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Assessing the cost of granular activated carbon (GAC) and ion exchange (IX) technologies for treating PFAS

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Background on PFAS and new regulations

Per- and polyfluoroalkyl substances (PFAS) are a broad class of chemical species containing one or more fluorinated carbons

- Sub-classified based on the diverse chemical structures[1]
- Display thermal stability and hydrophobicity[2]

PFAS are resilient compounds that accumulate in the environment

- Detectable levels in food, **drinking water**, and soils[2]
- Adverse human health effects of long-term exposure to PFAS

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[1] Su, Rajan. 2021. *Sci. Data.*
[2] Buck et al. 2011. *Integr. Envrion. Assess. Manag.*

Background on PFAS and new regulations

PFAS remediation is a modern issue

- Most research published during the past decade
- 29 species added to the Fifth Unregulated Monitoring Contaminants Rule (UMCR 5) in 2021[3]
- **6 species added to the National Primary Drinking Water Regulation (NPDWR) in 2023[3]**

PFAS National Primary Drinking Water Regulations[3]

Compound	Proposed MCLG	Proposed MCL (Enforceable)
PFOA	Zero	4.0 ppt (ng/L)
PFOS	Zero	4.0 ppt (ng/L)
PFNA	1.0 Hazard Index	1.0 Hazard Index
PFHxS		
PFBS		
HFPO-DA (GenX)		

MCLG, Maximum contaminant level goal
MCL, Maximum contaminant level

$$\text{Hazard Index} = \left(\frac{[PFNA]}{10\ ppt}\right) + \left(\frac{[PFHxS]}{9\ ppt}\right) + \left(\frac{[PFBS]}{2000\ ppt}\right) + \left(\frac{[HFPO\text{-}DA]}{10\ ppt}\right)$$

[3] US EPA. 2023. *https://www.epa.gov/pfas*

Designing adsorption systems for PFAS regulations

From prior state regulations and emerging research, some general design heuristics for PFAS removal by adsorption are apparent[4]

- Granular activated carbon (GAC) is effective removing long chain PFAS, but less effective for short chain
- Ion exchange (IX) is effective removing short chain PFAS, but less effective for long chain

The **process economics** and situational optimality of **selecting GAC and IX technologies** are underdefined

- **Cost assessments are largely limited** to pilot scale extrapolations of a given source water[4,5]

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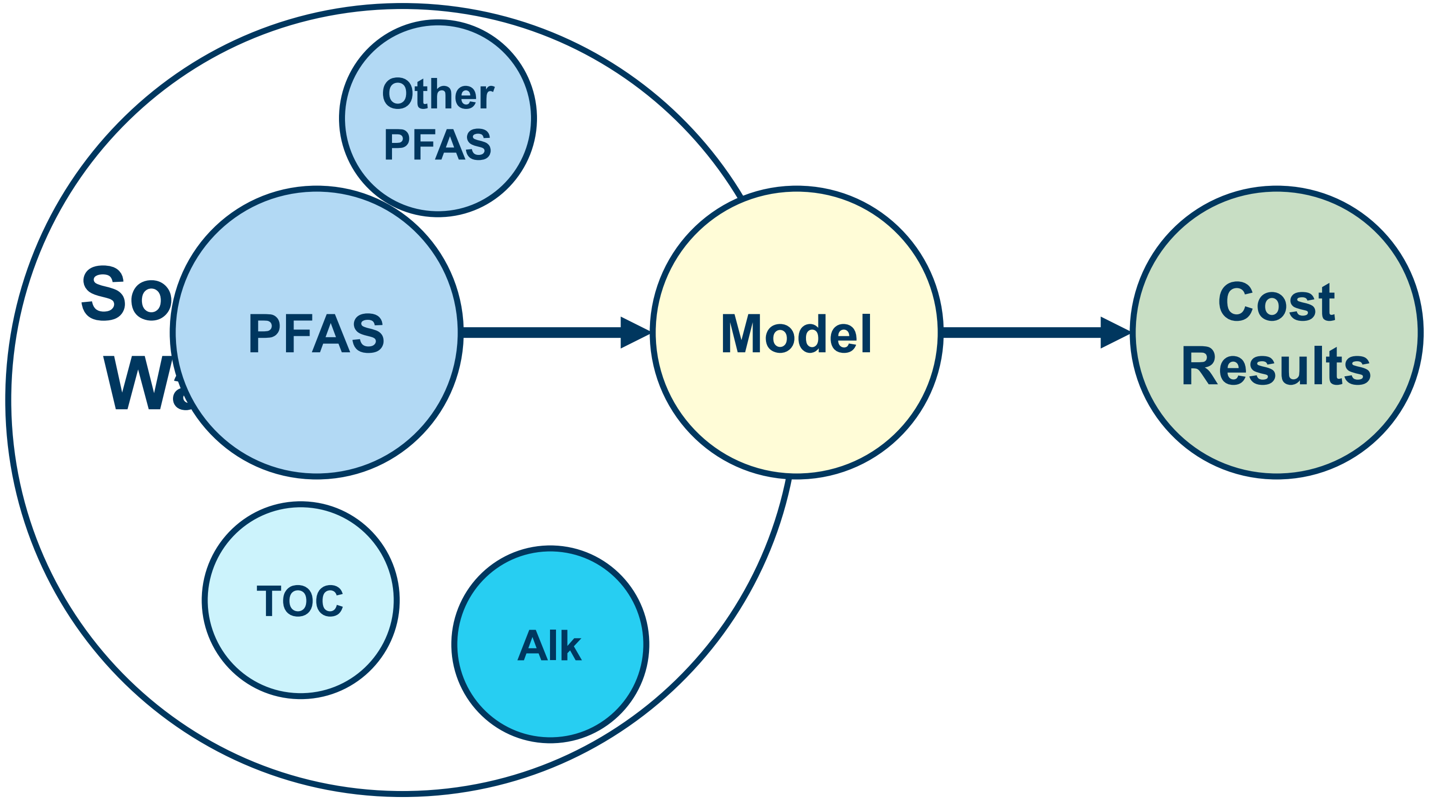
[4] Murray et al. 2021. *J. Water Process Eng.*
[5] Franke et al. 2021. *ACS ES&T Water.*

Challenges of modeling PFAS adsorption to design for minimal process costs

In a straightforward workflow:

- Define PFAS species (i.e., PFOA, PFOS, etc.) for treatment based on EPA regulations
- Select a model and use literature or regression of breakthrough data to parameterize that model
- Use model results to select the most cost-effective technology for design



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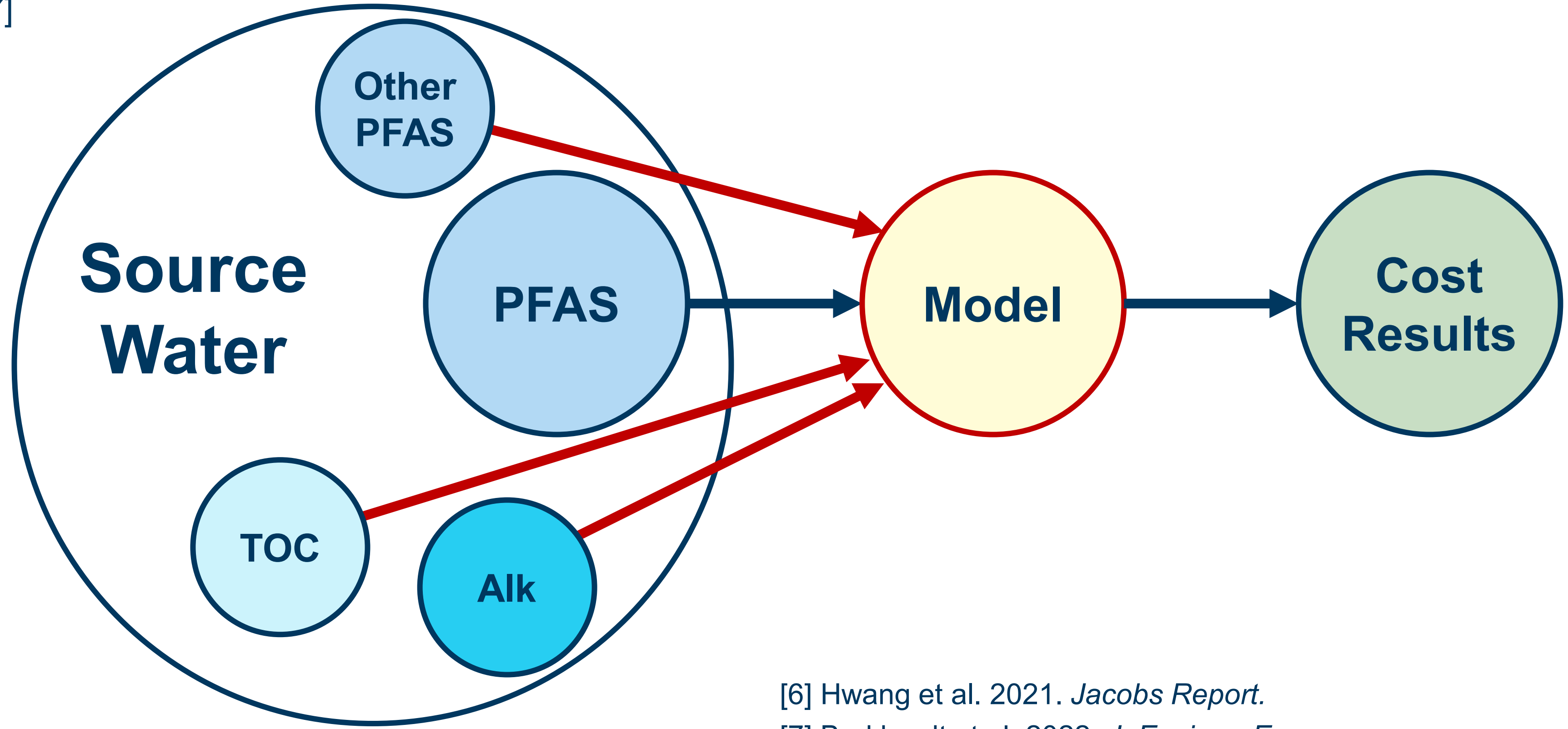
Challenges of modeling PFAS adsorption to design for minimal process costs

Current predictive models have low accuracy for PFAS adsorption

- Limited by low comprehension of PFAS adsorption mechanisms, background components influence, and low PFAS concentrations

The amount of data available is insufficient to develop new models or train surrogate models[6,7]



[6] Hwang et al. 2021. *Jacobs Report.*
[7] Burkhardt et al. 2022. *J. Environ. Eng.*

Objectives for this analysis

Employ available data to parameterize simplified models that **accurately simulates PFAS adsorption by GAC and IX technologies**

Statistically characterize the parameterization and generate corresponding economic results to evaluate and compare **cost distributions** of treatment by GAC and IX technologies

Present the methods for GAC and a simple example for the comparison GAC and IX economic results

WaterTAP’s GAC model features

GAC is simulated using the constant pattern homogeneous surface diffusion model (CPHSDM)

Assumptions:

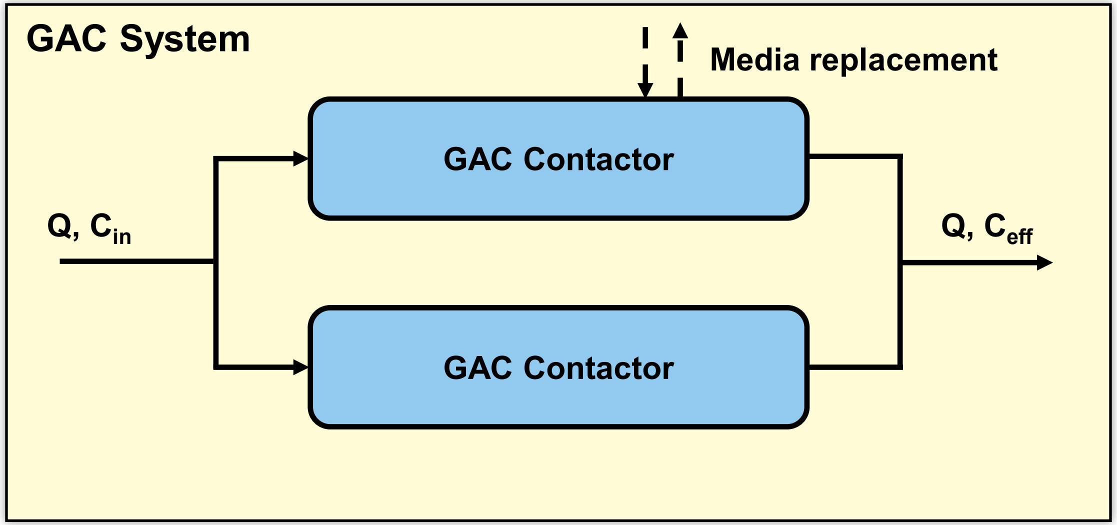
- Single species adsorption

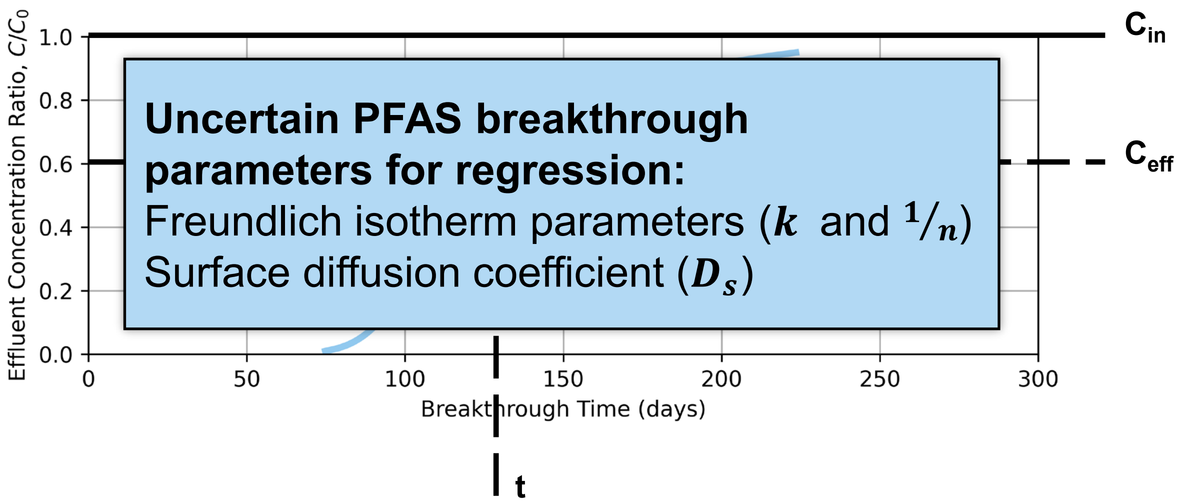
Inputs:

- Contactor design and configuration
- GAC media properties
- Influent conditions (Q, C_{in})
- Effluent target concentration
- **Breakthrough governing parameters**

Outputs:

- Breakthrough time
- Capital and operating costs





Breakthrough data availability and parameter fitting with Pyomo's parameter estimation

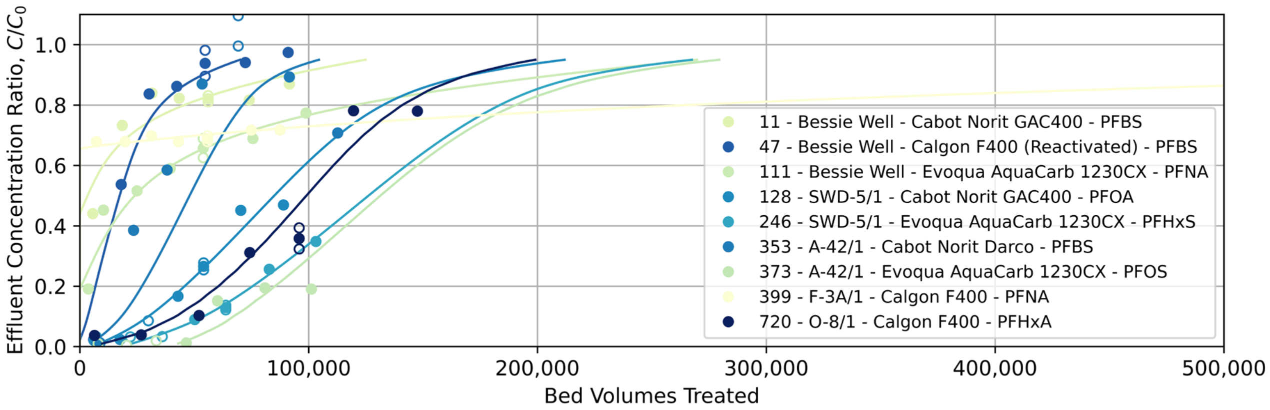
Rapid small-scale column test (RSSCT) data was made available by the teams at Orange County Water District (OCWD) and Jacob's[4]

- 864 breakthrough profiles
- 18 monitored species
- 11 GAC media
- 11 feedwater compositions

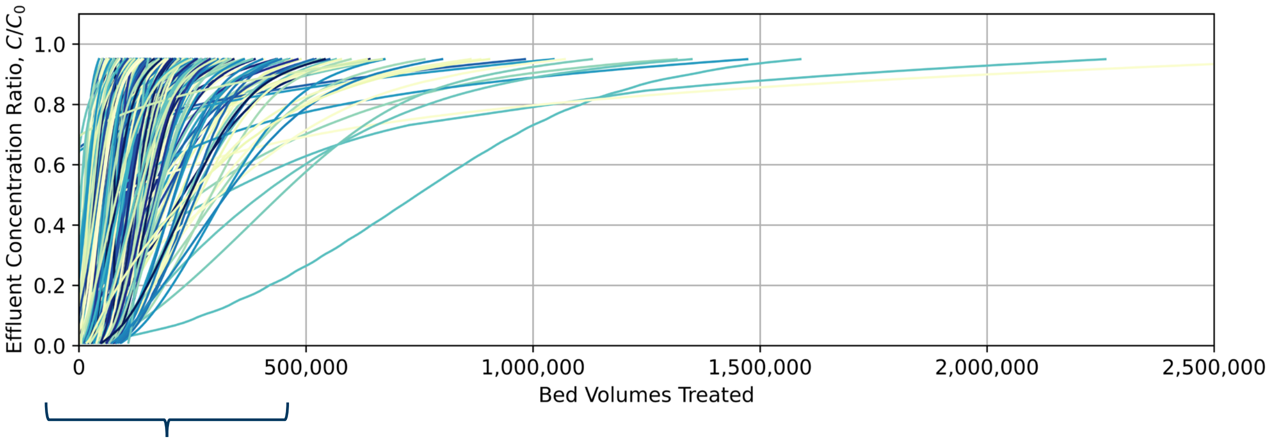
$\boldsymbol{k}$, $^{1}/_{n}$, and $\boldsymbol{D_s}$ **parameter estimation in Pyomo (*parmest*)**[9]

- Data filtering based on smoothness and omitting asymptotic regions
- Solved in WaterTAP at RSSCT scale with custom initialization and scaling

Subset of cases showing original data, filtered data, and regression



Regression of all cases shown at a larger BVT scale (x-axis)



Scale of subset

[4] Hwang et al. 2021. *Jacobs Report.*
[9] Klise et al. 2019. *Comput. Aided Chem. Eng.*

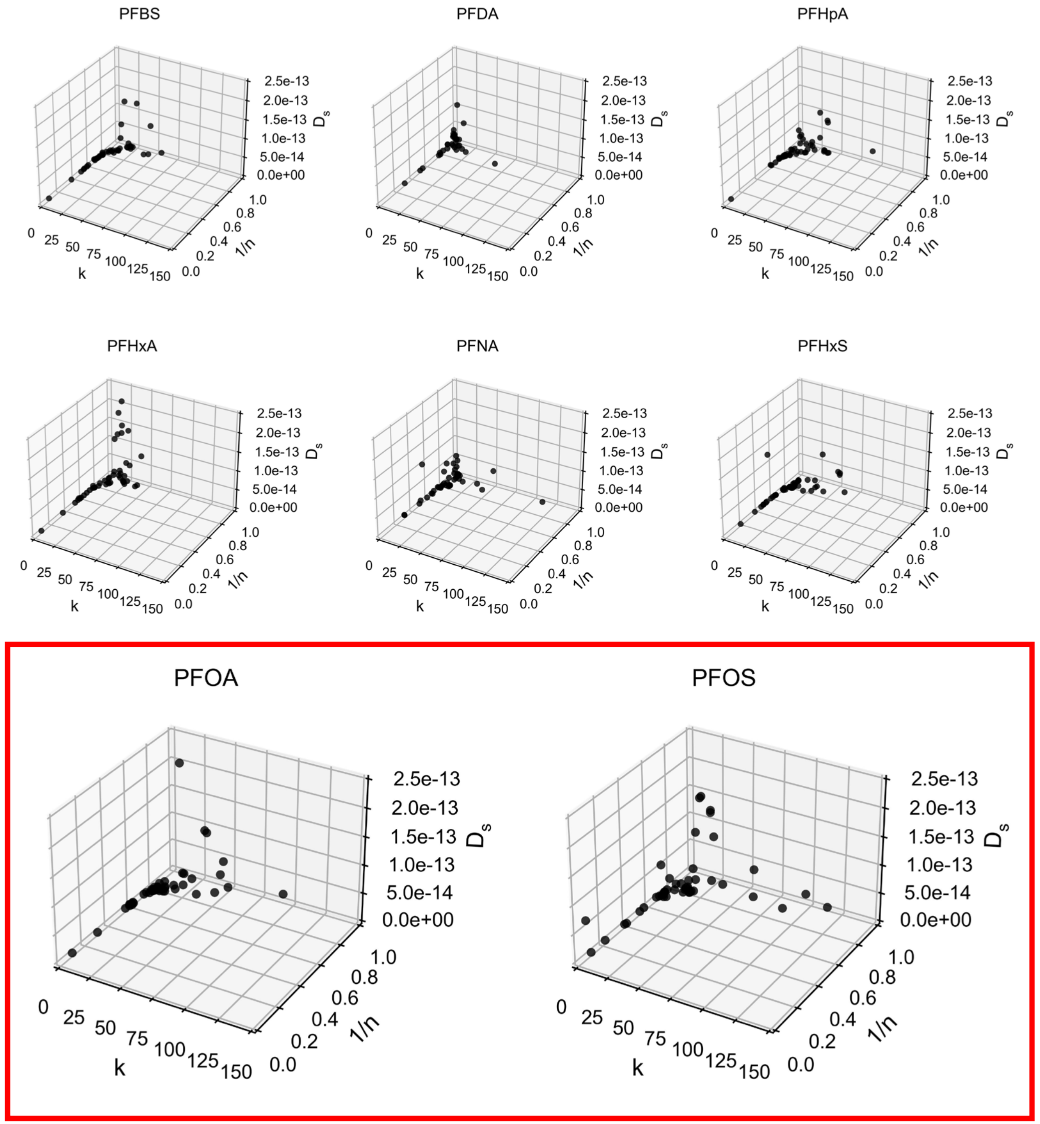
Assumptions when using regressed parameters

A set of regressed parameters is obtained for each species

Key assumptions for analysis

- The parameters are **scalable**
- The variability of parameters represents the **influence of factors not included in the model**
- The regressed parameter sets contain **enough samples to sufficiently represent expected source waters**

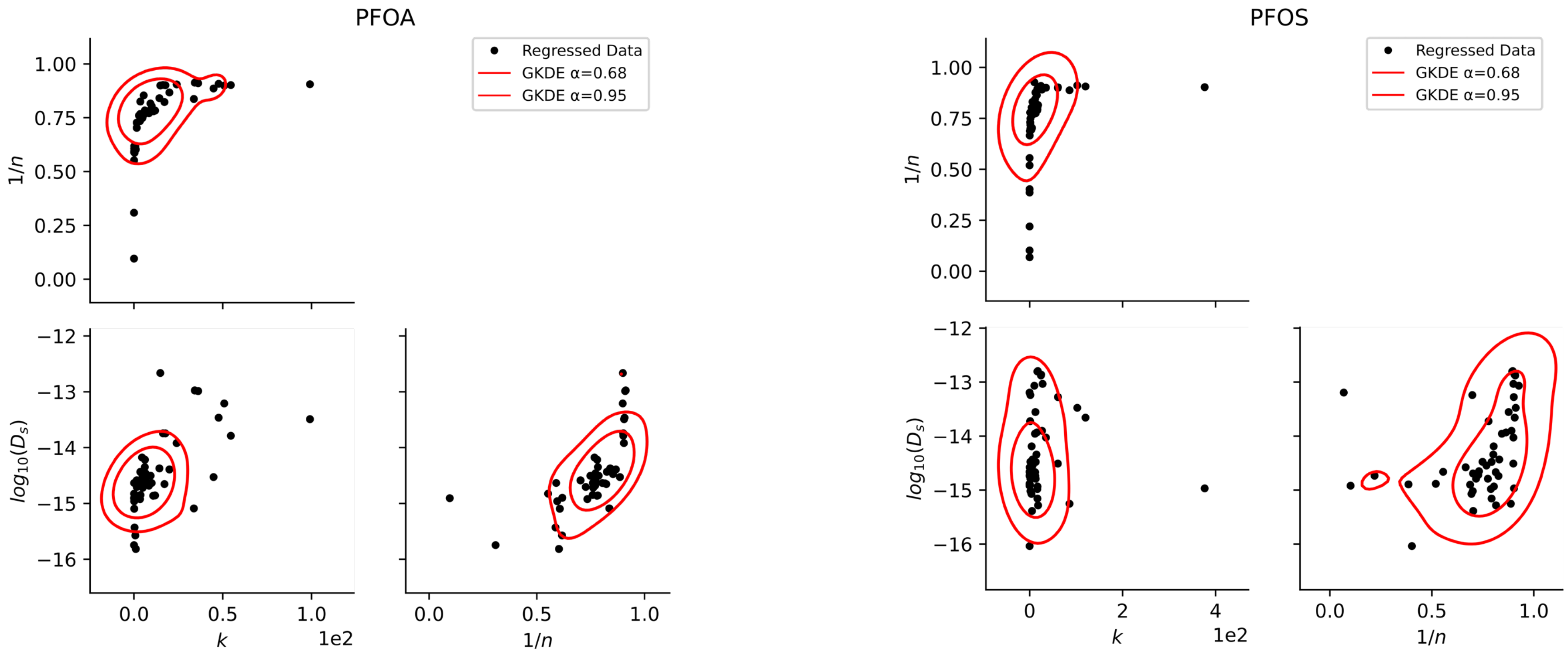
Further methods and results shown for PFOA and PFOS



Generalizing the regressed parameters through probability density functions

The parameter distribution is characterized through a **probability density function (PDF)**

- Train multivariate **Gaussian kernel density estimations (GKDE)** using ***SciPy*[10]**
- Resample the PDF if any parameter exceeds its bounds



Simulating and sampling for economic results

Specify GAC system design and sample regressed parameters (1,000 samples) for simulation

Fixed Variable	Value	
Influent flowrate	1	MGD
Influent concentration	10	ng/L
Effluent concentration at breakthrough	4	ng/L
Media apparent density	540	kg/m^3
Media particle diameter	1	mm
Empty Bed Contact Time	15	min
Bed voidage	0.4	-
Superficial velocity	8	m/h
Operating contactors	2	-
Redundant contactors	1	-
Fraction of spent media regenerated	0	-
Freundlich isotherm parameter k	**Sampled**	
Freundlich isotherm parameter 1/n		
Surface diffusion coefficient D_s		

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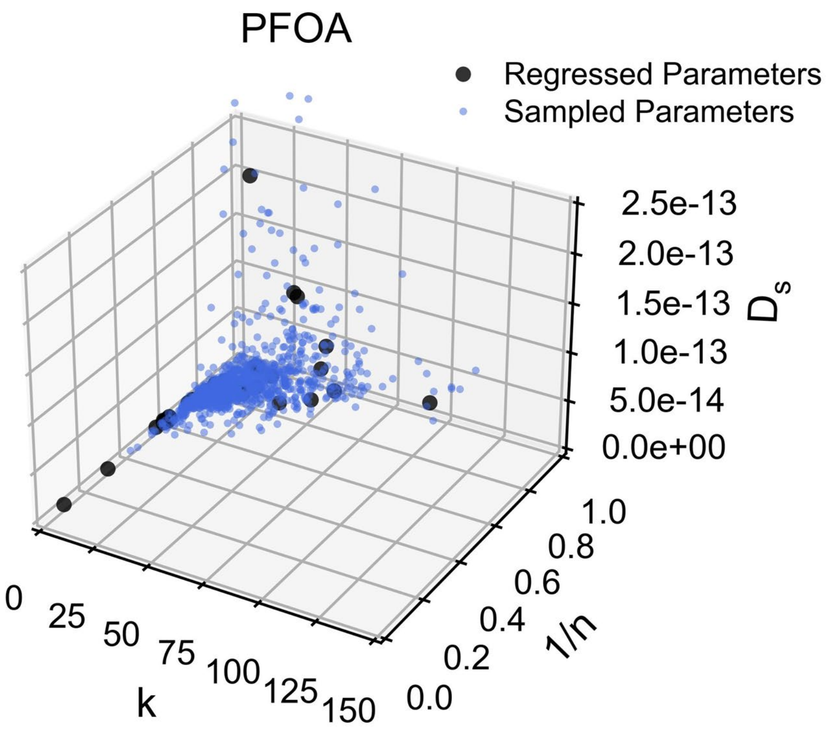

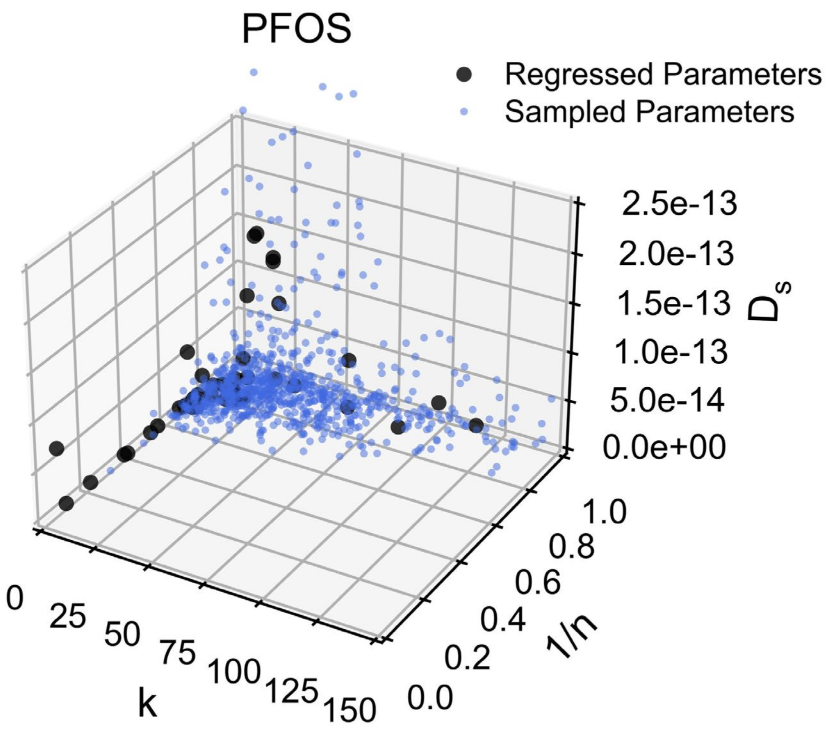

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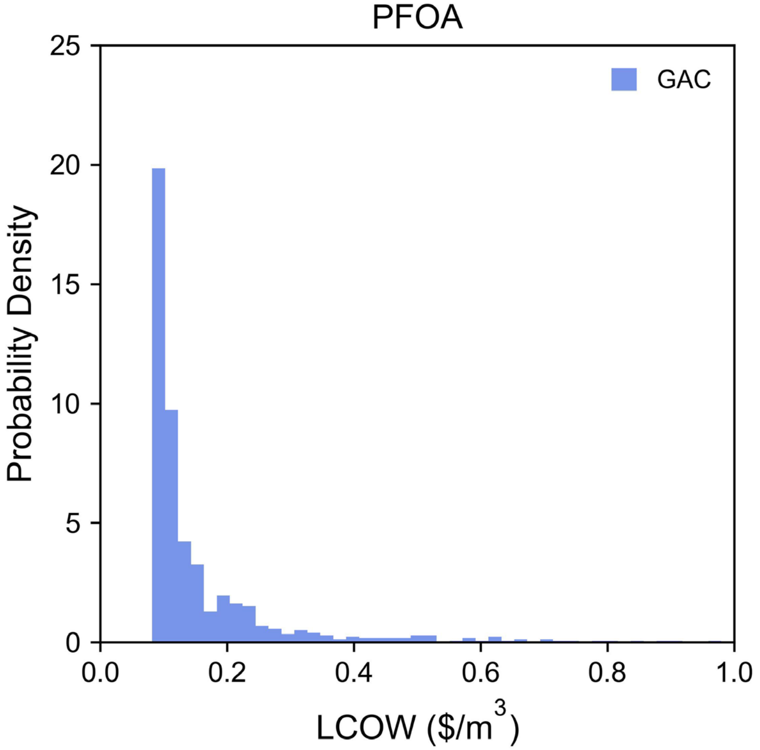

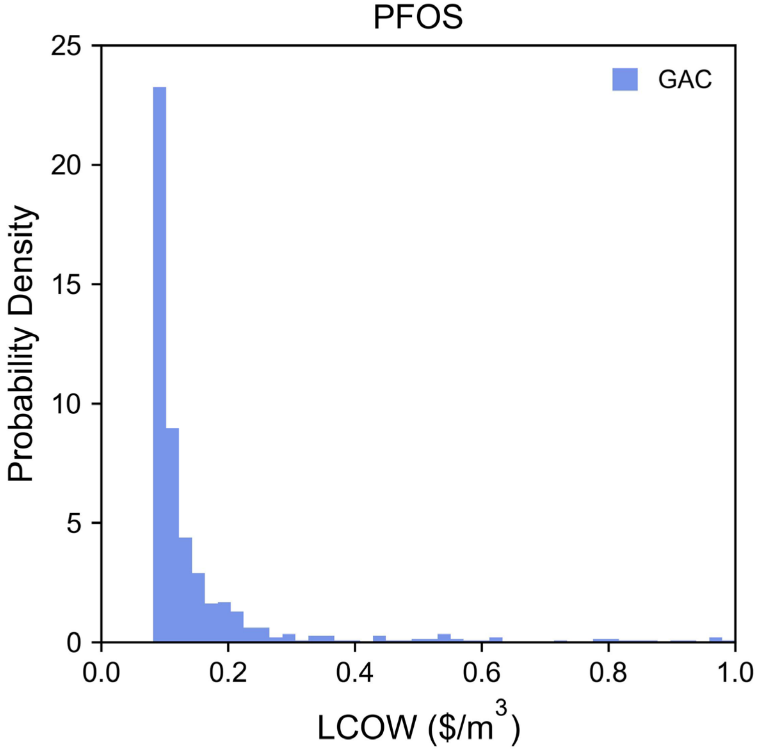

Comparison of GAC and IX results by PFAS species

Compare GAC and IX **process costs and cost variability** for the same conditions (with different designs)

Fixed Variable	Value	
Influent flowrate	1	MGD
Influent concentration	10	ng/L
Effluent concentration at breakthrough	4	ng/L

The methods for IX are not identical, but are **based on the same principles**

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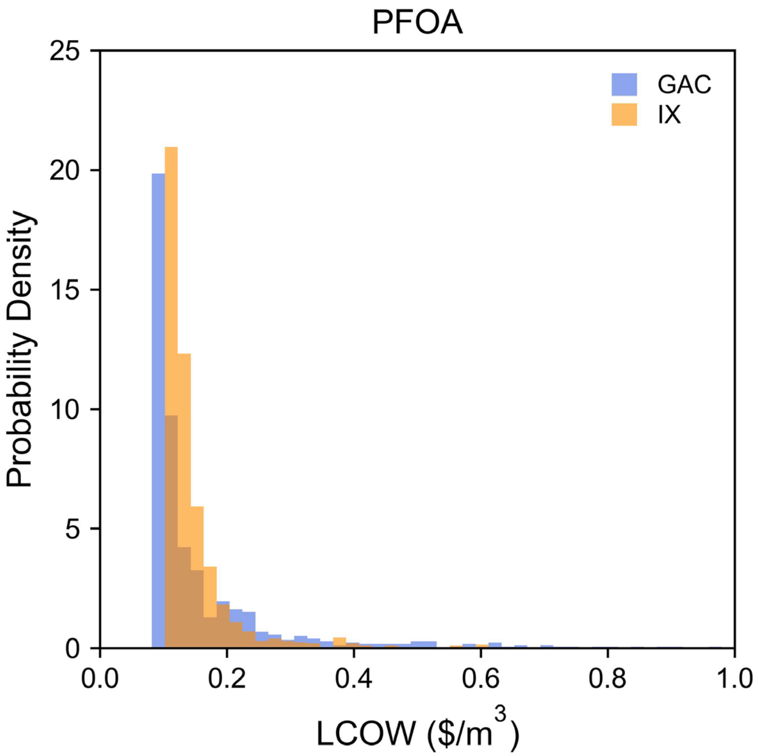

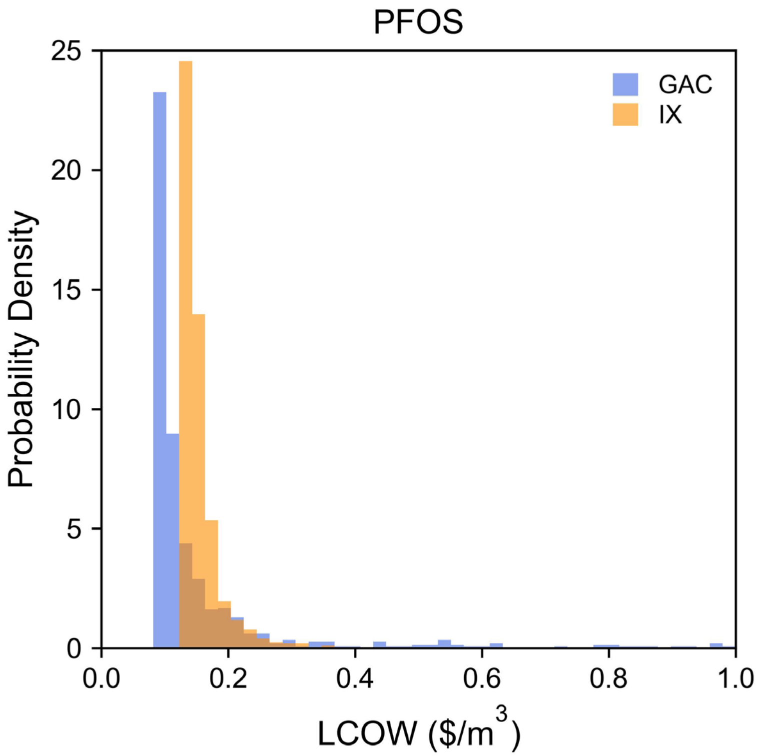

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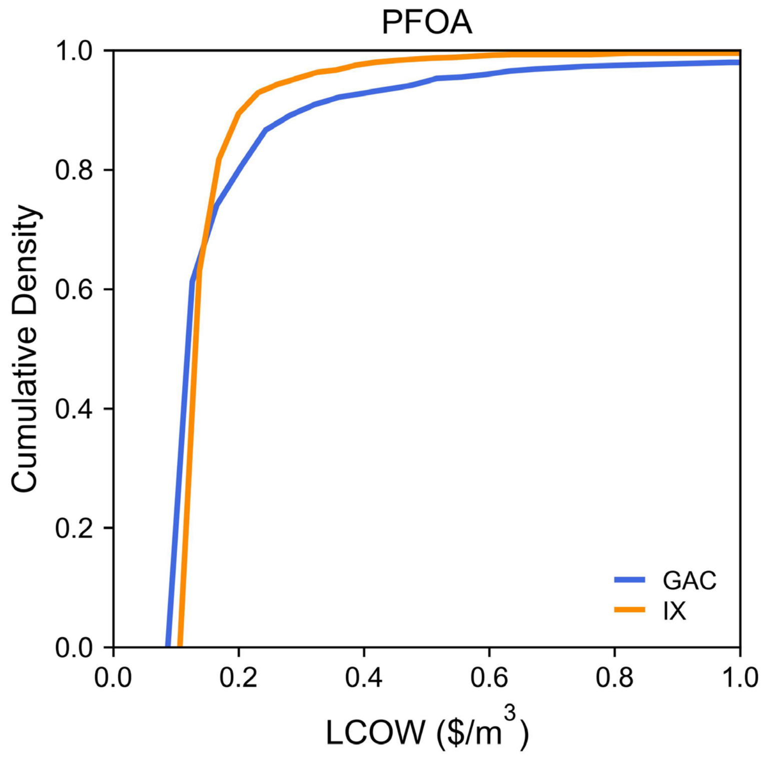
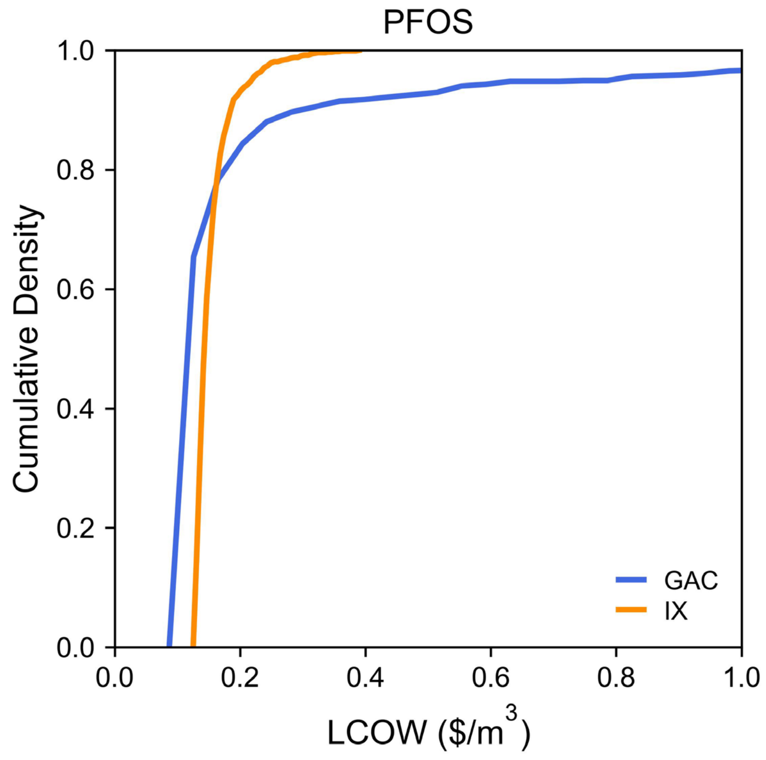
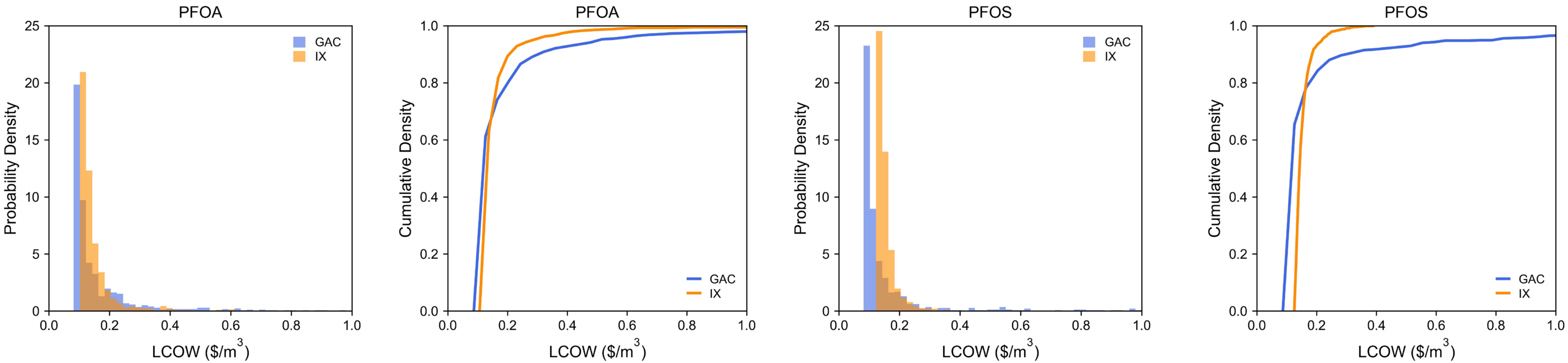




Comparison of GAC and IX results by PFAS species

Simple example comparing GAC and IX for PFOA and PFOS treatment

- **PFOA and PFOS have relatively equal costs for removal** as limiting adsorbed species
- **IX has marginally less variability in costs** under uncertain source water conditions
- Minimum costs are fixed by the initial capital costs, where **GAC is lower**



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Expanding the methodology for other analyses

Compare GAC and IX cost distributions for all species, **specifically those which may be a tipping point for technology selection**

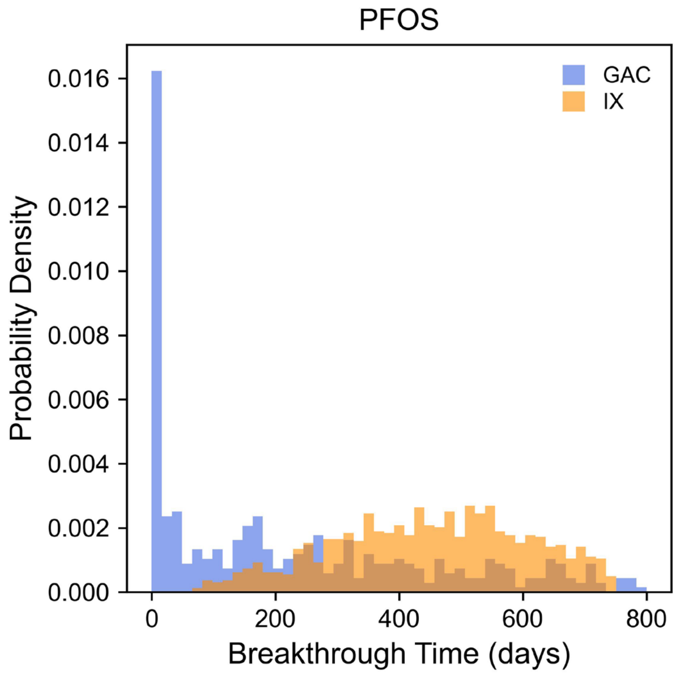
Assess cost distributions to include variable operating conditions

- Variable influent concentrations and flow rates of source waters
- **Decreasing MCLs** for PFAS species (effluent concentrations)

Compare GAC and IX systems for **technical factors**

- Time to breakthrough
- Mass intensity (replacement and disposal rates)
- Footprint

Optimize adsorption system design



Summary

Current adsorption models are insufficient for predictive modeling of PFAS treatment and adsorption data is limited

The statistical methodology used **may approximate costs and guide technology selection** for full-scale adsorption PFAS treatment systems

These analyses are performed and supported by the following team of collaborators working on preparing these analyses for publication

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Questions