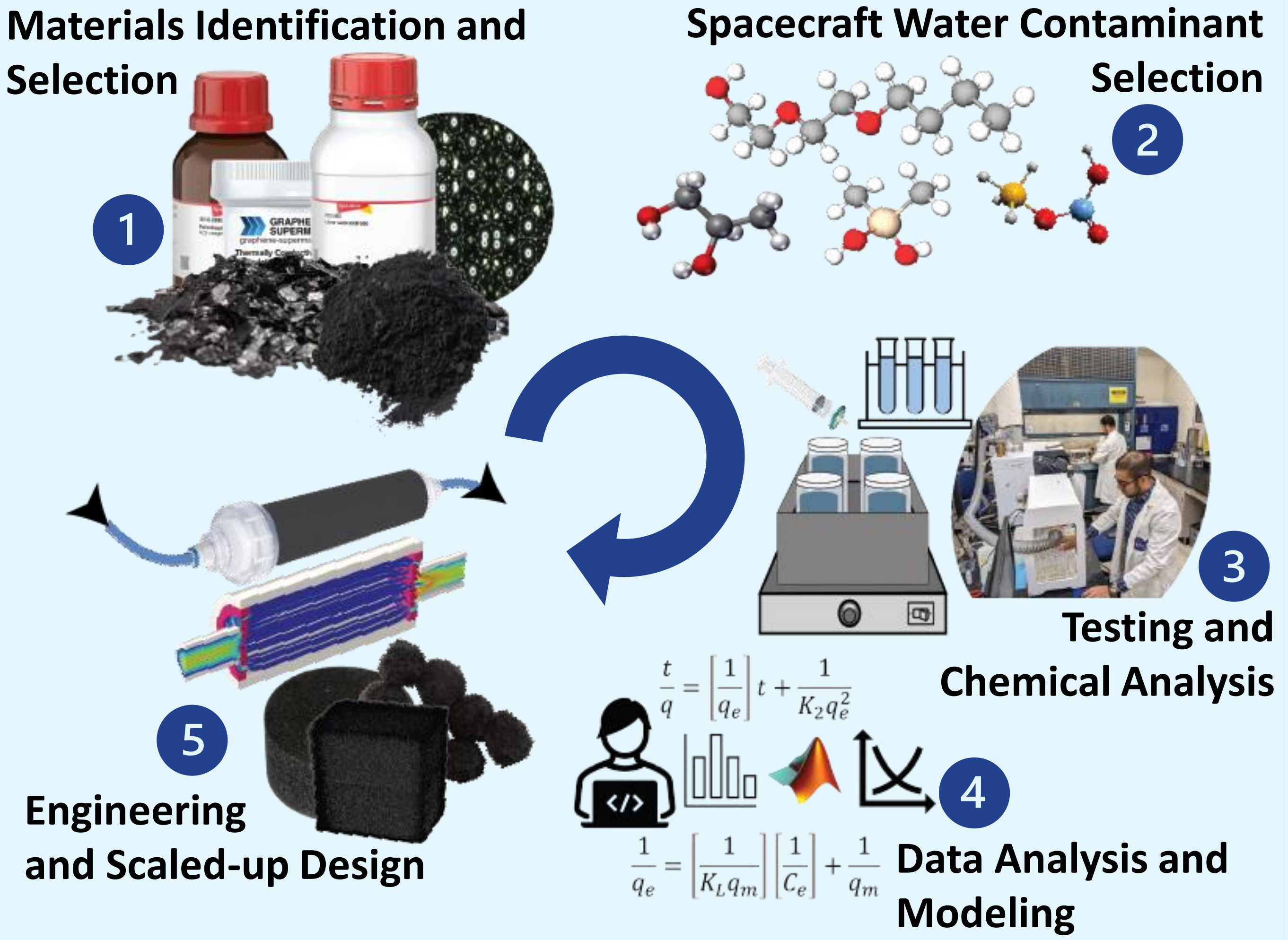
Graphene-based Filtration Media for Spacecraft Potable Water Systems: An Early Investigation - Rogelio Garcia Fernandez,* Michael Callahan,† Luke Gurtowski‡
JETS II Contract, NASA Life Support System Branch - Crew and Thermal System Division,† U.S. Army ERDC‡*

Johnson Space Center

What? The Promise of Graphene-based Materials (**GBMs**): High Surface Area and Chemical Affinity for Contaminant Adsorption.

Why? **GBMs** can help to close consumables gaps imposed by current SOA filtration media and improve filtration processes tailored for spacecraft operations.

How? By conducting scaled-down contaminant adsorption experiments, competitive **GBM** products can be initially identified and/or produced for tailored filtration processes in spacecraft water recovery operations.



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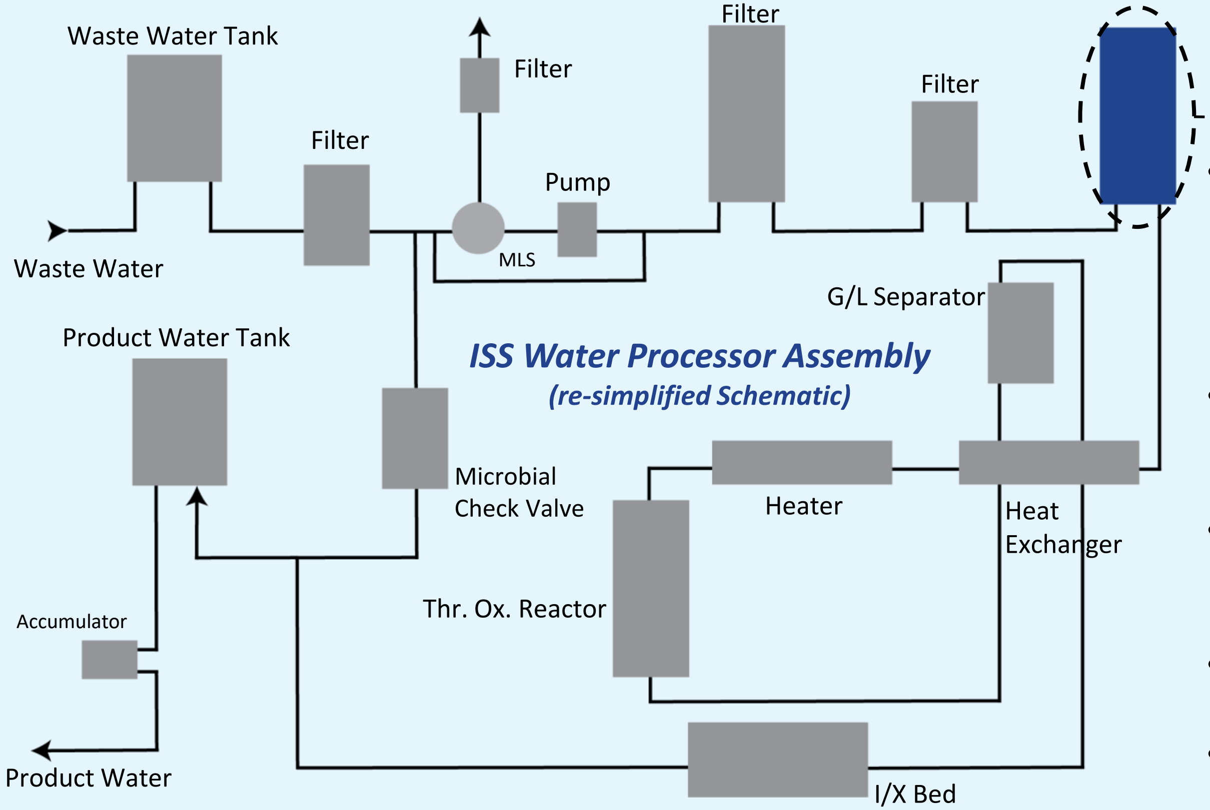
Graphene's Physical Properties

- Electron Mobility: ~200,000 cm²/Vs [1]
- Optical Transparency: ~97.4%[2]
- Specific Surface Area: up to 3300 m²/g [3]
- Thermal Conductivity: 3000-5000 Wm/K [4]
- Mechanical Strength: ~1.0 TPa [5]

Graphene's Adsorption Affinity

- Toxins
- Pharmaceuticals
- **Water-soluble organics**
- Volatile Compounds
- **Heavy Metals**
- Nuclear Waste constituents
- Oils
- Dyes

State-of-the-Art Spacecraft Water Recovery System



Multifiltration Bed

- Contains adsorbent and ion exchange media:
  - AmberSorb™ 4652.
  - AmberLite® IRN-150, IRN-77, or IRA67.
- Designed to ensure ionic breakthrough before non-volatile breakthrough.
- Considerable mass requirement for media, up to 14 kg.[6]
- ≥ One-year replacement cycle.[7]
- DMSD contaminant impacts filtration media's performance.

1. Zhang, Y., Tang, T.-T., Girit, C., et al. "Direct observation of a widely tunable bandgap in bilayer graphene," Nature, V. 459, No. 7248, 2009, pp. 820–3.
2. Blake, P., Brimicombe, P. D., Nair, R. R., et al. "Graphene-based liquid crystal device," Nano letters, V. 8, No. 6, 2008, pp. 1704–8.
3. Zhang, L., Zhang, F., Yang, X., et al. "Porous 3D graphene-based bulk materials with exceptional high surface area and excellent conductivity for supercapacitors," Scientific reports, V. 3, No. 1, 2013, p. 1408.
4. Booth, T. J., Blake, P., Nair, R. R., et al. "Macroscopic graphene membranes and their extraordinary stiffness," Nano letters, V. 8, No. 8, 2008, pp. 2442–6.
5. Kayatin, M. J., Carter, D. L., Schunk, R. G., et al. "Upgrades to the ISS water recovery system." International Conference on Environmental Systems. 2016.
6. Williamson, J., Gleich, A., and Wilson, J. "Status of ISS Water Management and Recovery," 2022.

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Typical Structure of Filtration Media Particle | Graphene Nanoplatelet

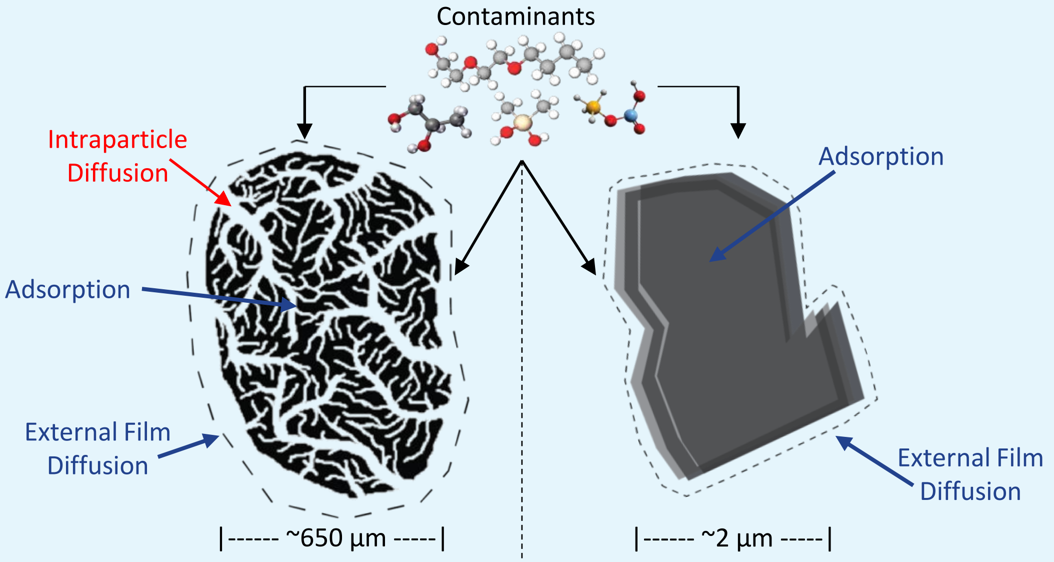

Table 1. Humidity Condensate Ersatz Recipe for Ground Testing[1] (Top-5 Spacecraft Water Contaminants)

Inorganic Compounds	*~ Conc. [mg/L]*	*Organic Compounds*	*~ Conc. [mg/L]*
Ammonium Bicarbonate	198.40	Ethanol	67.00
Zinc Acetate	15.00	DMSD	37.00
Ammonium Acetate	14.80	Propylene Glycol	27.00
Nickel Acetate	5.90	Methanol	6.50
Ammonium Formate	2.90	Benzyl Alcohol	1.50

Table 2. Identified Selection of Filtration Media

Graphene-based Materials	*SOTA/Commercial Adsorbents*
graphene nanoplatelets 750 m^2/g	Ambersep™ GT74 ★
graphene nanoplatelets 500 m^2/g	AmberSep™ IRC 748 UPS ★
graphene nanoplatelets 300 m^2/g	FiltraSorb™ 400 ★
granulated graphene	AmberSep™ 43600 ★
Chitosan-functionalized Graphene	AmberSorb™ 560 ★
	UltraClean™ UCW3600 ▲[2]
	AmberSorb™ 4652 ▲[3]
	AmberLite™ IRN 150 ▲[3]
	AmberLite™ IRN 78 ▲[3]
	AmberLite™ IRA 67 ▲[3]

★ Commercial product used in industries.

▲ Product used in ECLSS applications.

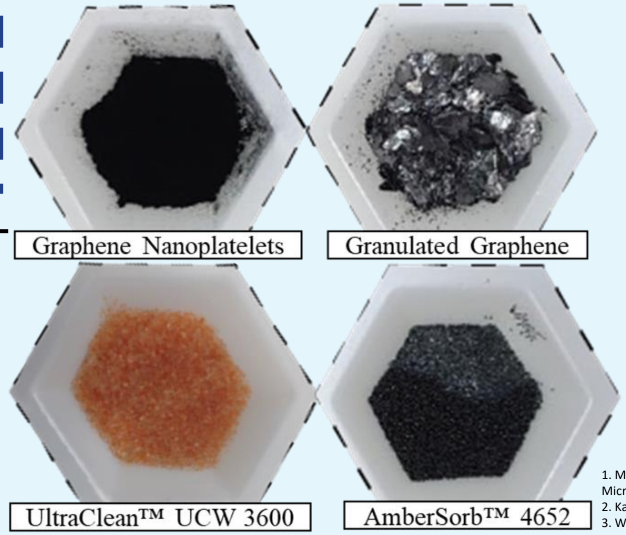

Table 3. Water Contaminant Selection

Adsorbate Solution	***Analyte***
Single Component	
Ethanol	TOC
Ammonium Bicarbonate	$NH4^+$, TIC
Propylene Glycol	TOC
Silver Fluoride	Ag^+
Iodine	I^-
DMSD	Si
2-(2-Butoxyethoxy)ethanol	TOC
Multicomponent	
Humidity Cond. Ersatz Solution	$NH4^+$, TOC, TIC

1. Muirhead, D., Moller, S., Adam, N., et al. "A Review of Baseline Assumptions and Ersatz Waste Streams for Partial Gravity Habitats and Orbiting Microgravity Habitats," 2022.
2. Kayatin, M. J., Carter, D. L., Schunk, R. G., et al. "Upgrades to the ISS water recovery system." International Conference on Environmental Systems. 2016.
3. Westhoff Larner, K., McPhail, C., and Romero, C. "Optimization of a Deionization Bed for an Oxygen Generator Assembly for Exploration Missions," 2022.

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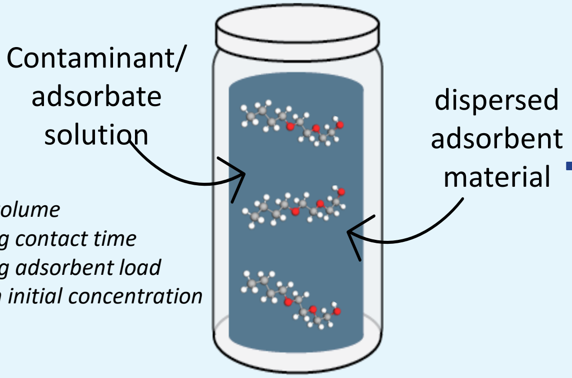
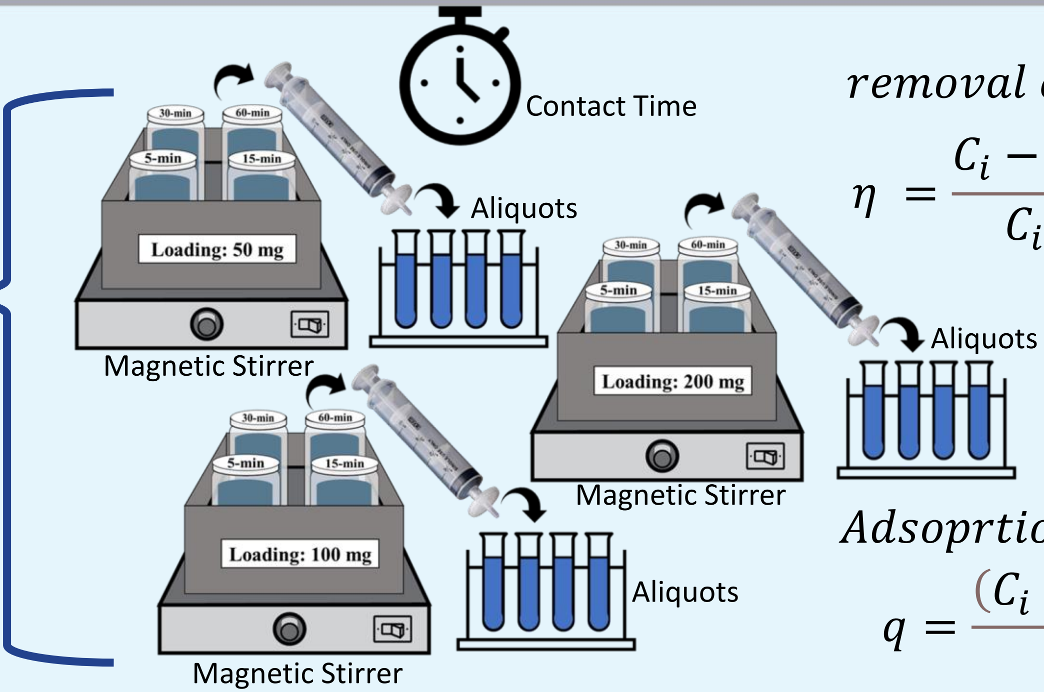
Graphene Adsorption Capacity Test



-fixed volume
-varying contact time
-varying adsorbent load
-known initial concentration

Test Subject

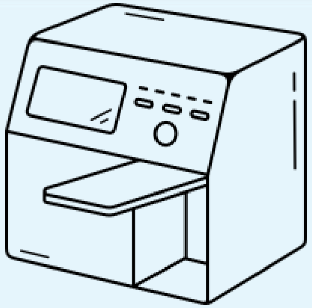


removal efficiency

$$\eta = \frac{C_i - C_f}{C_i} \times 100\%$$

Adsoprtion Capacity

$$q = \frac{(C_i - C_{ct})V}{m}$$

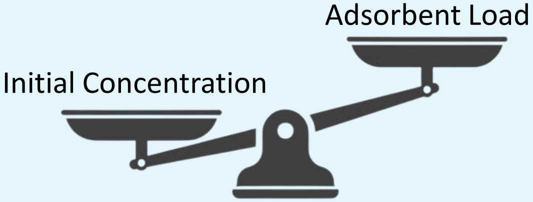


IC, TIC, TOC Analysis of Samples

Next

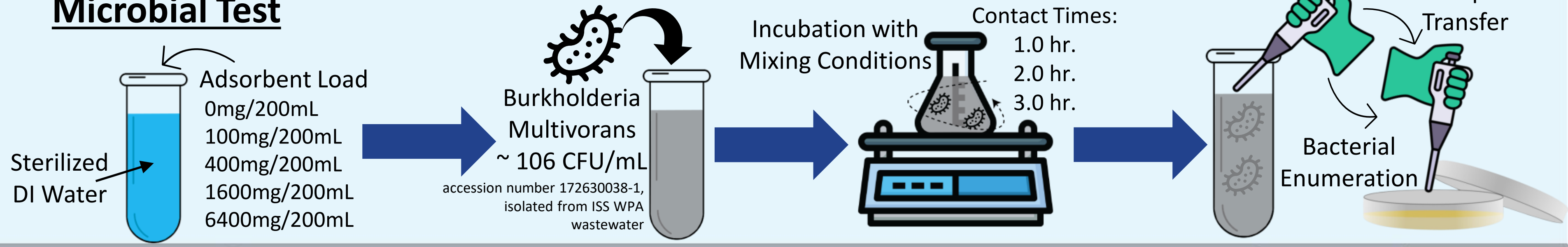
Data Wrangling & Processing

Test Adjustment



- fixed volume
- fixed limit of detection
- contact-time resolution

Microbial Test



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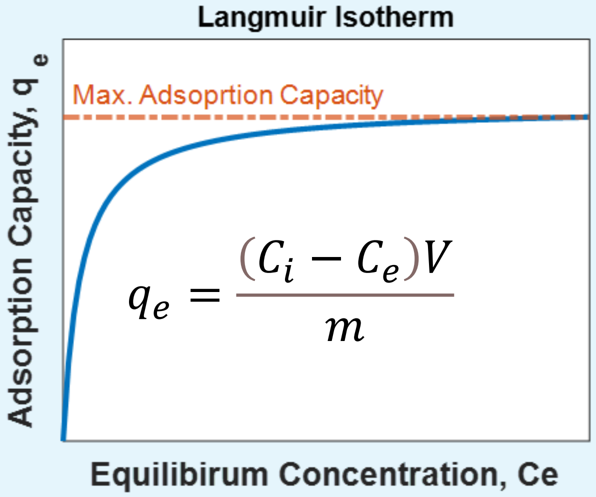
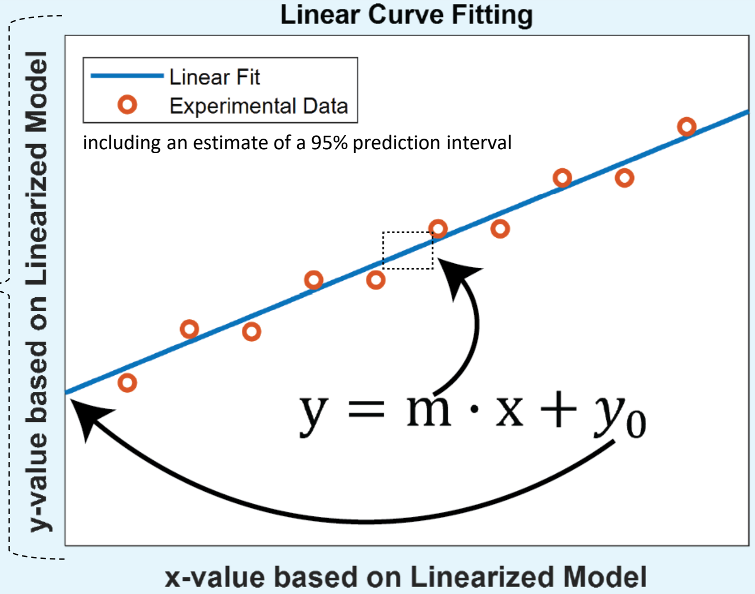
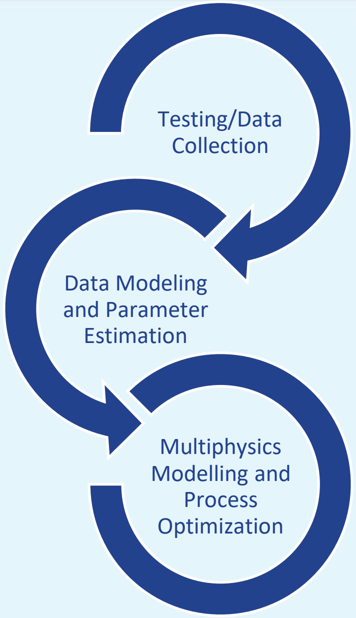
Modeling Batch Adsorption Data

- Isotherm Analysis
- Kinetics Analysis







Tablet 1. Adsorption Model and Their Linearized Forms

Adsorption Model	Expression	Linear Expression	Plot
Langmuir	$q_e = q_m\left[\frac{K_L C_e}{1+K_L C_e}\right]$	$\frac{1}{q_e} = \left[\frac{1}{K_L q_m}\right]\left[\frac{1}{C_e}\right] + \frac{1}{q_m}$	$\frac{1}{q_e}$ vs. $\frac{1}{C_e}$
Freundlich	$q_e = K_F C_e^{1/n}$	$ln(q_e) = ln(K_f) + \frac{1}{n} ln(C_e)$	$ln(q_e)$ vs. $ln(C_e)$
pseudo-1st order kinetic	$q = q_e^{(1-e^{-K_1 t})}$	$\ln(q_e - q) = -K_1 t + ln(q_e)$	$\ln(q_e - q)$ vs. t
pseudo-2nd order kinetic	$q = \frac{K_2 t q_e}{K_2 t + 1}$	$\frac{t}{q} = \left[\frac{1}{q_e}\right] t + \frac{1}{K_2 q_e^2}$	$\frac{t}{q}$ vs. t
intraparticle diffusion	$q = K_{id} t^{0.5}$	$q = K_{id} t^{0.5} + s$	q vs. $t^{0.5}$

S: thickness of the boundary layer

Tablet 2. Linear Regression Parameters

Adsorption Model	x-value	y-value	Slope (m)	y-intercept (y_0)
Langmuir	$\frac{1}{C_e}$	$\frac{1}{q_e}$	$\frac{1}{K_L q_m}$	$\frac{1}{q_m}$
Freundlich	$ln(C_e)$	$ln(q_e)$	$\frac{1}{n}$	$ln(K_f)$
pseudo-1st order kinetic	t	$\ln(q_e - q)$	$-K_1$	$ln(q_e)$
pseudo-2nd order kinetic	t	$\frac{t}{q}$	$\frac{1}{q_e}$	$\frac{1}{K_2 q_e^2}$
intraparticle diffusion	$t^{0.5}$	q	K_{id}	s

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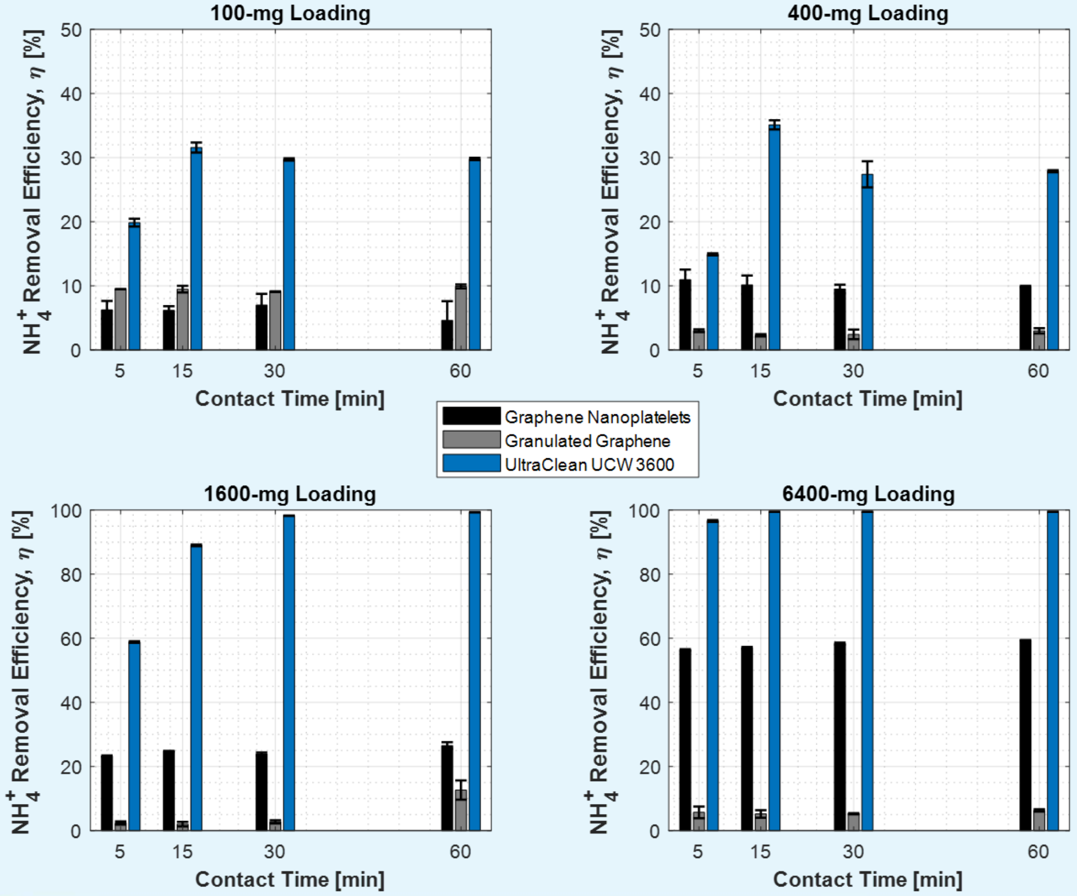
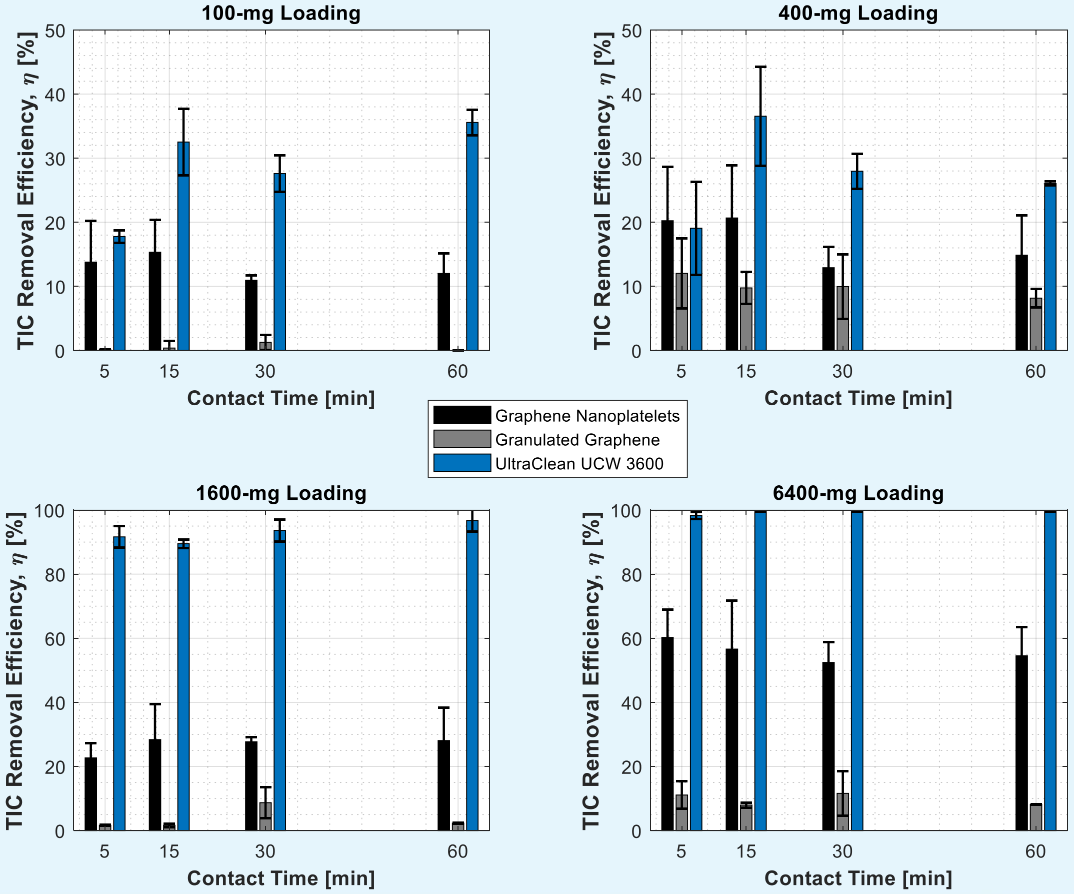
$NH4^+$ Removal



TIC Removal



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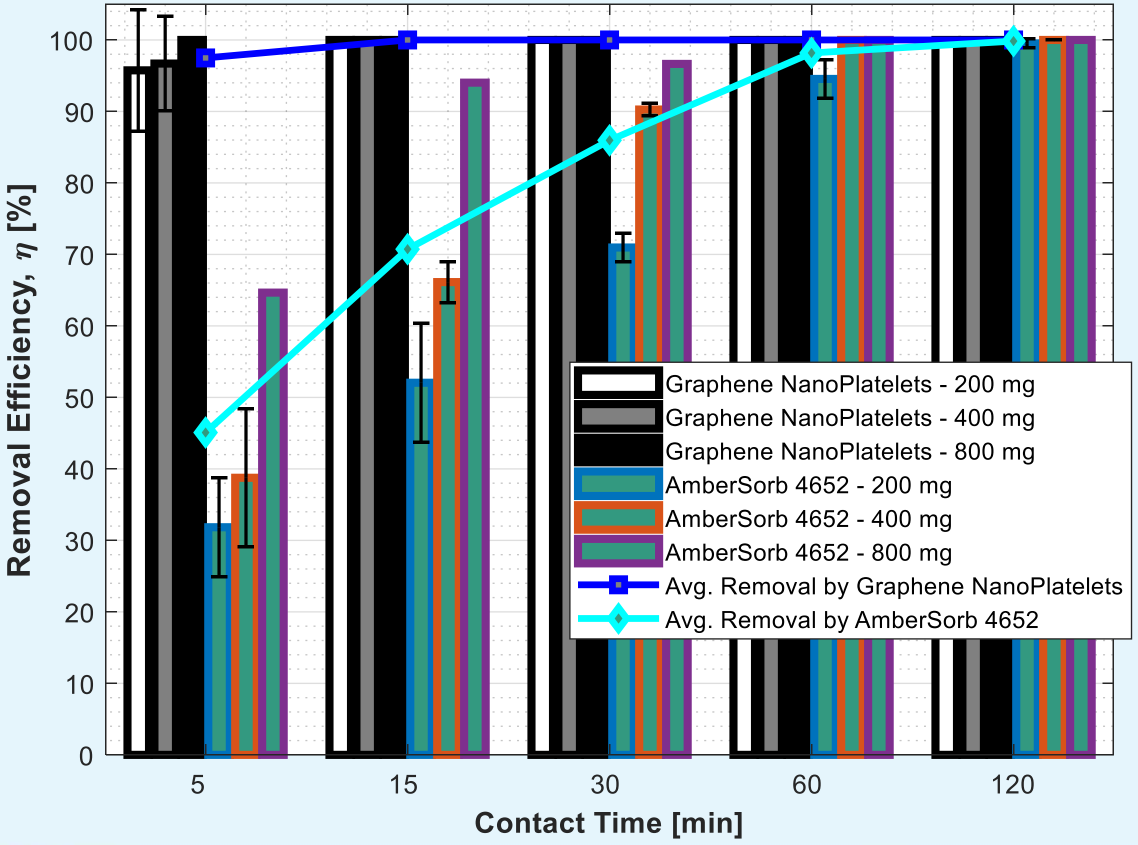
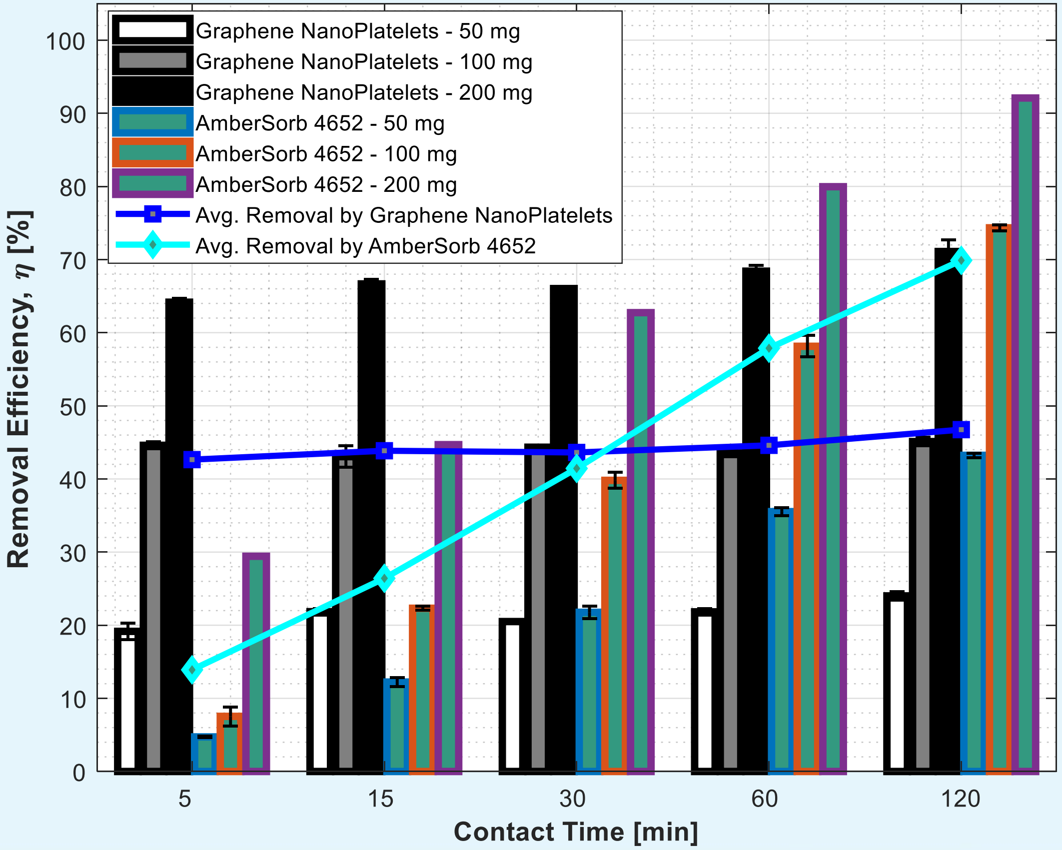
TOC Removal

Initial TOC: ~6.0 mg/L



Initial TOC: ~40.0 mg/L



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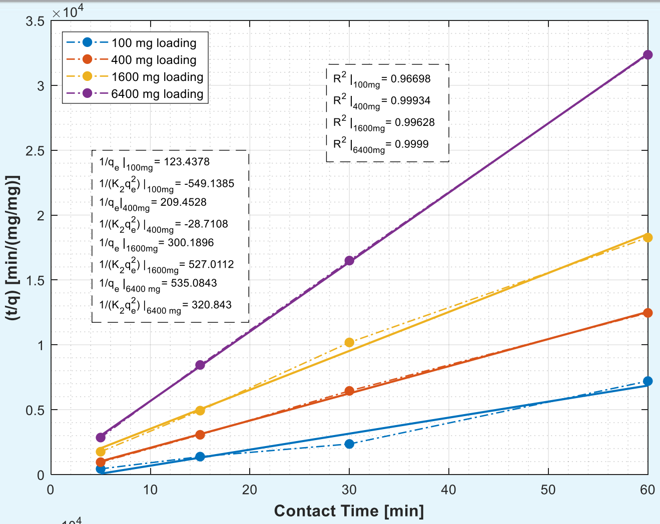
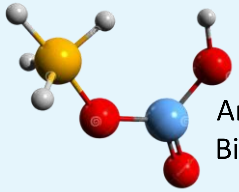
Linearized pseudo 2nd Order Kinetics

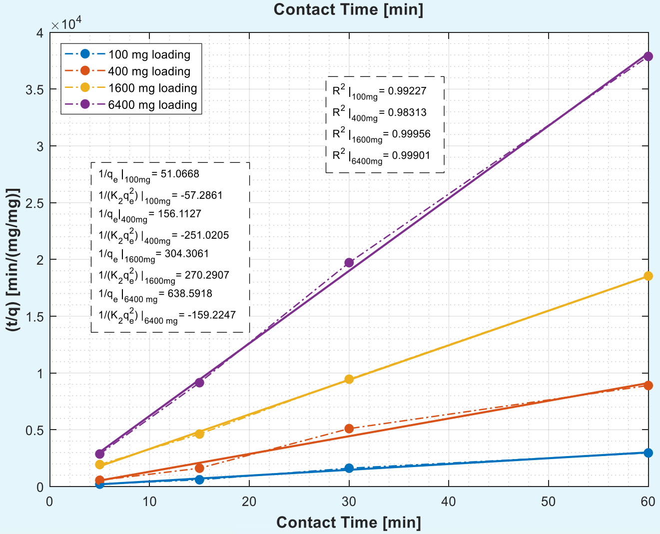
NH_4^+ Adsorption by Graphene Nanoplatelets



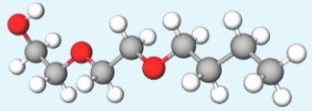


Ammonium Bicarbonate

TIC Adsorption by Graphene Nanoplatelets



Linearized Langmuir Isotherm



2-(2-Butoxyethoxy)ethanol

TOC Adsorption by Graphene Nanoplatelets, and AmberSorb™ 4652

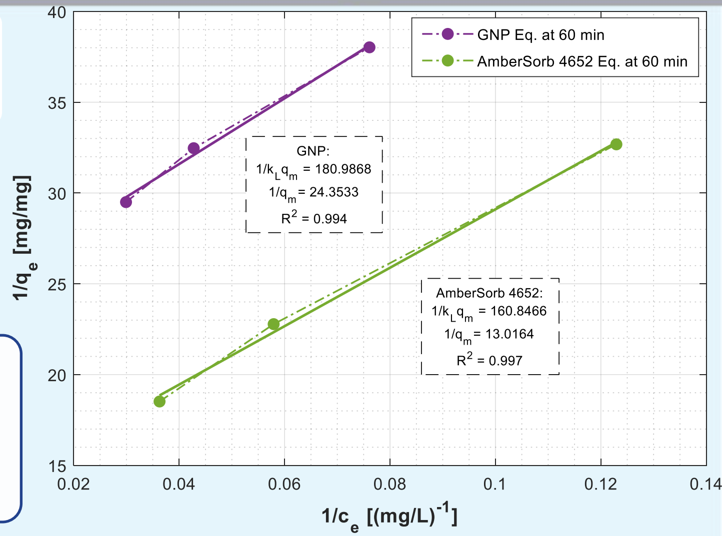


Table 1. Isotherm & Kinetics-based Parameter Estimation Summary

Adsorbent	Adsorbate	Best-fit Model	R^2	Parameter	
				q_e [mg/mg]	K_2 [mg/(mg min)]
Graphene Nanoplatelets	NH4+	Psudo-2nd Kinetics	0.9999	$1.87x10^{-3}$	$8.92x10^{+2}$
Graphene Nanoplatelets	TIC	Psudo-2nd Kinetics	0.9996	$3.29x10^{-3}$	$3.43x10^{+2}$
| |	| |	| |	| |	q_{max} [mg/mg]	K_L [L/mg]
Granulated Graphene	NH4+	Langmuir	0.8177	$1.22x10^{-3}$	$4.94x10^{-3}$
Granulated Graphene	TIC	Langmuir	0.7002	$5.51x10^{-4}$	$1.39x10^{-2}$
UltraClean™ UCW 3600	NH4+	Langmuir	0.9484	$2.69x10^{-2}$	$2.63x10^{-1}$
UltraClean™ UCW 3600	TIC	Langmuir	0.9731	$1.73x10^{-2}$	$3.99x10^{-1}$
Graphene Nanoplatelets	TOC	Langmuir	0.9940	$4.11x10^{-2}$	$1.35x10^{-1}$
AmberSorb™ 4652	TOC	Langmuir	0.9969	$7.68x10^{-2}$	$8.09x10^{-2}$

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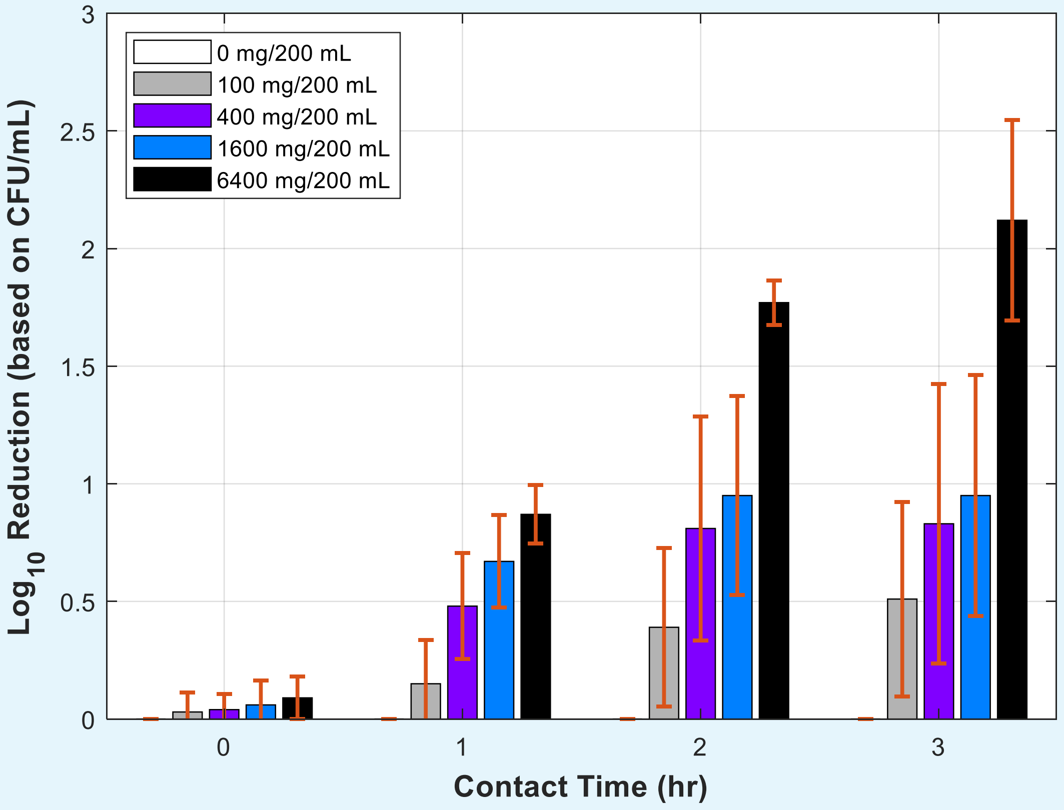
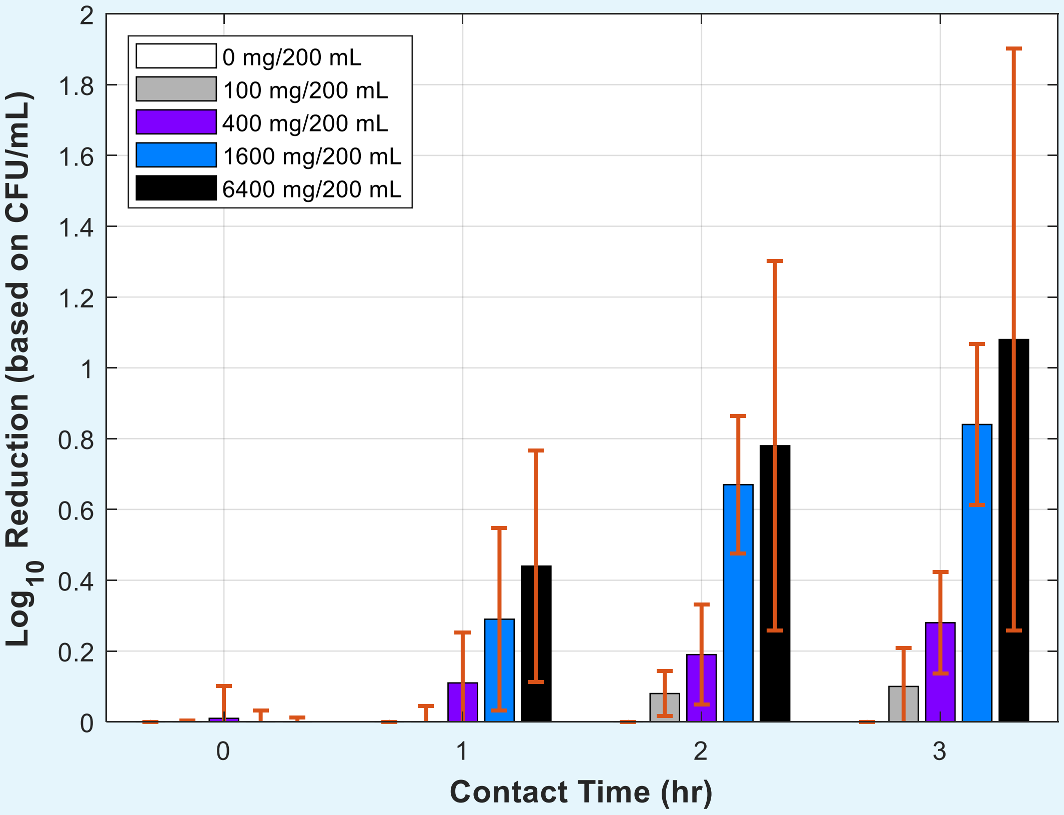
Microbial Removal

Graphene Nanoplatelets



AmberSorb™ 4652



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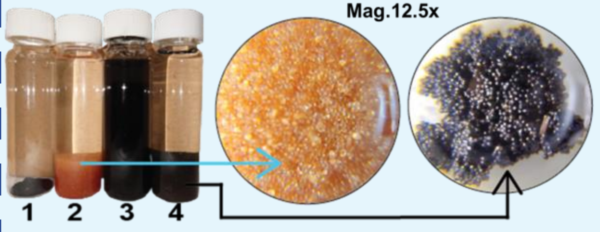
Remarks and Conclusions

- UltraClean™ UCW 3600 outperformed GNP and Granulated Graphene in removing inorganic contaminants.
- Graphene Nanoplatelets exhibited comparable (same order of magnitud) performance to AmberSorb™ 4652 in removing TOC without any preconditioning.
- Preliminary testing showed Graphene Nanoplatelets' antimicrobial properties with relevant bacterial strain from spacecraft environment.
- Further research on pressure-based experiments with graphene-based filtration media is warranted for microbial removal.
- Comparison of metrics between materials provides relevant performance baseline for graphene and SOA filtration media.
- Understanding of potential paths for optimization through graphene integration with other particles.
- Modeling generated parameters for Multiphysics simulations for realistic filtration components.
- Future research will investigate Graphene-based Materials with multicomponent contaminant solutions and in-house preparation of graphene-infused filtration media.
- Immobilizing GNP on other particles can prevent nanoplatelet aggregation and enhance antibacterial mechanisms.
- Next generation of ultra-high-capacity filtration media for spacecraft WRS applications is hoped to be realized.

Preparation of Graphene-loaded Filtration Media

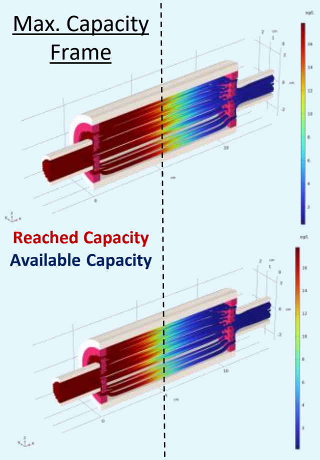


Loading Graphene onto Porous Matrix

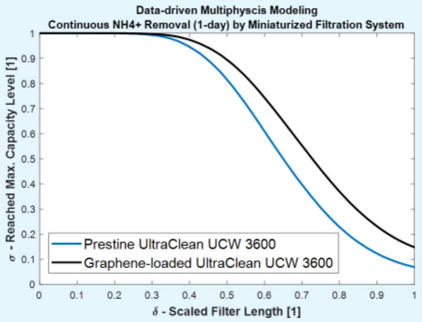
1. dry graphene powder
2. porous PSDB bead in water
3. water-based graphene suspension
4. graphene-loaded porous bead in water

Multiphysics Modeling

Max. Capacity Frame



Reached Capacity
Available Capacity



The results show how the capacity of UltraClean UCW 3600 is extended by graphene on the axial direction of the filter. Here, the pristine version of the filtration media will reach full capacity before the graphene-loaded version.

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Questions?