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Executive Summary

A planning and design tool for the removal of per- and polyfluoroalkyl substances (PFAS) and other industrial persistent, mobile and potentially toxic (iPMT) substances for drinking water treatment plants with source water with high dissolved organic matter (DOM) was developed.

Within PROMISCES, technologies to remediate PFAS and iPMT(s) in several environmental media have been studied. This deliverable reports on a tool developed to improve planning and design of drinking water treatment trains for PFAS and iPMT, especially focusing on the adsorption onto granular activated carbon (GAC), alternative adsorbents and removal using ion exchange (IX) resins. Despite several previous studies on PFAS and iPMT removal during drinking water treatment, informational gaps on how to best implement suitable treatment trains in practice remain. The design of a suitable treatment train will depend on the effectiveness of the adsorbent for the removal of various mixtures of chemicals, different background water qualities, and treatment goals. Modelling tools can be used to predict treatment performance under varying conditions and are especially helpful to improve the informative value of pilot tests. For example, potential changes in influent concentration, background water quality, flow rate, and adsorbent bed height not covered in pilot tests can be simulated using models. Whereas GAC adsorption of some organic micropollutants is already well studied, competitive adsorption of DOM and PFAS and iPMT in drinking water with elevated DOM-content is less understood, and design tools are lacking. The developed drinking water treatment and design tool (DWTDT) is applicable for fixed-bed adsorber design in water treatment trains. Using the tool, operational times until exhaustion of fixed-bed adsorbers using GAC or ion exchange resins can be predicted. This includes an estimation of ideal breakthrough using equilibrium isotherm data as main input data, as well as prediction of the dynamic breakthrough using additional input parameters describing internal and external mass transfer.

Dynamic breakthrough prediction is based on the pore surface diffusion model (PSDM) developed by the United States Environmental Protection Agency (EPA) and extended with the so-called tracer model (TRM), allowing the breakthrough of DOM and its competing effects on PFAS and iPMT removal to be mapped. Both the original model by the EPA as well as the DWTDT were developed using the programming language Python. A user interface was built for the DWTDT to make it more user friendly. The model was tested with experimental input data from the laboratory tests and validated with pilot plant data from the PROMISCES project. The DWTDT is publicly available on GitHub and Zenodo (<https://doi.org/10.5281/zenodo.13982527>). The tool allows users to simulate simultaneous DOM, PFAS and iPMT breakthrough in drinking water treatment trains using adsorbents or ion exchange resins, provided that the necessary input data including single solute isotherm data, external mass transfer coefficients, internal diffusion coefficients, and adsorption parameters for DOM background are known or can be estimated.

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List of abbreviations

Abbreviation	Full name
ADSA	Adsorption analysis
BTC	Breakthrough curve
DOC	Dissolved organic carbon
DOM	Dissolved organic matter
DWTD	Drinking Water Treatment and Design Tool
EBCM	Equivalent background compound model
EPA	Environmental protection agency
GAC	Granular activated carbon
GUI	Graphical user interface
IAST	Ideal adsorbed solution theory
iPMT	Persistent, mobile and potentially toxic substances
IX	Ion exchange resin
PFAS	Per- and polyfluoroalkyl substances
PSDM	Pore surface diffusion model
TRM	Tracer model

1 Introduction

A new planning and design tool to assist drinking water treatment plant operators in the removal of per- and polyfluoroalkyl substances (PFAS) and other persistent, mobile, and potentially toxic (iPMT) substances from drinking water rich in dissolved organic matter (DOM) has been developed.

Within PROMISCES, technologies to remediate PFAS and iPMT(s) in several environmental media have been studied. This deliverable reports on a tool developed to improve planning and design of drinking water treatment trains for PFAS and iPMT, especially focusing on the adsorption onto granular activated carbon (GAC), alternative adsorbents and removal using ion exchange (IX) resins. Although previous research has addressed PFAS and iPMT removal in drinking water treatment, knowledge gaps regarding the optimal implementation of effective treatment trains remain. The design of a suitable treatment system relies on the adsorbent's efficiency in removing different chemical mixtures, varying water qualities, and specific treatment objectives. Modelling tools can forecast treatment performance under different conditions, which is particularly valuable for refining pilot tests. For instance, models can simulate potential variations in influent concentration, water quality, flow rate, and adsorbent bed height that are not captured in pilot studies. While GAC adsorption has been extensively researched, the competitive adsorption of DOM with PFAS and iPMT is less understood, and there is a lack of design tools in this area.

The newly developed drinking water treatment and design tool (DWTDT) is suitable for fixed-bed adsorber design in drinking water treatment systems. It enables predictions of operation times until the exhaustion of fixed-bed adsorbents using GAC or ion exchange resins. This tool incorporates rough estimates of ideal breakthrough based on equilibrium isotherm data and can also predict dynamic breakthrough using additional parameters that describe both internal and external mass transfer.

GAC adsorbents are commonly used in drinking water treatment to remove organic chemicals such as PFAS and iPMT. The capacity of a GAC fixed-bed adsorber is influenced by both adsorption equilibrium and kinetics, with mass transfer processes like film diffusion, pore diffusion, and surface diffusion affecting the adsorption rate. To accurately describe the breakthrough curve (BTC) for different adsorbates, a suitable model and knowledge of equilibrium and kinetic parameters are necessary. However, the complexity of BTC models increases the number of parameters needed, making model selection a balance between accuracy and parameter estimation effort (Burkhardt et al. 2022). Despite the development of various BTC models, their application in drinking water treatment design is limited due to challenges in parameter estimation, particularly because drinking water is a complex multi-component system (Worch 2012).

The ideal adsorbed solution theory (IAST) is currently the most important and most commonly used thermodynamic model to predict multi-solute adsorption equilibria. Initially developed for gas adsorption by Myers and Prausnitz in 1965, it was later applied to liquid-phase adsorption by Radke and Prausnitz in 1972 for the first time. The IAST in its original form requires single-solute isotherm data of all mixture components and performs the calculation with molar quantities. However, in addition to PFAS and iPMTs, concentrations of which can be precisely determined by target analysis, natural waters contain a certain amount of DOM with a complex and unknown composition. DOM is therefore usually quantified in the form of the dissolved organic carbon (DOC) as sum parameter. The presence of DOM complicates the application of the IAST in two ways: first, no individual single-solute isotherms can be determined for the large number of DOM components, and second, the sum parameter DOC cannot simply be converted into molar substance quantities.

There are two important model approaches to circumvent these methodological problems in the IAST: the equivalent background compound model (EBCM) and the tracer model (TRM) (Worch 2010). The EBCM utilizes multi-solute adsorption data along with single-solute Freundlich parameters for PFAS and iPMTs to model the concentration and Freundlich parameters of a hypothetical equivalent background compound, which accounts for the adsorption competition caused by DOM. However, since the equivalent background compound is a purely fictitious quantity, it is not possible to model the DOC concentration in the filter effluent. The TRM is based on an adsorption analysis (ADSA). The core idea of the ADSA involves formally transforming the unknown multi-component system (e.g. DOM), into a defined mixture of a limited number of fictive components. Each of these fictive components represents a fraction of the measured DOC with specific adsorption characteristics. After additional fitting of the Freundlich parameters of the organic chemical to isotherm data in presence of DOM, the TRM is able to calculate the removal of the organic chemical as well as to quantify the DOC breakthrough. In contrast to the EBCM, this enables characterisation of the inlet of a second, downstream adsorber stage. Therefore, the TRM was implemented in the DWTDT to model the removal of PFAS from DOC-rich groundwater and drinking water with GAC.

The developed DWTDT includes modules for ADSA and TRM which feed into the PSDM and allow simulation of PFAS and iPMT breakthrough in fixed-bed systems.

2 Modelling approach and theoretical background

2.1 Structure of the DWTDT and integration of the EPA PSDM

The DWTDT is based on the open-source pore surface diffusion model (PSDM) Python application developed and provided by the US EPA and under license of the Massachusetts Institute of Technology. The PSDM uses orthogonal collocation on finite elements to solve the underlying set of differential equations. Detailed information on the PSDM and the applied numerical methods are given elsewhere (Mertz et al. 1999; Crittenden et al. 1980; Burkhardt et al. 2022). The PSDM application of the EPA already includes simple empirical correction factors to account for capacity and kinetic reduction due to fouling of GAC as described by Jarvie et al. (2005). The Python PSDM model is available on Github (US EPA 2024).

This original PSDM was extended by an ADSA and TRM module and wrapped in a GUI for the DWTDT. Furthermore, minor adjustments to the PSDM were necessary to guarantee compatibility with the TRM. The results from the ADSA and TRM module serve as input to the PSDM module. All modules are accessible through the GUI and can also be used independently as Python scripts.

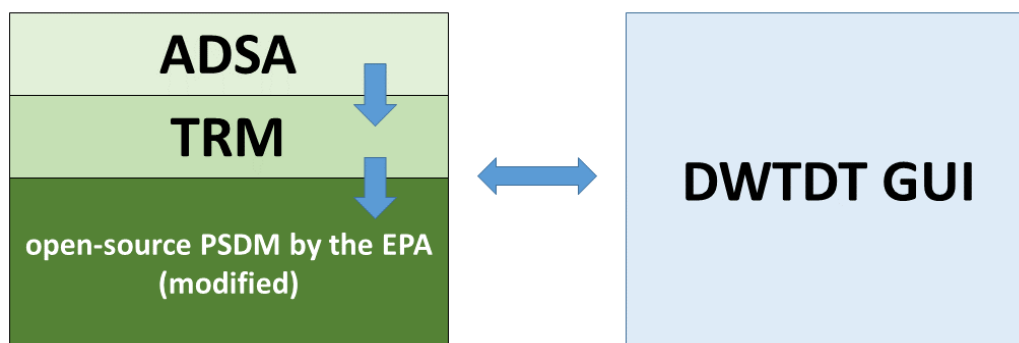


Figure 1 Structure of the DWTDT

2.2 Single-solute adsorption equilibrium

The adsorption equilibrium of one single-solute adsorbate is described with the empirical Freundlich isotherm equation (1):

$$q_i = K_i c_i^n \quad (1)$$

q_i : loading of adsorbate on the adsorbent in equilibrium

c_i : concentration of the adsorbate in the liquid phase in equilibrium

K_i and n : empirical Freundlich parameters

Isotherm data (c , q) needs to be determined with lab-scale batch experiments. Afterwards, a non-linear fitting approach (e.g. python `curve_fit` function) or linear fitting approach (after log transformation of c and q) can be applied to estimate K_i and n .

2.3 Modelling of multi-solute adsorption equilibrium with the IAST

The IAST is applied in the DWTDT to predict multi-solute adsorption equilibrium. To apply the IAST effectively, several conditions must be met. First, the model assumes that the adsorbed phase forms a two-dimensional layer in equilibrium with the liquid phase, where all adsorbates have equal access across the entire surface of the adsorbent. Consequently, competitive factors like size exclusion or pore blockage are not considered. Additionally, the IAST operates under the assumption of ideal behaviour in both the liquid and adsorbed phases. This is generally valid for the liquid phase, as adsorbates are typically well-diluted. However, in the adsorbed phase, interactions between adsorbate molecules can be significant and may lead to unsatisfactory results at high loading levels or when specific interactions occur (Worch 2012). A modified version of the Gibbs fundamental equation, often called the spreading pressure integral, serves as the foundation for the IAST (equation (2)):

$$\varphi_i = \frac{\pi_i A_m}{RT} = \int_0^{c_i^0} \frac{q_i^0}{c_i^0} dc_i^0 \quad (2)$$

The spreading pressure π is defined as the difference between σ_{ws} (the surface tension at the water-solid interface) and σ_{ss} (the surface tension at the adsorbate solution-solid interface). This difference determines how adsorbate molecules are distributed between the liquid and the adsorbed phases. It is developed for a component i within an N -component mixture and connects the spreading pressure to its equilibrium loading q_i^0 and the associated concentration c_i^0 . The spreading pressure term φ is included for simplification and is proportional to π , as the gas constant R , temperature T , and the adsorbent's surface area A_M can be considered constants. Similar to Raoult's law, the following equation (3) is applicable for multi-solute adsorption at a constant spreading pressure π or a fixed spreading pressure term φ , respectively:

$$c_i = c_i^0(\varphi) z_i \quad (3)$$

Equation (3) connects the concentration of a component c_i to the single-solute concentration $c_i^0(\varphi)$, which would generate the same spreading pressure as the mixture. Here, z_i represents the mole fraction of the component in the adsorbed phase. Therefore, it can be expressed with equation (4) as:

$$q_i = z_i q_T \quad (4)$$

With q_T being the total surface loading of all multi-solute components. The sum of the mole fractions follows per definition:

$$\sum_{i=1}^N z_i = 1 \quad (5)$$

q_T can as well be expressed as sum of the single-solute loadings $q_i^0(\varphi)$ and z_i at given φ , which results in equation (6):

$$q_T = \left[\sum_{i=1}^N \frac{z_i}{q_i^0(\varphi)} \right]^{-1} \quad (6)$$

A single-solute isotherm model (usually Freundlich, equation (1)) is employed to connect c_i^0 and q_i^0 and solve the the spreading pressure integral (equation (2)), resulting in equation (7):

$$\varphi_i = \frac{K_i}{n_i} (c_i^0)^{n_i} \quad (7)$$

Subsequently, solutions for q_i^0 (equation (8)) and c_i^0 (equation (9)) can be derived from equation (1) and (7):

$$q_i^0 = \varphi_i n_i \quad (8)$$

$$c_i^0 = \left(\frac{\varphi_i n_i}{K_i} \right)^{1/n_i} \quad (9)$$

A material balance (equation (10)) relates initial ($c_{0,i}$) and equilibrium concentration (c_i) with the adsorbent dose V_L/m_A .

$$q_i = \frac{V_L}{m_A} (c_{0,i} - c_i) \quad (10)$$

Inserting equation (9) in equation (3) and combining the results with equation (10) and (4) leads to equation (11):

$$z_i = \frac{c_{0,i}}{\frac{m_A}{V_L} q_T + \left(\frac{\varphi n_i}{K_i} \right)^{1/n_i}} \quad (11)$$

Following this, substituting equation (11) into equations (5) and (6) yields a set of equations (12 and 13) that can be solved numerically to determine the two unknowns q_T and φ .

$$\sum_{i=1}^N \frac{c_{0,i}}{\frac{m_A}{V_L} q_T + \left(\frac{\varphi n_i}{K_i} \right)^{1/n_i}} = 1 \quad (12)$$

$$\sum_{i=1}^N \frac{1}{\varphi n_i} \cdot \frac{c_{0,i}}{\frac{m_A}{V_L} q_T + \left(\frac{\varphi n_i}{K_i} \right)^{1/n_i}} = \frac{1}{q_T} \quad (13)$$

Finally, z_i , q_i and c_i can be calculated using equation (4), (10) and (11). The procedure of the IAST is summarized in [Figure 2](#).

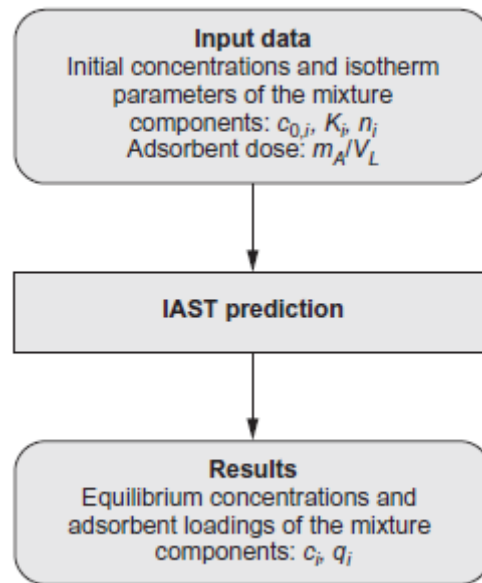


Figure 2 Calculation scheme of the IAST (Worch 2012). An IAST calculation in a defined mixture requires single-solute isotherm data for all adsorbates in the mixture.

2.4 Modelling of multi-solute adsorption equilibrium in presence of DOM: Adsorption analysis and Tracer model

The adsorption analysis (ADSA) is applied to model DOM breakthrough in the DWTDT. The fundamental concept of the ADSA involves transforming the unknown multi-component system of DOM into a defined mixture of a limited number of fictive components. The DOM is hereby quantified using the sum parameter DOC. Each of these fictive components represents a fraction of DOC with specific adsorption characteristics. During the adsorption analysis, the varying adsorption of the DOC fractions are defined by assigning them characteristic Freundlich isotherm parameters. To simplify the process, the exponent n is kept constant (e.g. $n = 0.25$), while different coefficients K_i can be employed to indicate the varying adsorption strengths. The non-adsorbable fraction is represented by setting K_i of one fraction to a very small value or to zero. Generally, selecting three to five fictive components is found to be effective for most practical scenarios. Once the number and isotherm parameters of the fictive components are defined, an IAST-based search routine is employed to determine the concentration distribution of the DOC fractions that best fits the measured DOC isotherm. The process of the ADSA is illustrated schematically in Figure 3. After completing the analysis, the DOC is characterized as a defined adsorbate mixture, meaning the isotherm parameters

and initial concentrations of the DOC fractions are known and can be utilized for further process modelling. The procedure of the ADSA is summarized in Figure 3.

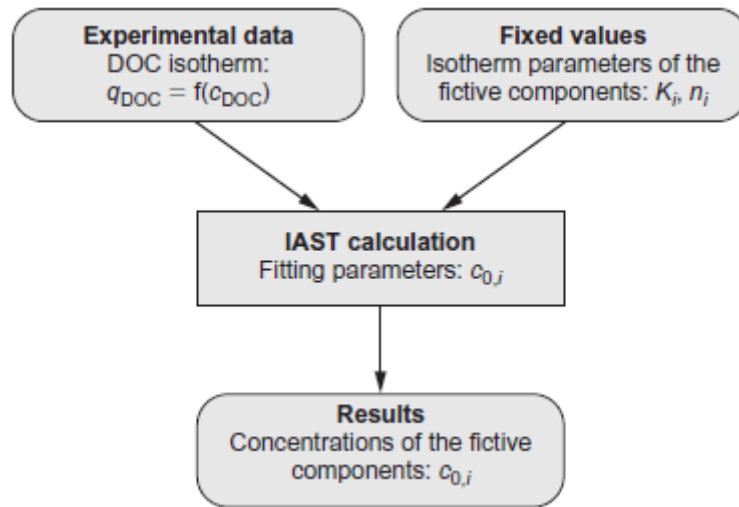


Figure 3 Calculation scheme of the adsorption analysis (Worch 2012).

The TRM relies on the findings from the ADSA, which are directly used as input data for calculating competitive adsorption between PFAS, iPMT, and DOM. To accurately represent this competitive adsorption with the IAST, adjustments are made to the single-solute isotherm parameters of the organic chemical. These corrected isotherm parameters are derived from experimental data on competitive adsorption (specifically, the organic chemical isotherm in the presence of DOM) through a fitting procedure based on the IAST. The outcome of this fitting process yields modified isotherm parameters for the organic chemical, enabling a more precise description of competitive adsorption when combined with the ADSA data. An overview of the TRM process is given in Figure 4.

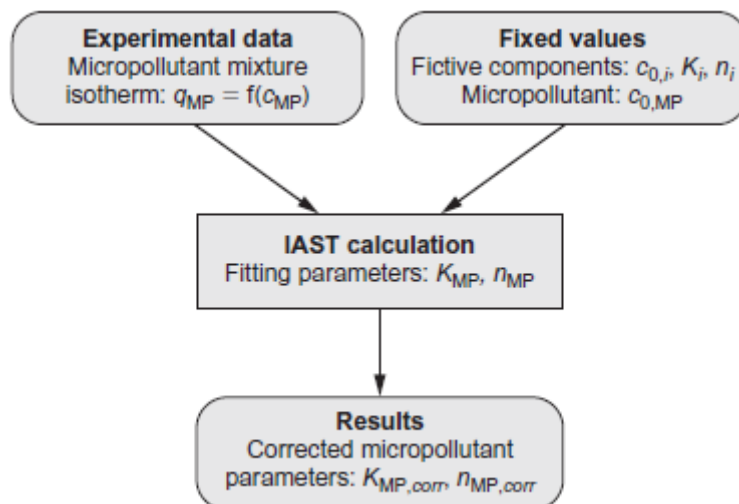


Figure 4 Calculation scheme of the tracer model (Worch 2012). A model run with DOM requires a DOC-isotherm as input for the ADSA as well as isotherm data of the adsorbate in the presence of DOM as input for the TRM.

2.5 Kinetic parameter estimation

2.5.1 Film diffusion

The film diffusion coefficient k_f is calculated using the Gnielski correlation (equation (14), Sontheimer et al 1988):

$$k_f = \frac{[1 + 1.5(1 - \varepsilon)]D}{d_p} [2 + 0.644 Re^{1/2} Sc^{1/3}] \quad (14)$$

with d_p being the adsorbent particle diameter, D the adsorbate liquid phase diffusivity and ε the adsorber bed void fraction. The dimensionless numbers Re and Sc are determined by equation (15) and (16):

$$Re = \frac{\rho d_p v}{\mu} \quad (15)$$

$$Sc = \frac{\mu}{\rho D} \quad (16)$$

in which ρ is the liquid density, v the liquid phase interstitial velocity and μ the liquid phase viscosity. The adsorbate liquid phase diffusivity D is determined from a correlation by Hayduk and Laudie (1974) (equation (17)), with V_b being the molar volume of the chemical at the normal boiling point:

$$D = \frac{13.26 \cdot 10^{-5}}{\mu^{1.14} V_b^{0.589}} \quad (17)$$

In case of a TRM run, the correlation by Worch (1993) (equation (18)) which uses the molar mass M of the adsorbate is employed:

$$D = \frac{3.595 \cdot 10^{-14} T}{\mu M^{0.53}} \quad (18)$$

2.5.2 Surface diffusion

The surface diffusion coefficient D_s is determined by an empirical correlation (equation (19)) according to Sontheimer (1988), with ρ_a as apparent adsorbent density and SPDFR being the surface to pore diffusion flux ratio:

$$D_s = \frac{D \varepsilon c_{0,i}}{\tau \rho_a q_{0,i}} \cdot SPDFR \quad (19)$$

2.5.3 Pore diffusion

The pore diffusion coefficient D_p is related to the adsorbate liquid phase diffusivity D (equation (20)) and depends on the tortuosity τ of the adsorbent:

$$D_p = \frac{D}{\tau} \quad (20)$$

3 Introduction to the GUI and functionality of the DWTDT

3.1 Code availability

The DWTDT is published according to the FAIR principles, meaning that it will be findable, accessible, interoperable and reusable. In accordance with the PROMISCES data management plan, the code is available in a GitHub repository, which is linked to a Zenodo resource within the PROMISCES community page on Zenodo (<https://doi.org/10.5281/zenodo.13982527>).

3.2 Installation

The DWTDT requires the installation of Python (it was developed under Python 3.12.7, so python 3 is recommended). The user can check their python installation and version by entering the following command in the command window:

```
python --version
```

If Python is installed, the user will receive a notification with the version number. The next step is to download and save the 'Water_treatment_models' folder locally on the computer. The user should then navigate to the 'Water_treatment_models' folder using the following command in the command window:

```
cd <local path to 'Water_treatment_models' >
```

Following that, the user should enter the following command from the install.txt file:

```
pip install -r requirements.txt
```

This should automatically install all packages listed in the requirements.txt file.

3.3 Start

To start the model after installation from the 'Water_treatment_models' folder, the following command must be entered in the command window:

```
shiny run ShinyPy-GAC/app.py
```

A URL is displayed in the command window that can be opened in the browser. The user can now operate the model.

3.4 Input Data

3.4.1 Import and export of DWTDT projects

The DWTDT enables the user to save and reload projects as .json files. The tab of the GUI where the user can upload/ save project files is shown in **Fehler! Verweisquelle konnte nicht gefunden werden..** All entries from 'Adsorbent Characteristics', 'Adsorber Specifications', 'Adsorbate Properties', 'Adsorption Properties' and 'Treatment Train' are saved in the .json file. The influent and effluent data from the 'Data'.xlsx file as well as the isotherms for the ADSA and TRM ('DOM' tab) are not saved and must be reuploaded. Under the 'Input Data' menu, users first enter all the information about the model input, while the 'Simulation' menu allows for the configuration of calculation settings.

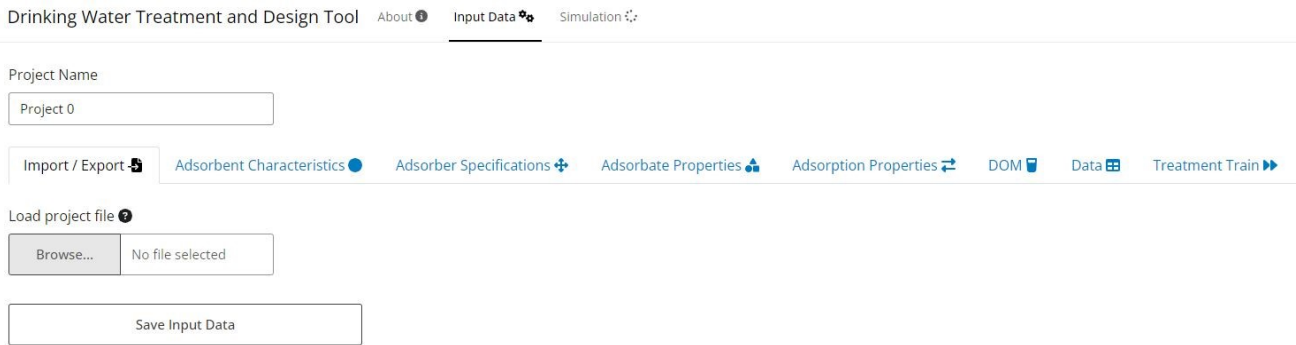


Figure 5 DWTDT menu with import/ export functionality

3.4.2 Adsorbent characteristics

Information on the adsorbent can be entered under 'Adsorbent Characteristics'. Each data entry must be confirmed using the 'add/update' button to be available for model runs. To revise the adsorber data, first select it from the right-hand menu ('Adsorbent Selection'), make modifications, and then confirm via 'add/ update'. The tab of the GUI that shows the settings for the adsorbent characteristics is shown in Figure 6.

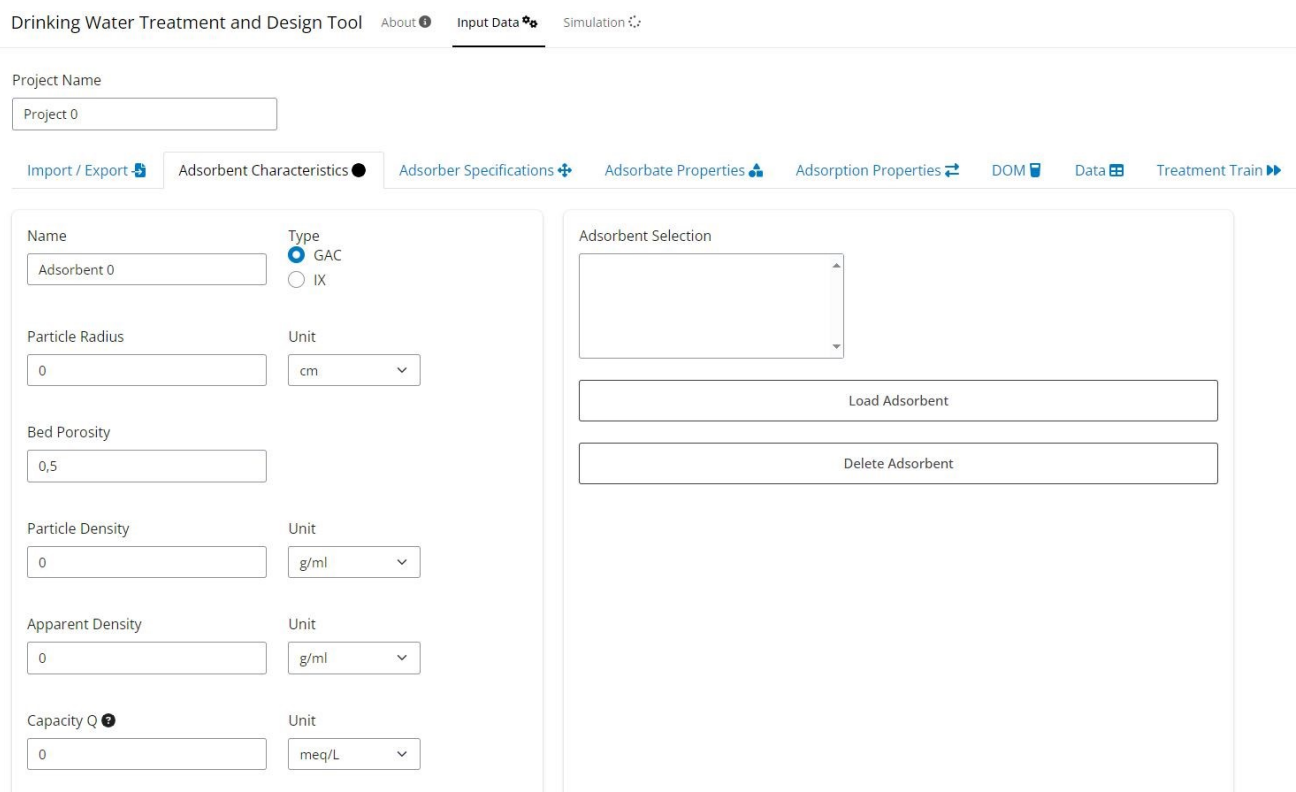


Figure 6 Adsorbent Characteristics menu of the DWTDT

3.4.3 Adsorber specifications

The data for the fixed-bed filter is stored under the 'Adsorber Specifications' tab (compare Figure 7). This includes, for example, the dimensions of the filter and the volume flow. This information is not adsorbent-specific and can be accessed for various adsorbents as part of a treatment train.

Project Name

Import / Export

Adsorbent Characteristics

Adsorber Specifications

Adsorbate Properties

Adsorption Properties

DOM

Data

Treatment Train

Adsorber Name <input type="text" value="Column 0"/>	Adsorber Selection <div style="border: 1px solid gray; height: 50px; width: 100%;"></div>
Length Unit <input type="text" value="0"/> <input type="text" value="cm"/>	<input type="button" value="Load Adsorber"/>
Diameter Unit <input type="text" value="0"/> <input type="text" value="cm"/>	<input type="button" value="Delete Adsorber"/>
Flow Rate Unit <input type="text" value="0"/> <input type="text" value="L/h"/>	
Temperature Unit <input type="text" value="20"/> <input type="text" value="degreeC"/>	
<input type="button" value="Add/Update Adsorber"/>	

Figure 7 Adsorber specifications menu of the DWTDT

3.4.4 Adsorbate properties

All substance-specific data is stored under 'Adsorbate Properties' (compare Figure 8). The molar mass, the molar volume, and the density are used for the empirical correlations to calculate the diffusion coefficients. The sum formula is only required if calculating with the TRM, where the amount of substance is converted into mass of carbon (given as [mgC]). The valence is only needed if IX calculations are performed.

Project Name

[Import / Export](#)
[Adsorbent Characteristics](#)
[Adsorbent Specifications](#)
[Adsorbate Properties](#)
[Adsorption Properties](#)
[DOM](#)
[Data](#)
[Treatment Train](#)

Name <input type="text" value="PFBA"/>	Formula <input type="text" value="C4HF7O2"/>	Compound Selection <input type="text" value="PFBA"/> GenX PFBS PFDA PFHpA <input type="button" value="Load Compound"/> <input type="button" value="Delete Compound"/>
Molar Weight <input type="text" value="214,03853314099996"/>	Unit <input type="text" value="g/mol"/>	
Molar Volume <input type="text" value="129,72"/>	Unit <input type="text" value="mol/L"/>	
Boiling Point <input type="text" value="121"/>	Unit <input type="text" value="degreeC"/>	
Density <input type="text" value="1,65"/>	Unit <input type="text" value="g/ml"/>	
Valence <input type="text" value="1"/>		
<input type="button" value="Add/Update Compound"/>		

Figure 8 Adsorbate properties menu of the DWTDT

3.4.5 Adsorption properties

The actual isotherm data is entered under 'Adsorption properties', as shown in Figure 9. In the current version of the tool, only the Freundlich model can be used. When entering the K_i value, various units can be selected, while the Freundlich exponent n is dimensionless. The corresponding adsorbent and adsorbate must first be selected for input. In order to perform a calculation, it is essential that the adsorbent is stored under 'Adsorbent Characteristics' and the adsorbate is stored under 'Adsorbate Properties'. For the corresponding isotherm data to be accepted, it is necessary to confirm the entries using the 'Add/ Update Properties' button. Under the 'Advanced' settings, manual diffusion coefficients can be defined if these were determined using experimental data or are to be fitted to the breakthrough curve.

Project Name

<p>Adsorbent <input type="text" value="H3ON"/></p> <p>K <input type="text" value="10,131394"/></p> <p>n <input type="text" value="0,45"/></p> <p>Advanced</p>	<p>Adsorbate <input type="text" value="PFBA"/></p> <p>Unit <input type="text" value="(ug/g)/((ug/L)*"/></p>
--	---

Add/Update Properties

Adsorption Properties Selection

- H3ON:PFBA
- H3ON:PFHxA
- H3ON:PFOS
- H3ON:PFHxS

Figure 9 Adsorption properties menu of the DWTDT

3.4.6 DOM

If a calculation is to be carried out with the TRM, it is necessary to enter additional data under the 'DOM' menu item (compare Figure 10). To carry out an ADSA, a DOC isotherm (with DOC in mg/L as 'c' and adsorbent in g/L as 'm') must be entered. Only .xlsx file format is accepted. Any number of K_i values for the fictitious fractions can be specified in the 'Input K values' input field. Good results are usually achieved with 3-5 fractions. The Freundlich exponent n of the fractions and the mean molar weight can also be adjusted manually: the default values are '0.25' and '1000' in g/mol. After pressing 'Run ADSA', the calculation results are plotted and the IAST data is output in a table format. Following the ADSA, a TRM run can be carried out. This requires entering additional isotherm data of the organic chemical in the presence of DOM. The results of the ADSA are used as unmodified input to the TRM run. After the TRM calculation, it is possible to add the results of TRM and ADSA as inputs to the BTC simulation. It is important to know that this feature will overwrite any isotherm data of the modelled organic chemical inserted under 'Adsorption Properties'.

Project Name:

Adsorption Analysis

Select .xlsx file with DOC Isotherm

H3ON_DOC.xlsx

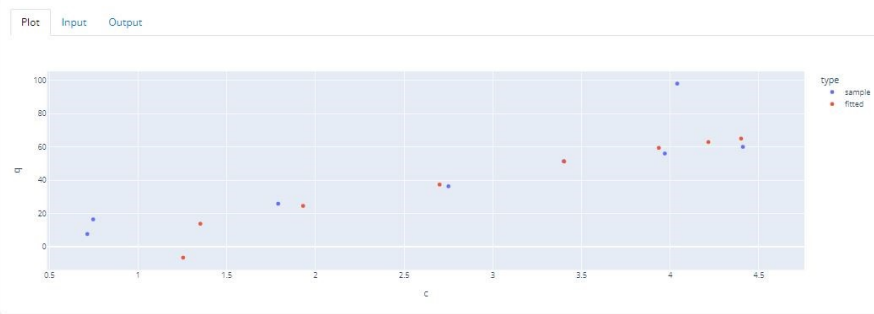
Adsorbent:

Input Molecular Weight:

Input Ki Values:

Input n:

Plot:



Tracer Model

Adsorbate:

Select File with Isotherm in DOC presence

No file selected

Plot:

Figure 10 DOM input menu for ADSA and TRM

3.4.7 Data

Influent and effluent data is inserted under 'Data', as shown in Figure 11 The DWTDT accepts .xlsx file formats for this purpose. The specification of effluent data is optional, but the specification of influent data is essential. It is important to define the influent concentration at time 0. By default, the maximum simulation time is set to the last influent time. While influent data can be entered at any resolution, highly variable influents or very low concentrations can lead to long calculation times and numerical instability.

Drinking Water Treatment and Design Tool About Input Data Simulation

Project Name

Select .xlsx file with influent and (optional) effluent data of your adsorber.

Influent Keyword

Effluent Keyword

Time Unit

Concentration Unit

Influent Data

time	concentration	compound	step	scenario
0	1256.7832082219	TRM_0		
0	1356.6600374522	TRM_1		
0	545.5297109459	TRM_2		
0	1371.0270433801	TRM_3		
0	1256.7832082219	TRM_0	0	
0	1356.6600374522	TRM_1	0	
0	545.5297109459	TRM_2	0	
0	1371.0270433801	TRM_3	0	
225.9166666667	1256.7832082219	TRM_0	0	
225.9166666667	1356.6600374522	TRM_1	0	
225.9166666667	545.5297109459	TRM_2	0	
225.9166666667	1371.0270433801	TRM_3	0	
0	0.405	PFOS	0	
1.9583333333	0.405	PFOS	0	
0.0583333333	0	PFOS	0	

Viewing rows 1 through 15 of 32

Effluent Data

time	concentration	compound	step	scenario
1.9583333333	0	PFOS	0	
0.0583333333	0	PFOS	0	

Figure 11 influent and effluent data

Treatment train

The ‘Treatment train’ menu enables the user to define different ‘scenarios’ for drinking water treatment trains (compare Figure 12). Within the DWTDT, the term ‘Treatment Train’ refers to one or a combination of fixed-bed adsorbents in series (with the same or different adsorbents equipped). The term ‘scenario’ describes the entire calculation example. This includes not only which adsorbents are used, but also which substances are modelled and at which influent concentrations. A ‘Treatment train’ can therefore be modelled in different ‘scenarios’.

Each treatment step requires information about the adsorbent and the adsorber. The menu offers automatically all adsorber and adsorbent data entered in the previous menu steps. To guarantee compatibility, it is necessary that labelling of adsorbents is consistent within all menus of one project file. It is possible to add several adsorbents in series, although it should be mentioned that this option

can lead to long model runtimes. The menu options ‘Water type’ and ‘Chemical type’ refer to the empirical GAC-fouling correlations from the original EPA model (more information about these correlations can be found in (Mertz et al. 1999)). They can also be applied in the DWTDT for comparison purposes, or if no suitable isotherm data is available to carry out an ADSA and TRM run.

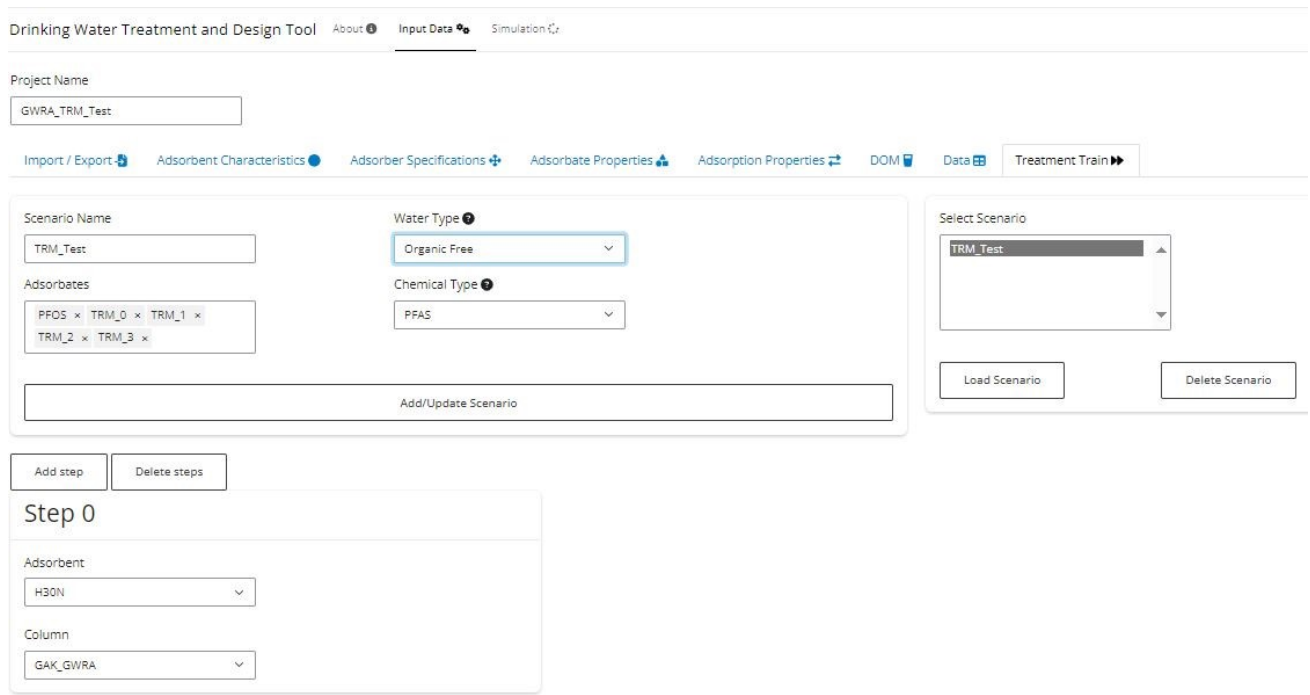


Figure 12 Treatment train menu of the DWTDT

3.5 List of input parameters

Abbreviation	Full name	Available units
D	diameter of adsorber	cm, mm, m
D	liquid phase diffusion coefficient	cm ² /s
D _p	pore diffusion coefficient	cm ² /s
D _s	surface diffusion coefficient	cm ² /s
K _i	Freundlich parameter	(ug/g)/(ug/L) ⁿ , (ug/mg)/(ug/L) ⁿ , (mg/g)/(mg/L) ⁿ , (mmol/mg)/(mmol/L) ⁿ
k _f	film diffusion coefficient	cm/s
L	length of adsorber	cm, mm, m
M	molar weight	g/mol
n	Freundlich parameter	
Q	capacity	meq/L
r	particle radius	cm, mm, m

T	temperature	C
T _b	boiling point	C
V	flow rate	L/h, L/min, m ³ /h, m ³ /min
V _b	molar volume	mol/L
e	bed porosity	
rho_a	adsorbate density	g/ml
rho_b	apparent density	g/ml, kg/L
rho_p	particle density	g/ml, kg/L

3.6 Simulation

The settings of the simulation are defined under ‘Setup’ (compare screenshot in Figure 13). The number of radial and axial collocation points can be defined here. The PSDM uses orthogonal collocation on finite elements as numerical solving method. Increasing the number of collocation points and/or finite elements increases the resolution of the calculation and can improve the accuracy of the model and prevent numerical instability. Numerical instability can be recognized, for example, by oscillation and extreme outliers. However, a high number of collocation points can also lead to very long calculation times (several hours). For practical applications, it is recommended to start with the default settings (or even a lower number) and to increase these gradually until the results look plausible or satisfactory.

The default for the number of finite elements is ‘1’. If numerical instability occurs, it can be helpful to minimize the axial collocation points and control collocation with the number of finite elements (e.g. 20-30 finite elements and low numbers (1-3) for axial and radial collocation) instead. This can be helpful for complex model runs in multi-solute systems. Clicking the ‘Run Analyses’ button will start the simulation. The user can view the results in a plot window and save as .png (example plot shown in Figure 14) and save all calculation results as .xlsx.

Test About Input Data Simulation

Setup Results

Select Scenarios to Simulate / Save Results from

- GWRA_A2_A3_A4
- GWRA_A2
- GWRA**

Radial Collocation Points

3 7 18

Axial Collocation Points

3 12 18

Number of finite Elements

1 100

Run Analyses

Save Results

Figure 13 simulation setup



Figure 14: Example of a results output window. The user has the option to change the x-axis from bed volumes to time, deactivate or activate data series, and zoom in or out.

4 Calculation example and conclusions

Figure 15 shows an example calculation (PFOS BTC in presence of DOM) for a GAC adsorber at the pilot plant in Berlin-Tegel. The model was run using the TRM, building on an ADSA run with four fictive DOM fractions (TRM0-TRM3) with different K values ($K = 1, 20, 40, 60 \text{ mg/g}/(\text{mg/L})^n$ and $n = 0.25$). The model is able to give a realistic order of magnitude for the breakthrough of PFOS. The number of days until breakthrough of 10 % of the PFOS influent concentration (BV10) is underestimated by the model by about 26% (model: 48 days; measurement data: 65 days) and the number of days until breakthrough of 50 % of the PFOS feed concentration (BV50) is slightly overestimated by about 12 % (model: 190 days, measurement data: 190 days). An additional improvement of the model could be achieved by calibrating the diffusion coefficients to the effluent data or entering experimentally determined kinetic parameters. This optimization is always possible if effluent data is already available for a site and would not be possible for a purely theoretical modeling scenario without site data. In order to further verify the robustness of the model, it would be advisable to carry out further studies in which the model is tested with different substances and waters with different DOM concentrations and compositions.

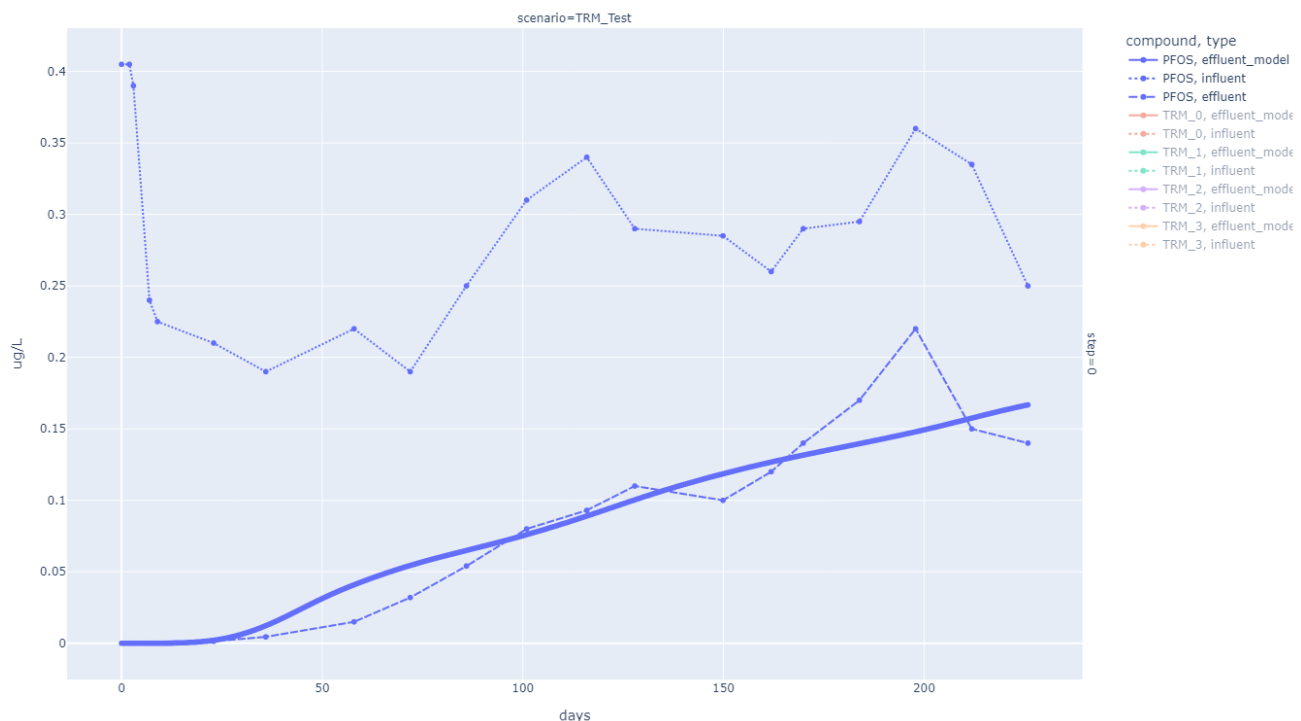


Figure 15 calculation example (PFOS BTC in presence of DOM with TRM) for a GAC-adsorber in Berlin-Tegel. ADSA run with $K = 1, 20, 40, 60 \text{ mg/g}/(\text{mg/L})^n$ and $n = 0.25$.

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