PFAS interaction with aquifer materials: Implications on PFAS transport in groundwater

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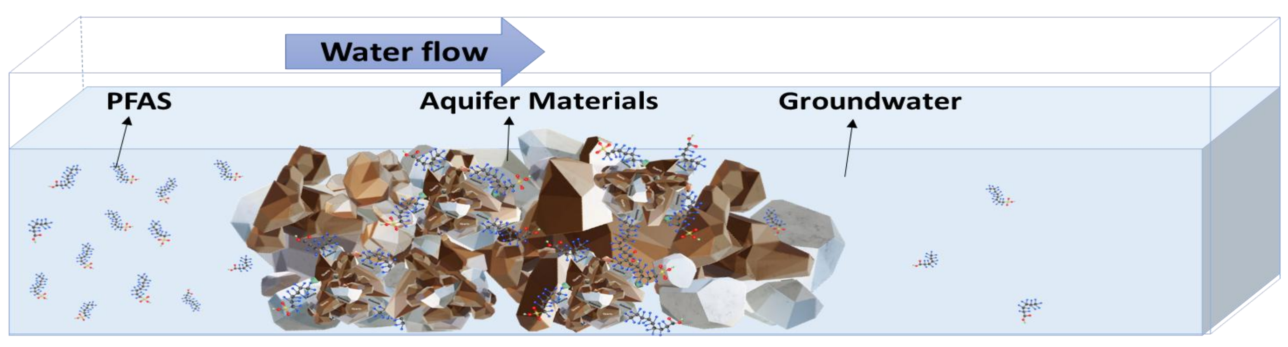
Introduction

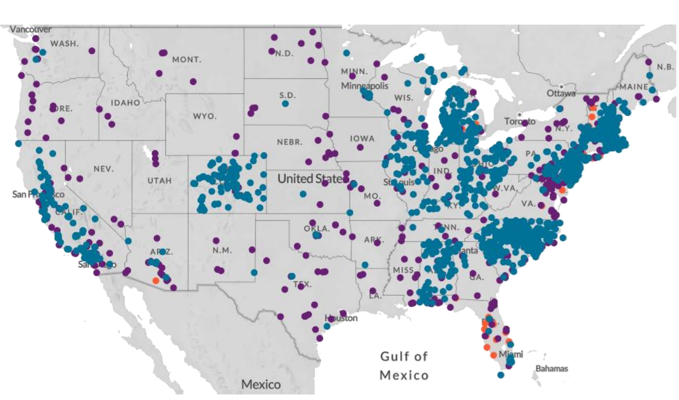
- **Per- and polyfluoroalkyl substances (PFAS)**
  - PFAS are a large class of synthetic organic chemicals used in a variety of applications, such as surface coatings, firefighting foams, carpets, clothing, food packaging, etc.

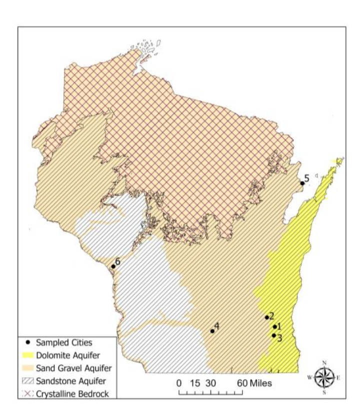


  - Per- and polyfluoroalkyl substances (PFAS) in groundwater adsorption on to aquifer materials when PFAS pass through the aquifer material with groundwater.

Methods

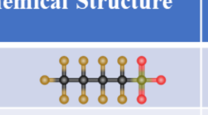
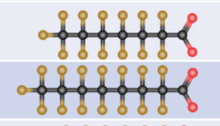
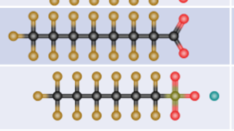
- **Aquifer Materials selection**





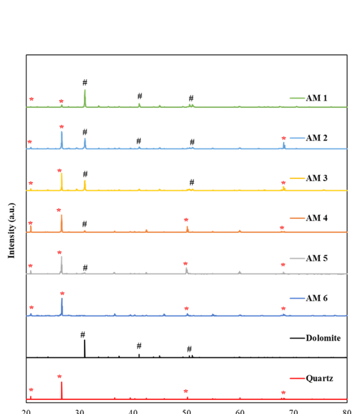
  - Sites were selected according to the contamination site, geographical coverage and aquifer material composition.

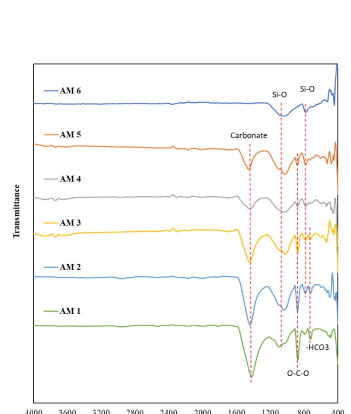
- **Adsorption isotherm study**
  - Mixture of 6 PFAS: PFHpA, PFOA, PFNA, PFBS, PFHxS, PFOS
  - Concentration range: 100 – 5,000 ng/L for each PFAS
  - Natural groundwater: pH ~8.5
  - Aquifer materials loading: 100 g/L
  - Contact time: 7 days

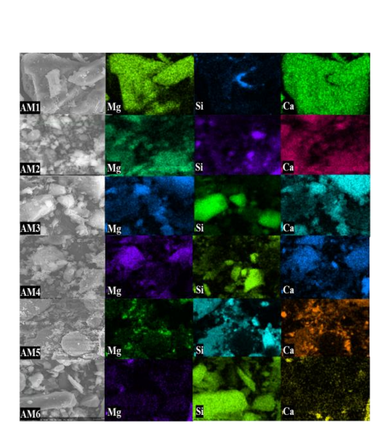
PFAS	Chemical Structure	Molecular Weight (g/mol)	log K_{ow} [1]	log D_{ow} at pH 8.5 [1]
PFBS		300.1	2.63	0.25
PFHpA		364.06	4.41	0.88
PFOA		414.07	5.11	1.58
PFHxS		400.12	4.03	1.65
PFNA		464.08	5.81	2.28
PFOS		500.13	5.43	3.05

Results

- **Aquifer Material Characterization**



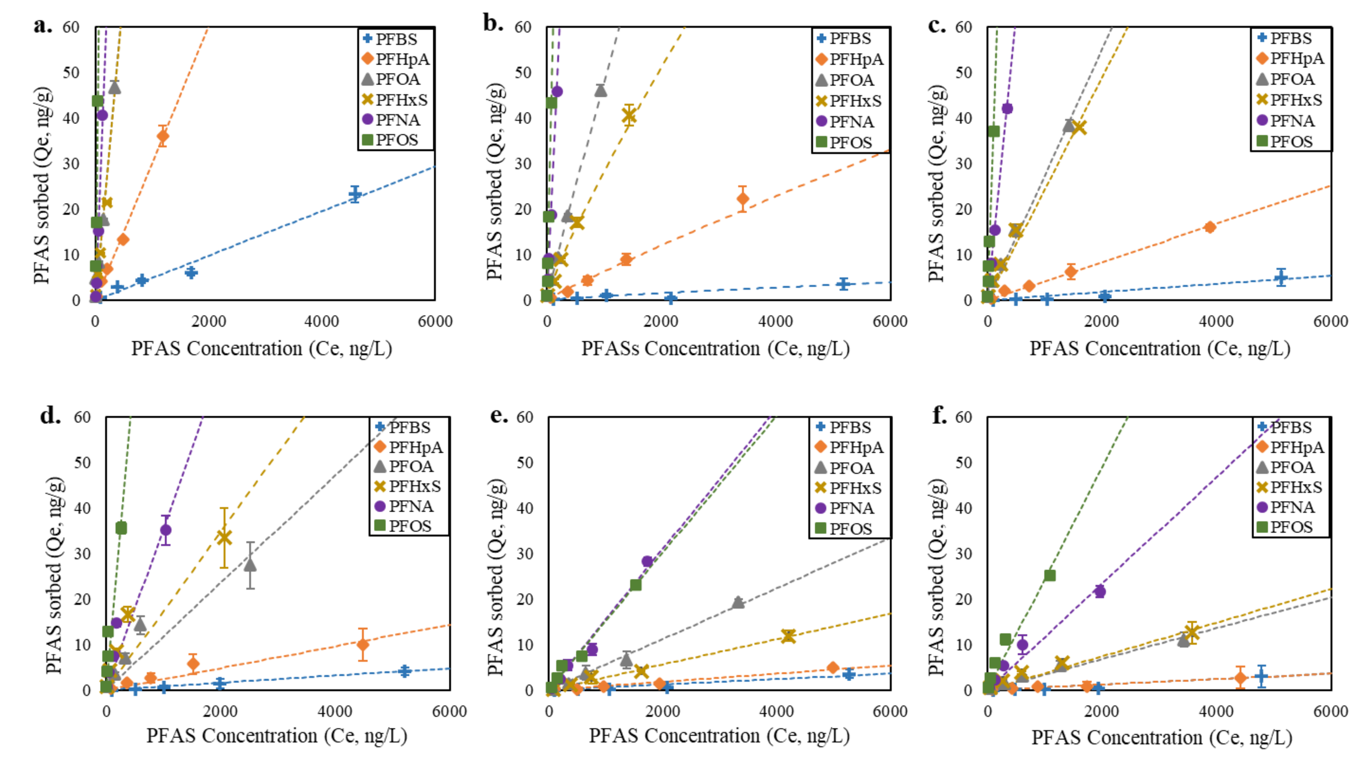




Dolomite content in the aquifer materials used in this study followed the trend: AM6 < AM5 ≈ AM4< AM3 < AM2 < AM1

- **Adsorption Isotherm Results**

Freundlich Model: $Q_e = K_F * C_e^{\,n}$ → n ≈ 1 → Linear Model: $Q_e = K_d C_e$ → $K_d = Q_e / C_e$ K_d: solid-water partition coefficient (L/kg)

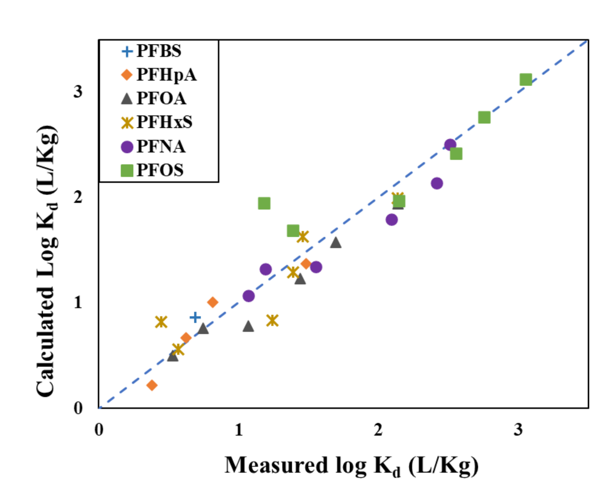


- Adsorption isotherms of PFAAs onto aquifer materials (a) AM1, (b) AM2, (c) AM3, (d) AM4, (e) AM5, (f) AM6
- PFAAs matrix in groundwater with 100 g/L aquifer material.
- Dash lines represent linear isotherm model fits

Conclusions

- **Multilinear Regression Model**

$$log\ K_d = 1.68 \cdot C_{dolomite} + 0.81 \cdot log\ D_{ow} - 0.81$$

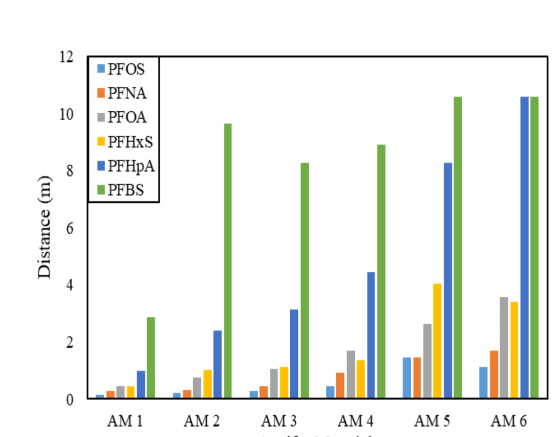


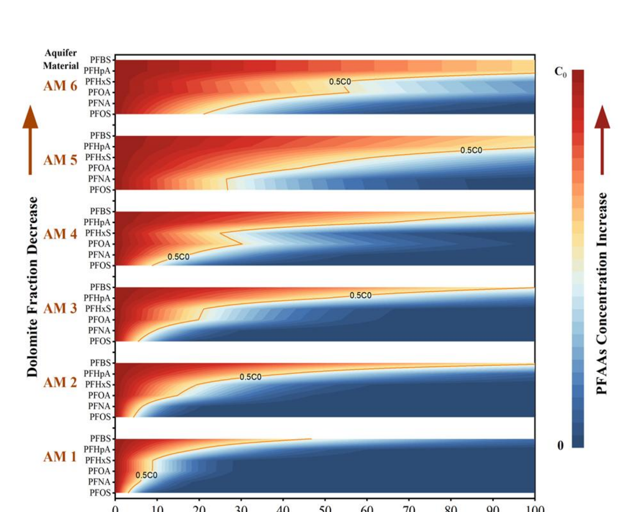
The comparison between the model calculated log Kd and measured log Kd shown that the data points fell closely along the 1:1 line, suggesting that the multilinear regression model may be used to estimate the adsorption affinity of various PFAS onto aquifer materials with varied fractions of dolomite.

- **Retardation Factor: R**

$$R = 1 + K_d \frac{\rho}{\theta}$$

K_d: solid-water partition coefficient, L/kg
ρ: bulk density, kg/L
θ: porosity



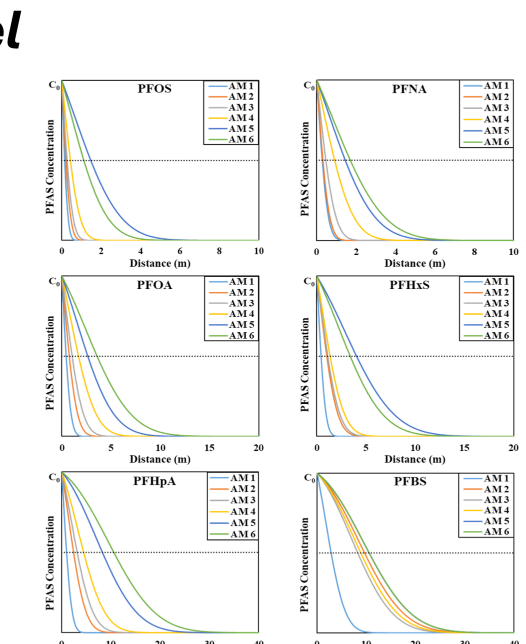


- ***1-D transport model***

$$\frac{\partial C}{\partial t} = -\frac{v}{R}\frac{\partial C}{\partial x} + \frac{D}{R}\frac{\partial^2 C}{\partial x^2}$$

$$C = \frac{C_0}{2}\text{erfc}\left[\frac{Rx - vt}{2\sqrt{DRt}}\right] + \frac{C_0}{2}e^{\frac{vx}{D}}\text{erfc}\left[\frac{Rx + vt}{2\sqrt{DRt}}\right]$$

C: PFAS conc., ng/L
C_0: PFAS conc. in the source, ng/L
x: travel distance, m
t: travel time, s
R: retardation factor
D: hydrodynamic dispersion coefficient, m^2/s
v: average linear pore water velocity, m/s



For comparison purposes, we selected half of the source concentration(C_0/2) and calculated the corresponding PFAAs travel distance. Compared with a sand-rich aquifer , the travel distance of PFAAs could be reduced by 4 to over 10 folds in a dolomite-rich aquifer.

- ***Environmental implications***
  - Dolomite are abundant in groundwater aquifers, its impact on the transport of emerging contaminants such as PFAS has been largely overlooked. Our results suggested that dolomite had a strong adsorption affinity with PFAAs and thus could play an important role in the transport of PFAAs in groundwater systems.

Acknowledgments

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Publications

Adsorption of per-and polyfluoroalkyl substances (PFAS) by aquifer materials: The important role of dolomite. *Environmental Science & Technology Letters*, 2023,10(10), pp: 931-936.