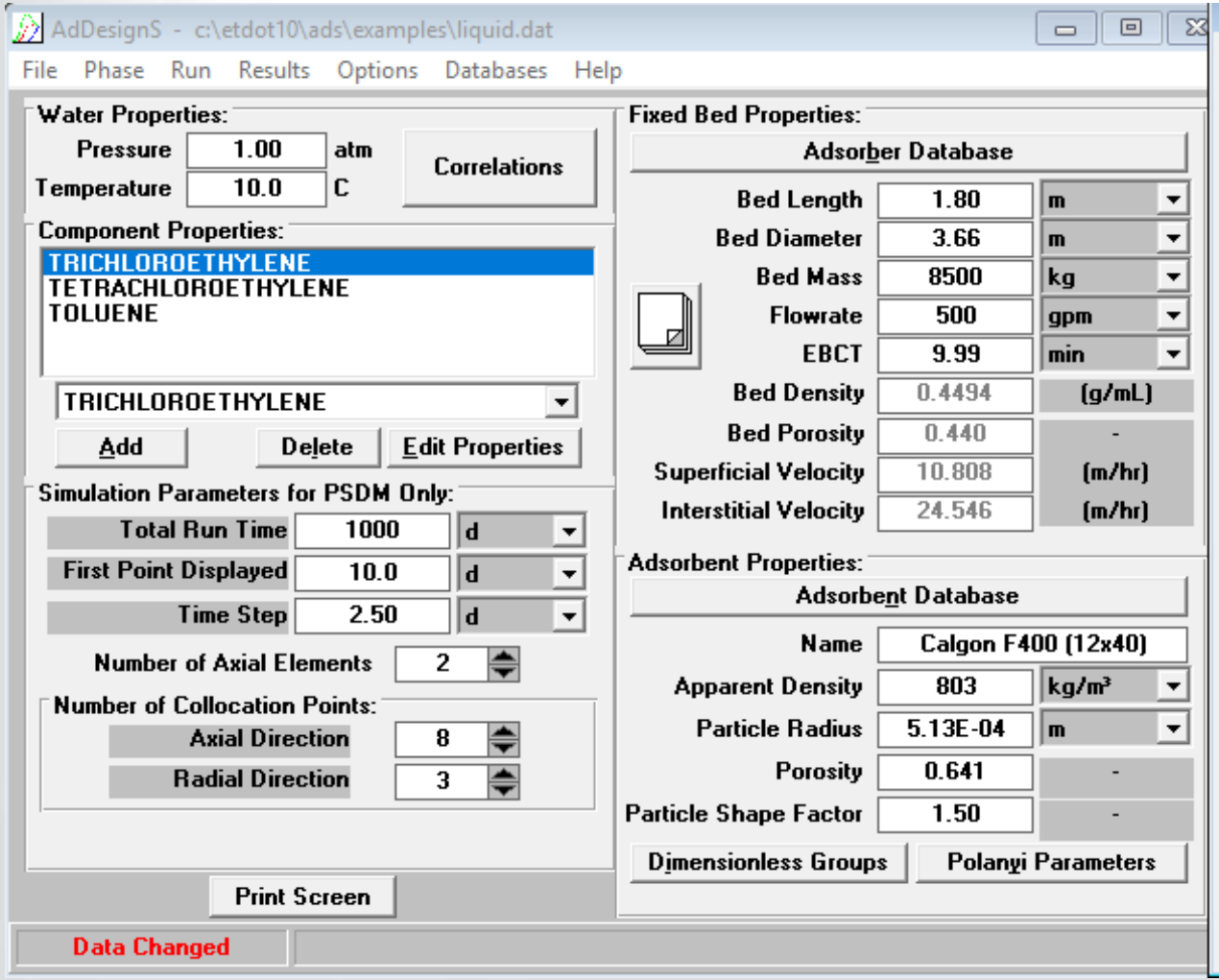


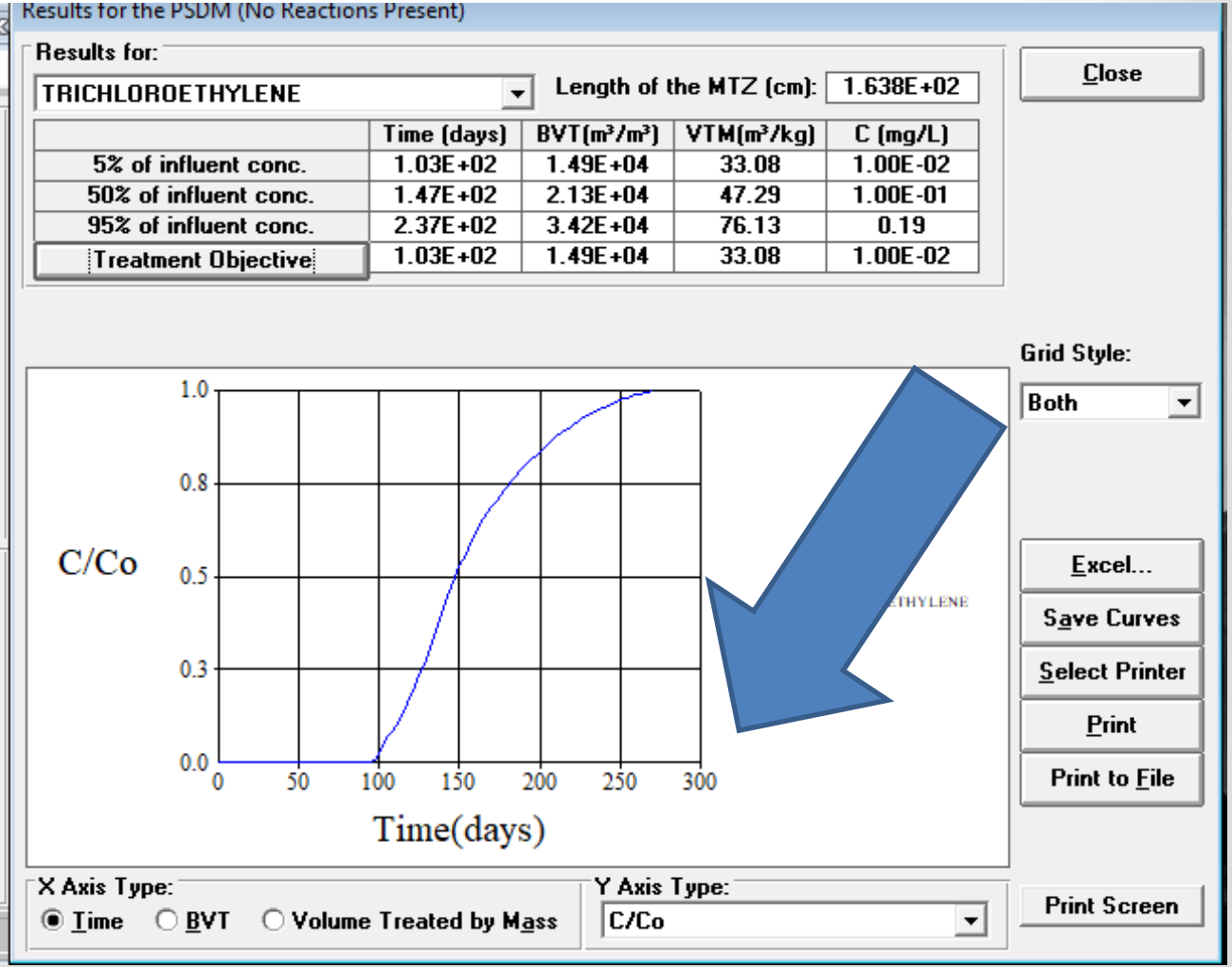
Under Kinetic Properties For TCE



- **Single Compound – Rhine River Fouling, halogenated alkene**

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





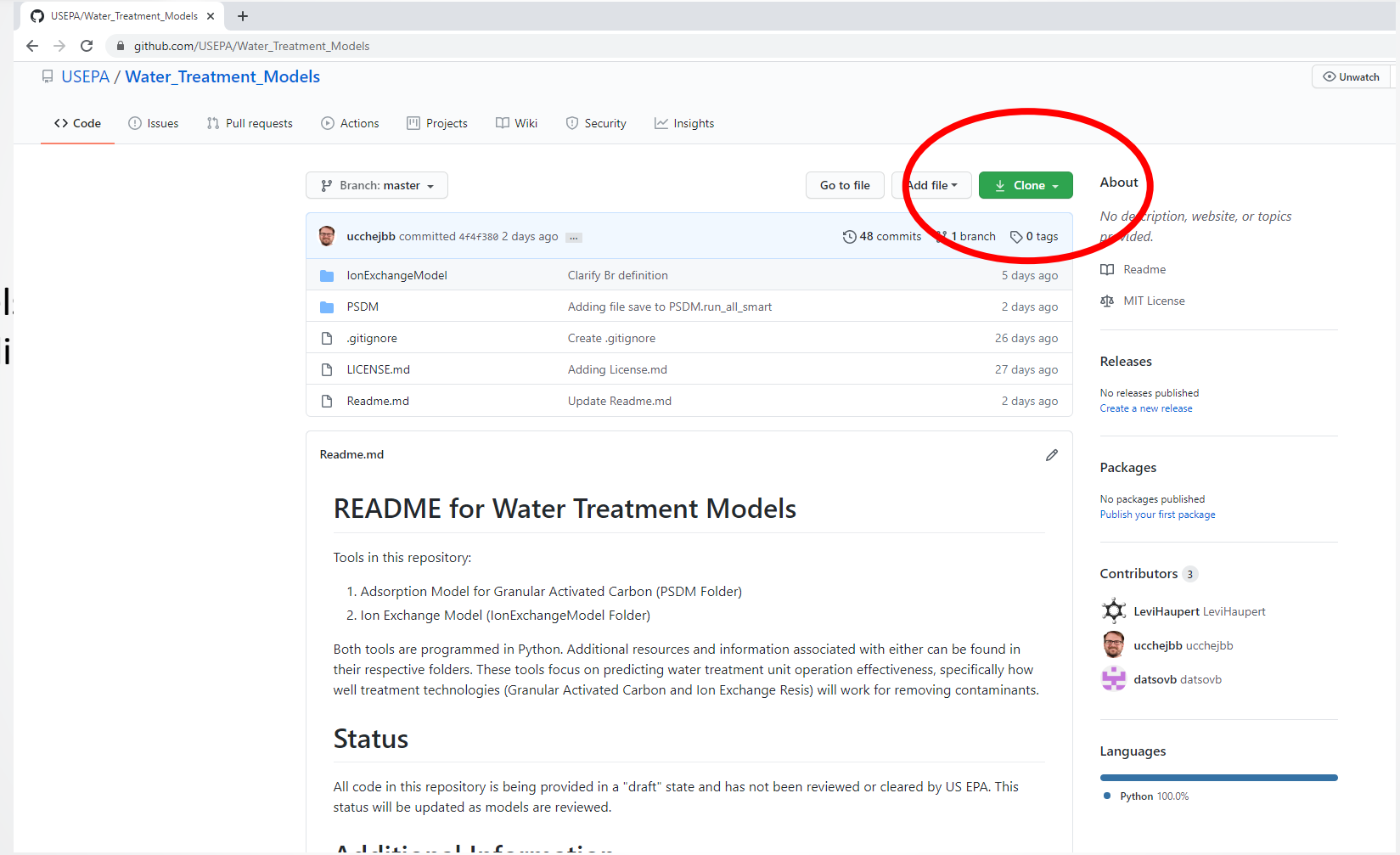
Water Treatment Models

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

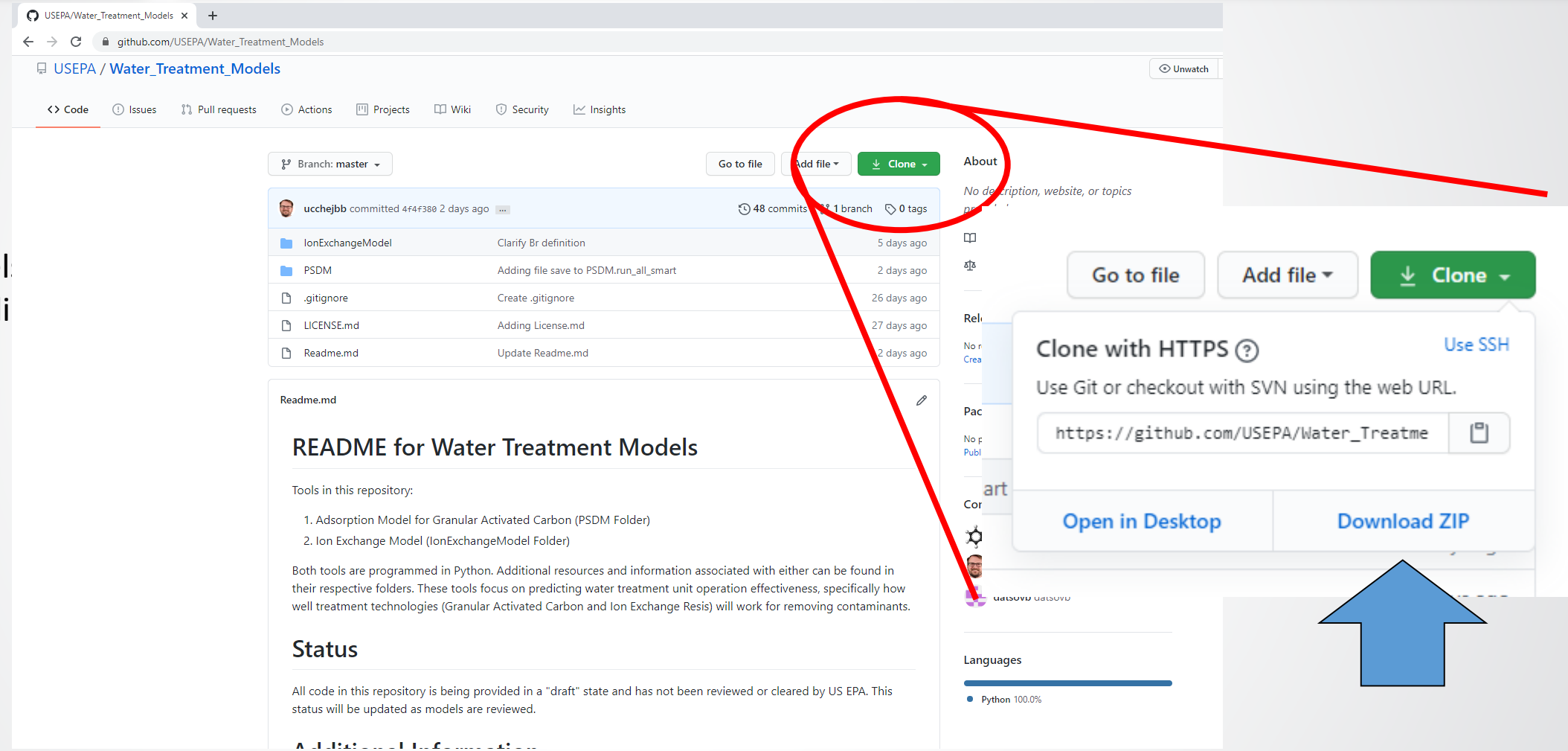
Python Tools:
Ion Exchange Model
PSDM – GAC Modeli



https://github.com/USEPA/Water_Treatment_Models

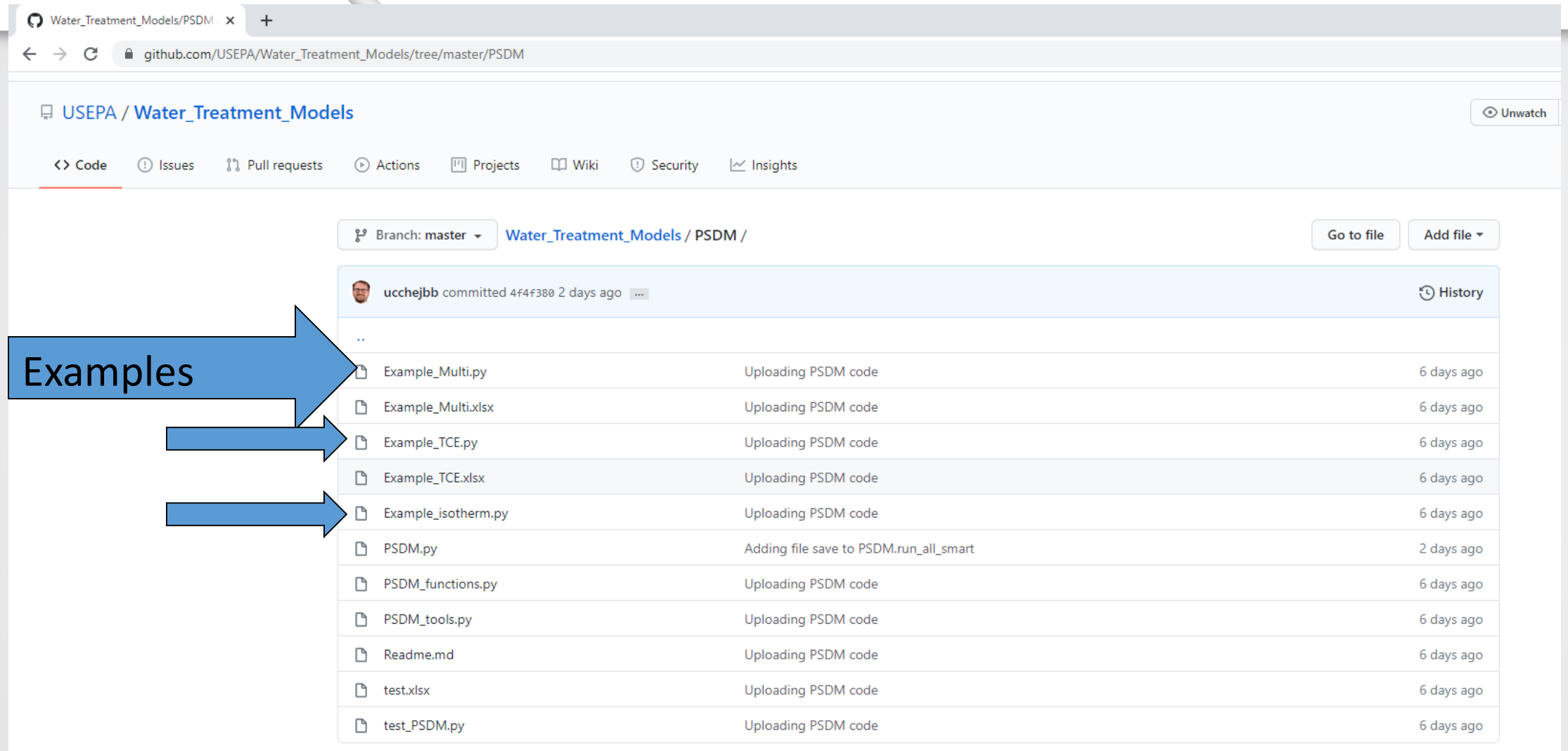
Water Treatment Models

Python Tools:
Ion Exchange Model
PSDM – GAC Modeli



https://github.com/USEPA/Water_Treatment_Models

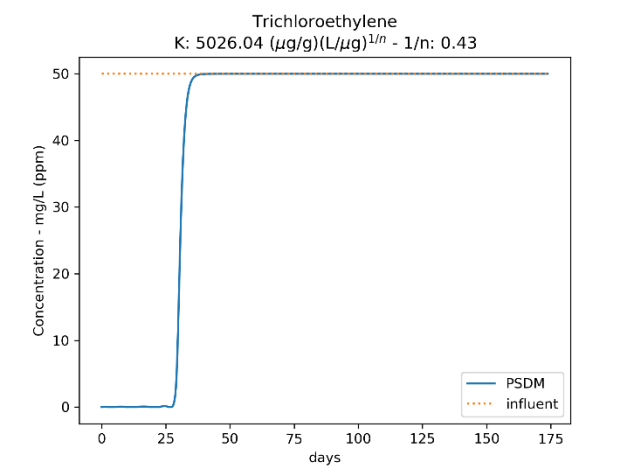
Pore and Surface Diffusion Model (PSDM)



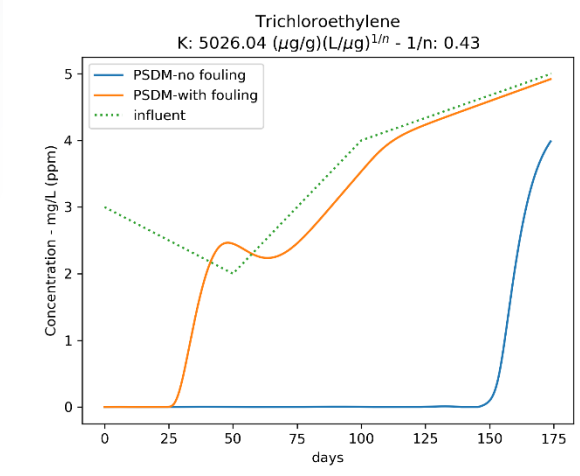
Examples

https://github.com/USEPA/Water_Treatment_Models

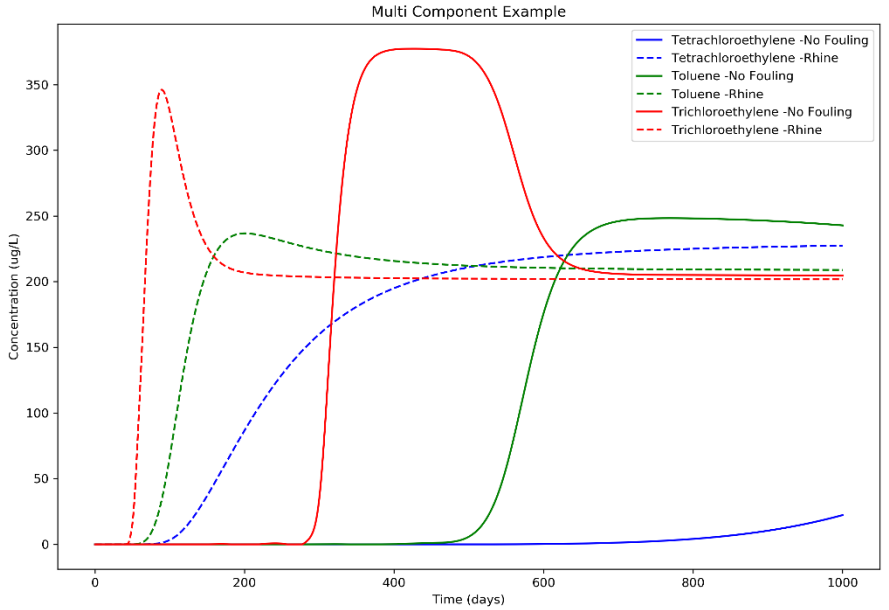
PSDM Model Examples



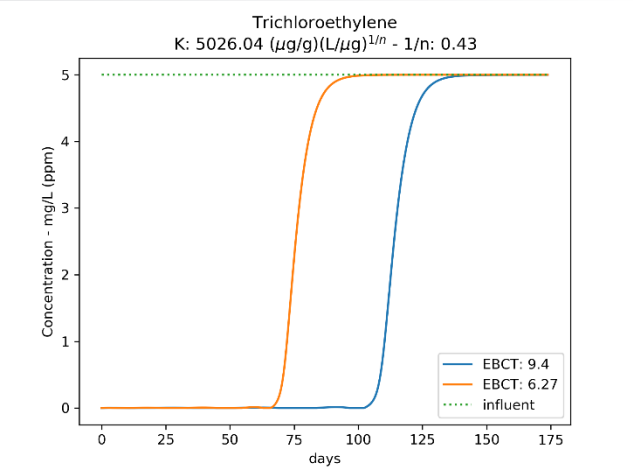
Single Compound



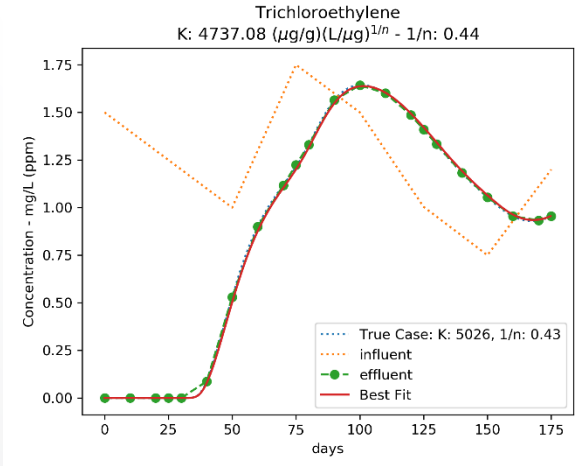
Modeling Fouling



Multicomponent competitive modeling



Comparing EBCT

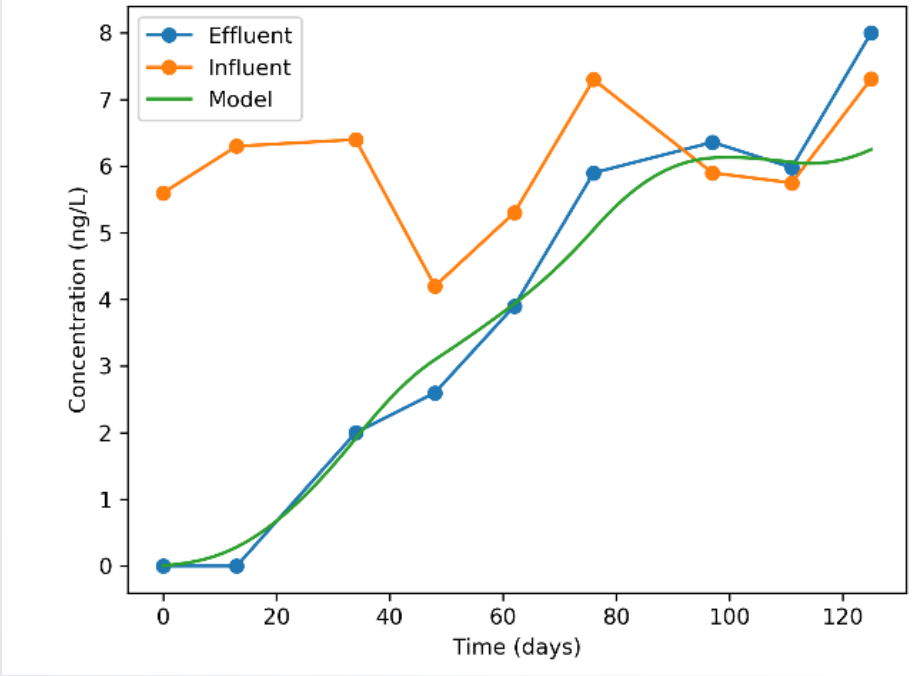


Fitting Pilot Data

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

Applying the PSDM Mode

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.

Contacts

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