Diffusion Coefficients of PFAS-Surrogates in Agarose Gels for Passive Samplers (ER20-1363)

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Objective: Develop and validate a diffusive gradients in thin-films (DGT) passive sampling device (PSD) to quantify time-weighted average aqueous phase concentrations of 24 PFAS prioritized by DoD.

Technical Approach

- Task 1: Measure PFAS diffusion coefficients in agarose gels ($D_{PFAS:Gel}$) as a function of water chemistry and temperature
  - Develop methods using dyes (e.g., PFAS-surrogates) with similar molecular weights as target PFAS (320-830 g·mol^{-1}) due to ease of measurement (e.g., UV absorbance)
  - Assess diffusive boundary layer (DBL) thickness as a function of mixing speed (e.g., dyes initially then PFAS)
  - 24 PFAS as single compounds and various mixtures
- Task 2: Validate DGT-PSD components
  - Housing, gel type, gel thickness (*g*), outer membrane (if any) must be neither source/sink for PFAS
  - Binding layer with high capacity and rapid PFAS uptake
  - Measure $D_{PFAS:Gel}$ in DGT-PSD and validate against Task 1
- Task 3: Determine DGT-PSD method detection limits and concentration ranges for each PFAS (ng·L^{-1} to µg·L^{-1} levels)
  - Engineer binding layer to minimize competitive sorption effects of short- and long-chain PFAS

Schedule

- Start Date: July 9, 2020; Final Report: July 9, 2024
- Task 1: Anticipated Completion of June 30, 2021

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Results to Date

- Designed and fabricated diffusion cell machined from ultra-high-molecular-weight polyethylene (UHMWPE, Fig. 1)
- Measured $D_{Dye:Gel}$ for:
  - Methylene Blue (MB), Acid Orange 7 (AO), and Acid Black (AB)
  - For MB, *g* = 0.078 and 0.200 cm
- Fig 2: Mean $D_{Dye:Gel}$ = 0.8-10.5×10^{-6} cm^2·s^{-1} and decreased with increasing dye MW

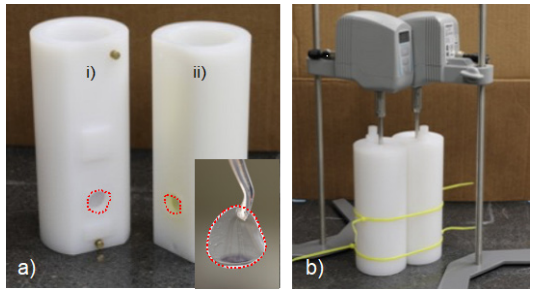

Fig. 1 – UHMWPE two compartment diffusion cell (a) disassembled compartments showing (i) source and (ii) sink with the porthole for diffusive gel red-lined and shown in inset and (b) assembled cell with mixers installed.

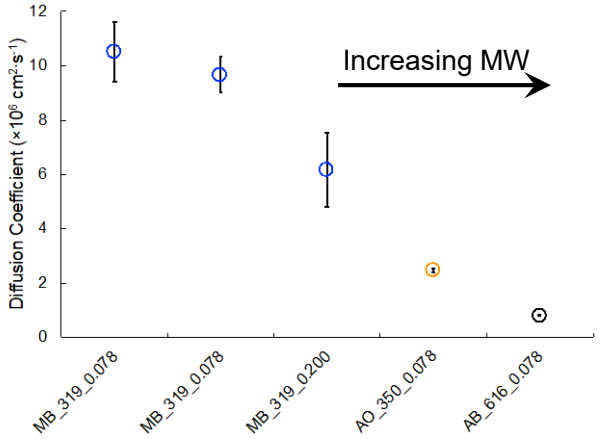

Fig. 2 – $D_{Dye:Gel}$ of MB, AO, and AB at pH 7 and 25 ℃. X-axis label: *Dye Type_MW_g*.

- Less error in $D_{Dye:Gel}$ by optimizing sampling times for a given *g*
  - Need to repeat MB tests
- Next steps: measure DBL thickness as a a function of mixing speed, water chemistry, and temperature (4 to 30 ℃)
  - Need to account for DBL in measurement of $D_{Dye:Gel}$

Lessons Learned and/or Data Gaps

- Determine DBL thickness over a range of mixing speeds prior to measuring PFAS diffusion coefficients
  - To complete Task 1, measure $D_{PFAS:Gel}$ as a function of pH, conductivity, natural organic matter concentration, and water temperature