Hot Water, Cold Reality: Experimental Analysis of Sorption Constraints in Iodine Filtration Media Under Heated-Water Conditions

Rogelio Garcia Fernandez*, **Mary Lou Nadeau**†, **Phillip Hicks***, **Jaione Romero Mangado***, **Michael Callahan**‡

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What?

A potential risk has been identified in potable water systems: insufficient biocide levels may occur when iodine removal technology is installed upstream rather than at terminal dispensing points, as in the ISS Potable Water Dispenser. This risk grows in relevance for future exploration architectures with dormant water lines.

Why?

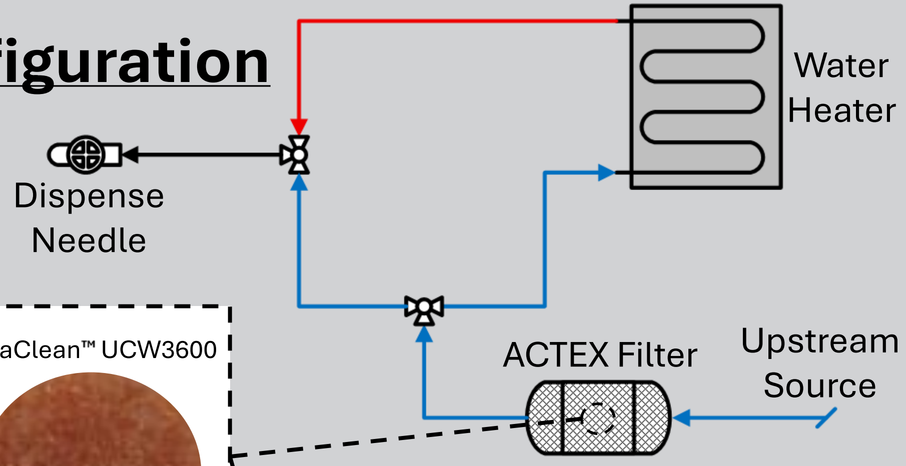
Current iodine-removal media are not recommended for elevated-temperature water, and thermal limitations may degrade performance. To ensure effective iodine removal, systems position the media upstream where water remains at ambient temperature.

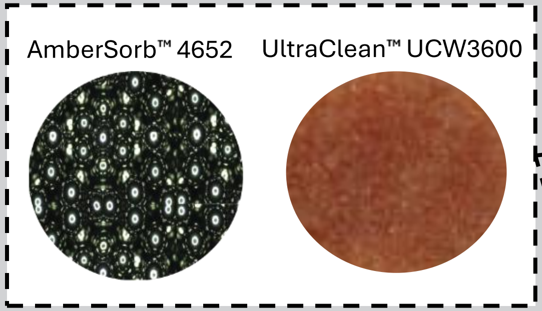
How?

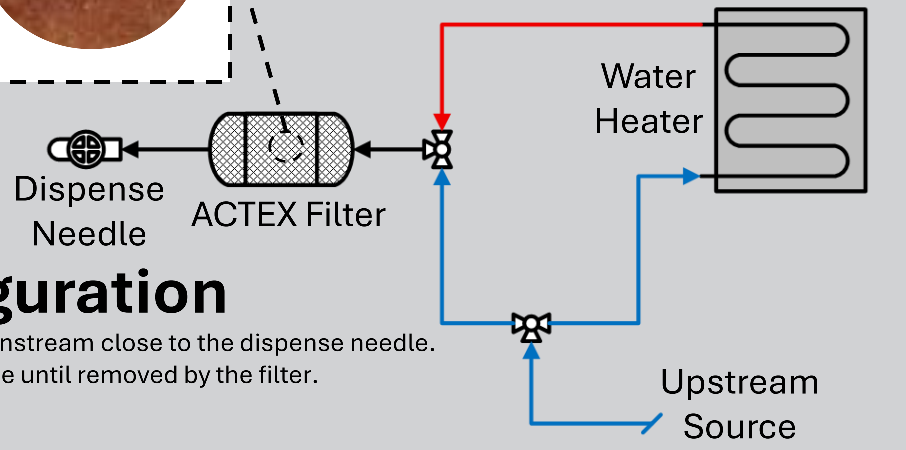
This study evaluates whether state-of-the-art iodine-adsorption materials truly exhibit the reported thermal limitations and whether these effects propagate to potable dispenser operations. Batch adsorption tests at heated and ambient conditions provide the first experimental data quantifying this risk.

PWD Configuration

- Iodine is removed upstream.
- Water in ambient and hot legs do not contain biocide.







Alt. Configuration

- Iodine is removed downstream close to the dispense needle.
- All lines contain biocide until removed by the filter.

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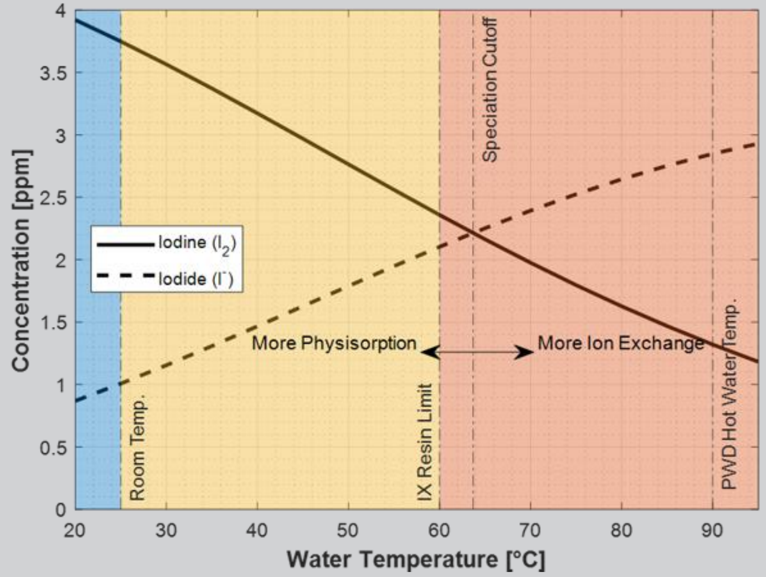
Iodine Speciation and Temperature Effects

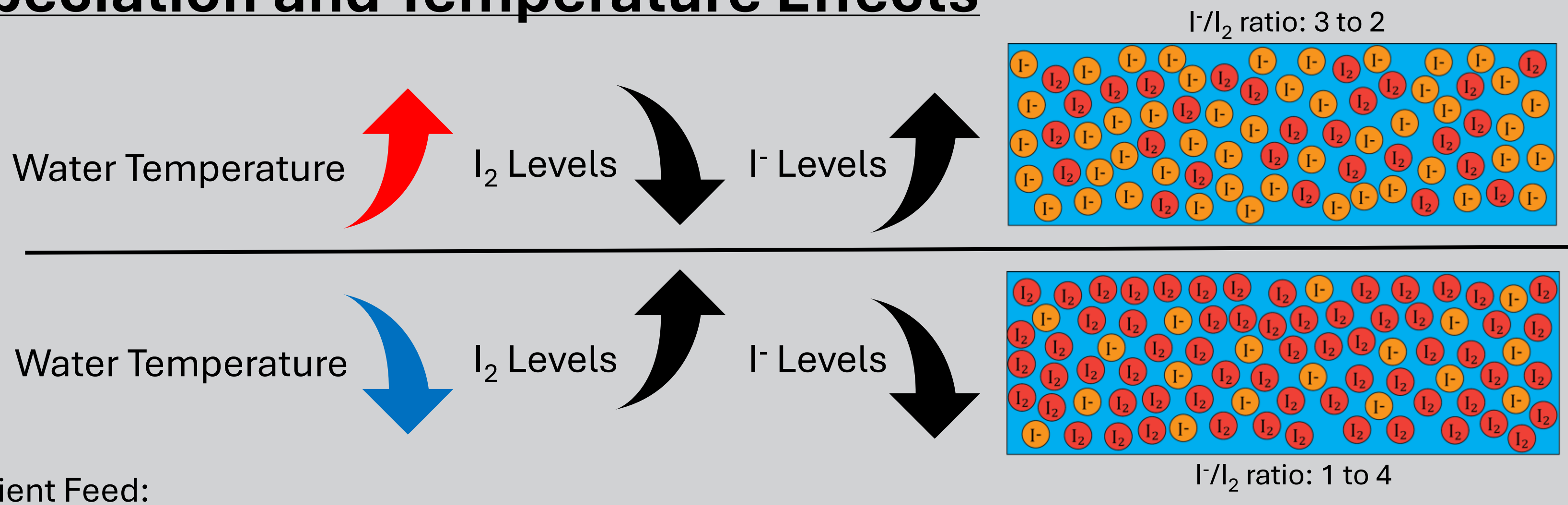
Iodine (I_2) Hydrolysis Reaction

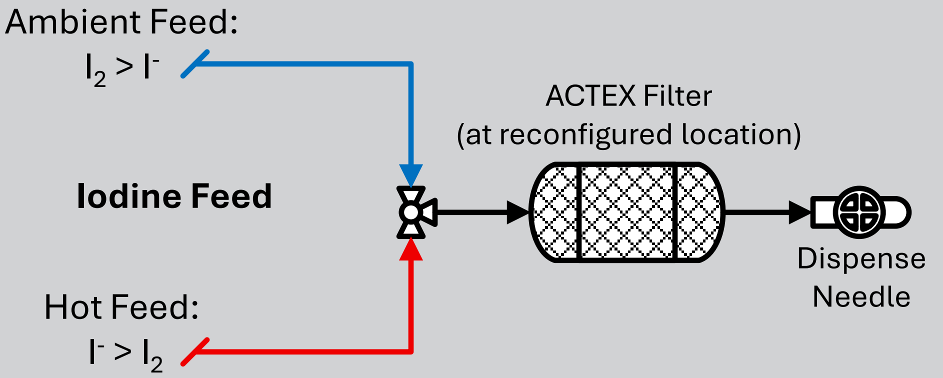
$$I_2 + H_2O \rightleftharpoons HOI^- + I^- + H^+$$

Temperature Effect on Speciation of 5 mg/L Iodine in Water.



Predicted via e-NRTL thermodynamic package.





Considerations

- Hydrolysis, ionic formation, and pH-shift are coupled processes.
- The filtration media formulation depends on the iodine specification in the upstream feed.
- The current IX/GAC ratio might not be optimal to process ambient and hot feeds.

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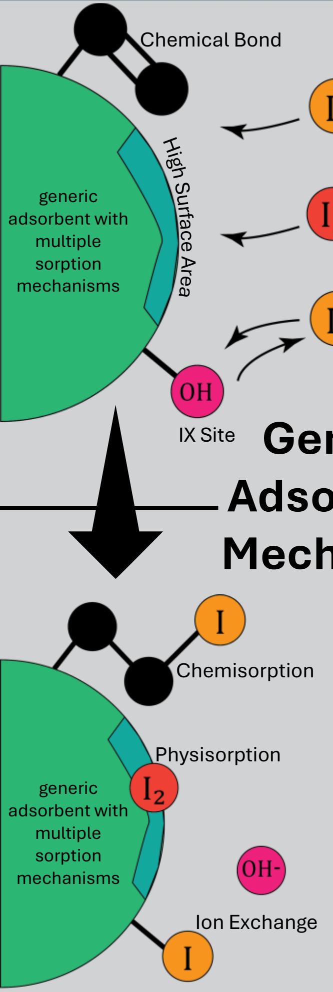
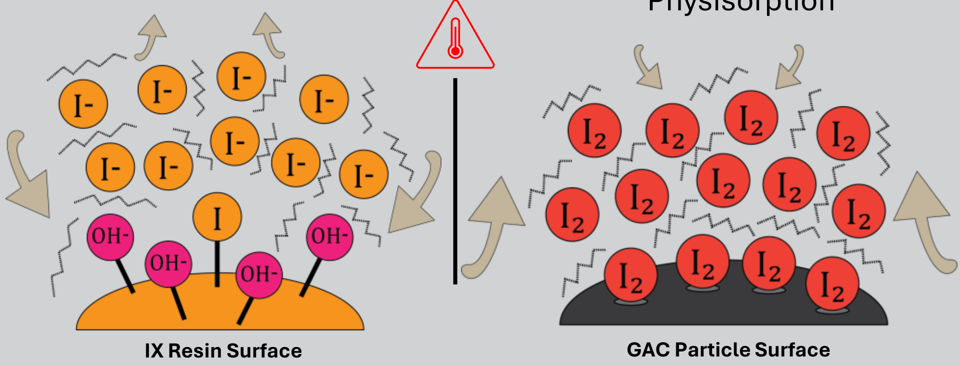


General Adsorption Mechanism

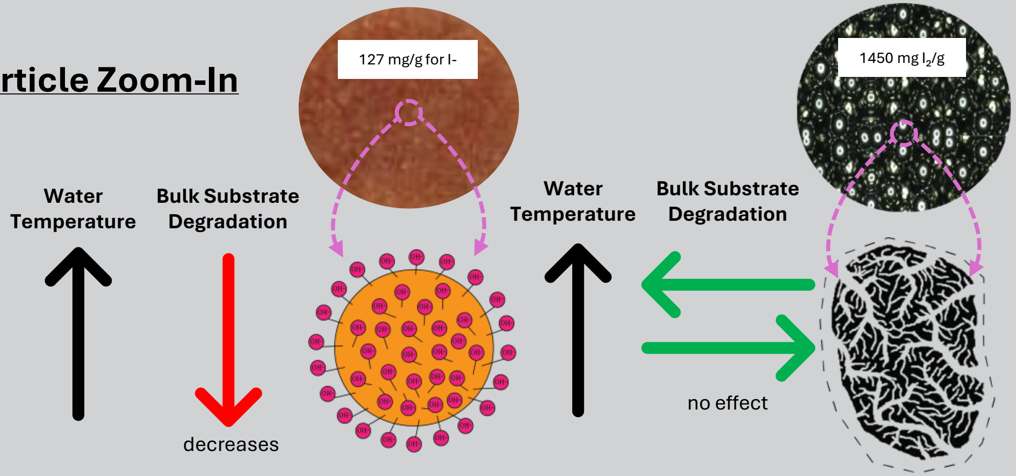
Sorption Mechanisms and ACTEX Media Behavior

Potential Impact of Hot Water on ACTEX Filtration Media

Iodine Sorbent	*UltraClean™ UCW3600*	*AmberSorb™ 4652*
Matrix Material	*polystyrene–divinylbenzene*	*carbon*
Targeted Iodine Species	I^-	I_2
Speciation-Capacity Consideration	*more ionic iodine is present in water at 90°C*	*less molecular iodine is present in water at 90°C*
Sorption Effect	*IX is enhanced with temperature increase*	*physisorption diminish with temperature increase*
Thermal Effect	*matrix material and IX sites likely to degrade above 60°C*	*matrix is not impacted*



Particle Zoom-In



Considerations

- Filtration media components rely on different iodine adsorption mechanisms which proceed differently to thermal changes.
- While higher thermal conditions do not physically affect the dense phase of the GAC material, the IX resin might be susceptible to material degradation after expected periods.
- Adsorption capacity of the SOA filtration media must be sustained at higher water temperatures to main the same configuration. Otherwise, reformulation or re-sizing will be needed to accommodate new thermal condition.

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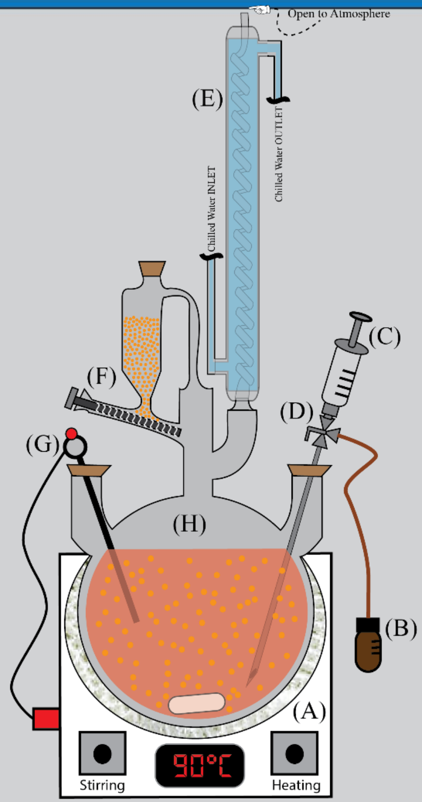


Experimental Apparatus. *(A) Heating Mantle; (B) Sample Vial; (C) Withdrawal Glass Syringe; (D) Three-way Stopcock Valve; (E) Graham Condenser; (F) Air-tight Solid-dispensing Funnel; (G) Thermocouple; (H) One-liter Glass Flask.*

Batch Experimental Setup & Rationale

Equilibrium capacity provides a clear, comparable measure of an adsorbent's intrinsic uptake performance.

Test Matrix

Test Item	Adsorbent Loading [mg] Room Temp. Test/ Hot Temp. Test
1	50
2	100
3	400
4	800
5	1600

$$q_{eq,I_2} = \frac{\left(c_{0,I_2} - c_{eq,I_2}\right)V_0}{m_{abs}} [=] {}^{mg}/_{g}$$

Where:

c_{0,I_2}: *total* I_2 *concentration, [mg/L]*

c_{eq,I_2}: *total* I_2 *equilibrium concentration, [mg/L]*

V_0: *batch volume, [L]*

m_{abs}: *added adsorbent amount, [g]*

Stirred batch tests offer rapid, low-cost screening

Tightly controlled mixing and temperature

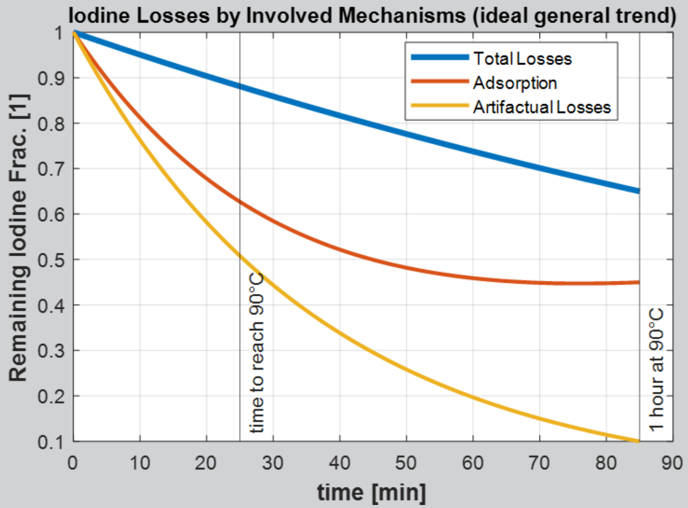
stirred batch adsorption testing

Equilibrium measurements are more straightforward

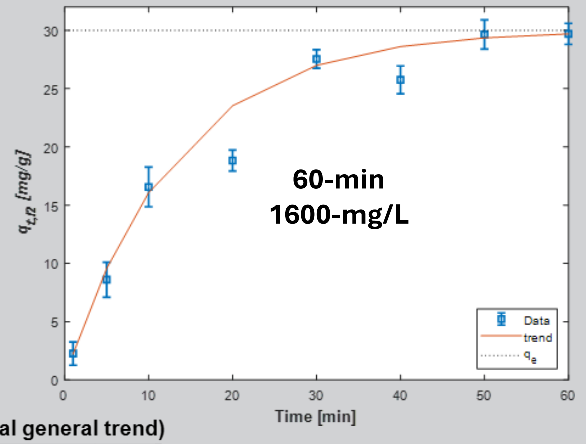
Simplified setup enables fast experimental turnaround

Adjustment of Concentration Measurements

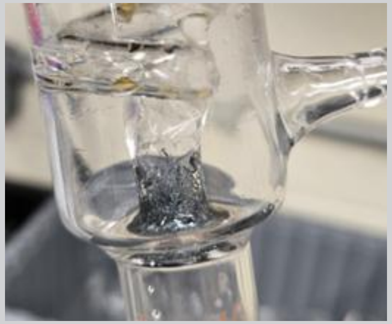
$$\hat{c}_{I_2}^{end} = c_{I_2}^{end}\left(1 - \delta_{I_2}^{loss}\right)$$



Total Contact Time



Iodine Vapor Crystallization



Condenser Inlet

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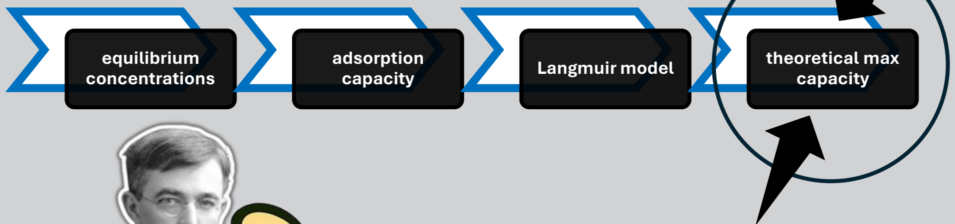
Data Processing and Dimensionless Analysis

Data Processing Scheme



$$q_{e,I_2} = \frac{k_L q_{max,I_2} c_{e,I_2}}{1 + k_L c_{e,I_2}}$$

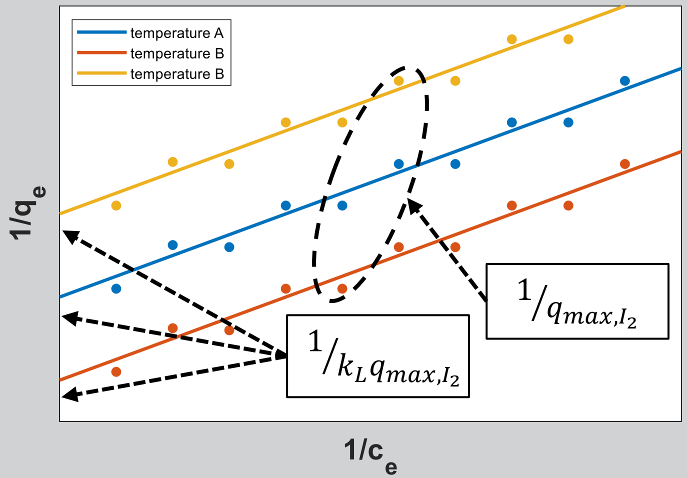
Linearization

$$\frac{1}{q_{e,I_2}} = \left(\frac{1}{k_L q_{max,I_2}}\right)\left(\frac{1}{c_{e,I_2}}\right) + \frac{1}{q_{max,I_2}}$$

The Langmuir model describes how adsorbate loading approaches a monolayer limit q_{max}, while the affinity parameter k_L changes with temperature and governs the concentration-dependent shape of the isotherm.

Where:
q_{e,I_2}: *equilibrium iodine adsorption capacity, [mg/g]*
c_{e,I_2}: *equilibrium iodine concentration, [mg/L]*
k_L: *Langmuir constant, [L/mg]*
q_{max,I_2}: *maximum iodine adsorption capacity*

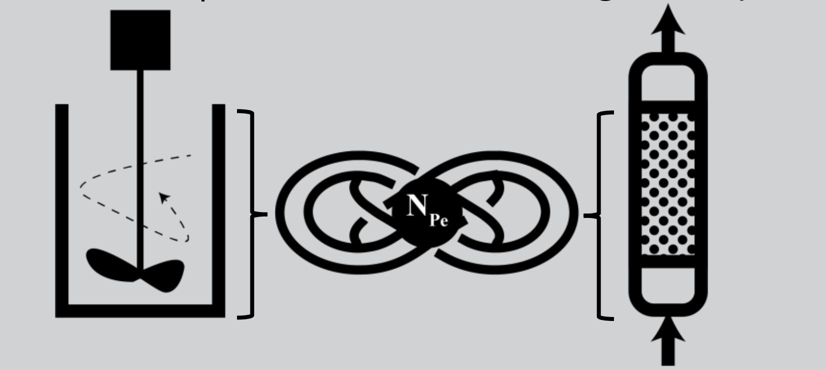
Ideal Linearized Isotherm Behavior



$$N_{Pe} = \frac{uL}{D_{I_2}} = \frac{\pi N d^2}{D_{I_2}} [=] 1$$

Where:
u: fluid velocity, [m/s]
L: characteristic length, [m]
D_{I_2}: *I_2 diffusion coefficient in water, [m²/s]*
N: rotational speed, [rev/s]
d: stirrer diameter, [m]

Applying the Peclet Number as a Scaling Framework for Mapping Batch Adsorption Data to Plug-Flow Systems



This Peclet-based scaling framework provides physical continuity by preserving the underlying transport relationships when translating from batch measurements to plug-flow operation.

$$\frac{N_{Pe}\varepsilon D_{I_2}}{L_b} = u_b$$

Where:
u_b: *avg. bed fluid velocity, [m/s]*
L_b: *bed length, [m]*
ε: *rotational speed, [rev/s]*

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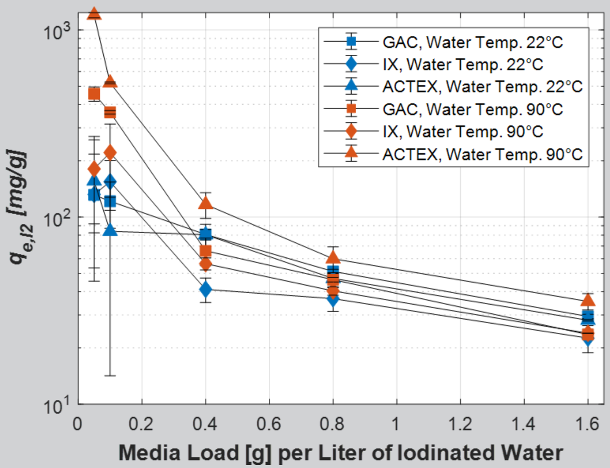
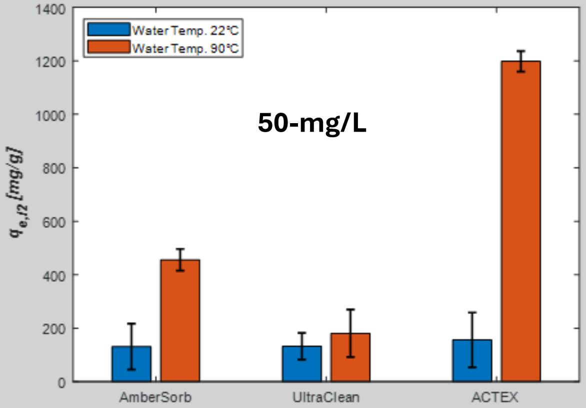
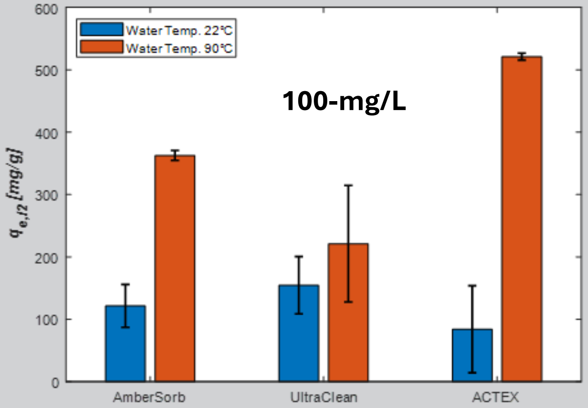
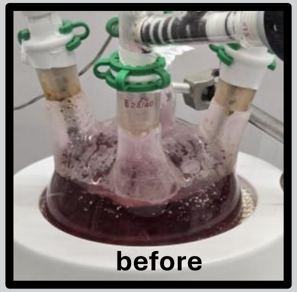
Equilibrium Results & Temperature Effects on Each Sorbent

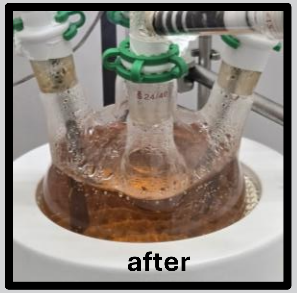


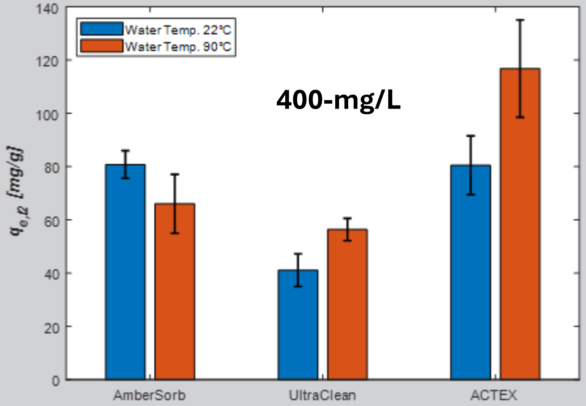


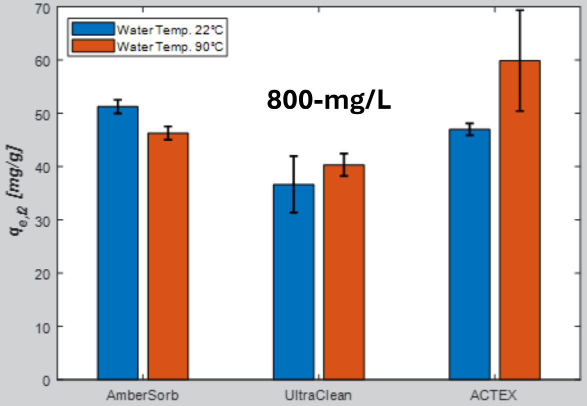


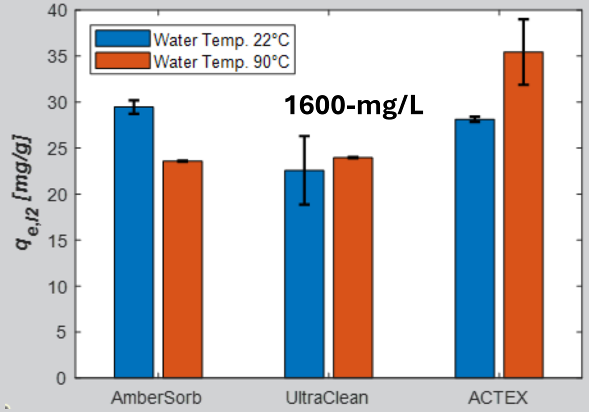
heated experiments











Key Points

- IX Resin: Slight ↑ capacity at 90 °C (thermokinetic enhancement).
- GAC: ↓ capacity at 90 °C (physisorption weakened).
- ACTEX: ↑ capacity dominated by IX resin's trend.
- High-load data most reliable; low-load heating artifacts.

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N_{Pe} Scaling & Langmuir Fits

N_{Pe} System Characterization

Parameter, [unit]	Units	Parameter	Value	Equation/Notes
		Batch Process		
I_2 diffusion coefficient in water	[m²/s]	D_I2	1.00E-09	I_2 in water
stirrer rotational speed	[rpm]	N_rpm	250	
stirrer rotational speed	[rev/s]	N_rps	4	=N_rpm/60
stirrer diameter	[m]	d_st	0.03	
batch Péclet number	[1]	Nb_Pe	1.18E+07	=(PI()*N_rps*d_st^2)/D_I2
		Assumed Flowthrough Process		
bed diameter	[in]	Dь_in	1.62	[17]
bed diameter	[m]	Dь_m	0.041	=Dь_in/39.3701
nominal bed flow rate	[mL/min]	Qь_mlpmin	1059	
nominal bed flow rate	[m3/s]	Qь	1.77E-05	=Qь_mlpmin/60000000
bed nominal fluid velocity	[m/s]	vь	1.33E-02	=Qь/(PI()*(Dь_m/2)^2)
bed length	[in]	Lь_in	10.5	[17]
bed length	[m]	Lь_m	0.267	=Lь_in/39.3701
media void fraction	[1]	ε	0.3	educated guess
plug flow Péclet Number	[1]	Nf_Pe	1.18E+07	=(vь*Lь_m)/(ε*D_I2)

Key Points

- N_{Pe} links hydrodynamics across test platforms.
- $N_{Pe} \gg 1$ → advective transport dominates.
- Batch results become predictive only when N_{Pe} alignment is maintained.
- Linear velocity for columns must be set via N_{Pe}, not intuition.
- N_{Pe} independent of iodine concentration or media mass.

Summary of Estimated Langmuir Adsorption Parameters and Associated Regression Statistics

Media	Data-point Input	Temp. [°C]	Max. Capacity [mg/g]	Langmuir Constant [L/mg]	R^2
AmberSorb™ 4652	single	22	77.406	0.2785	0.3043
AmberSorb™ 4652	averaged	22	135.418	0.0927	0.9661
AmberSorb™ 4652	single	90	279.852	0.1318	0.5911
AmberSorb™ 4652	averaged	90	549.366	0.0549	0.7216
UltraClean™ UCW3600	single	22	-573.320	-0.0021	0.4170
UltraClean™ UCW3600	averaged	22	-51.559	-0.0133	0.8432
UltraClean™ UCW3600	single	90	72.261	1.8475	0.6041
UltraClean™ UCW3600	averaged	90	81.584	1.2243	0.7207
ACTEX	single	22	35.982	4.0593	0.0001
ACTEX	averaged	22	147.635	0.0545	0.9357
ACTEX	single	90	86.652	-8.0488	0.0001
ACTEX	averaged	90	65.427	-0.3170	0.0294

Key Points

- Linearized Langmuir fits show low R^2 across all materials.
- Parameter values sometimes non-physical → caution required.
- Averaging improves R^2 but not underlying reliability.
- Equilibrium data trends more credible than regression outputs.
- Poor fits likely driven by low-mass normalization artifacts.
- Future work requires non-linear or alternative isotherm models.

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Conclusions & Forward Work for Future Water-System Design

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Key Findings

- Elevated temperature measurably **alters** iodine-removal behavior of ACTEX media.
- **UCW3600 (IX resin)**: slight performance improvement at 90 °C (thermokinetic enhancement).
- **AmberSorb 4652 (GAC)**: reduced capacity at 90 °C due to weakened physisorption.
- Combined ACTEX mixture **dominated** by IX behavior → slight thermal improvement overall.

Design & System-Level Implications

- Thermal effects + iodine speciation impose constraints on **placement** of iodine-removal units.
- GAC performance loss at high temperature raises concerns for **hot-water dispensing** architectures.
- Iodine mass-balance instability at elevated temperature highlights need for improved volatilization control.

Scientific Takeaways

- **Foundational link** established between temperature, speciation, and sorbent performance.
- Current ACTEX configuration adequate at ambient conditions but may not meet exploration-mission reliability **margins** under heated-water operation.

Future Work

- Transition from batch to **flow-through** testing with N_{Pe}-aligned scaling.
- High-fidelity **modeling** of temperature-dependent speciation and sorption kinetics.
- Evaluate **alternative or hybrid sorbents** with improved thermal robustness.
- Conduct **long-duration** thermal exposure studies to assess IX-resin durability.

Ultraclean™ UCW3600 at 🔥 💧

dense polymer bead ↑ susceptible to deterioration for long heated periods

slight performance increase, but smaller than ACTEX

AmberSorb™ 4652 at 🔥 💧

porous carbon structure ↓ less effective at removing ionic iodine

performance decrease

ACTEX Formulation at 🔥 💧

comprised of more IX resin than GAC ↑ media reformulation might be needed

slight performance increase

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