Nanoplastic-facilitated transport of lead through reactive porous media

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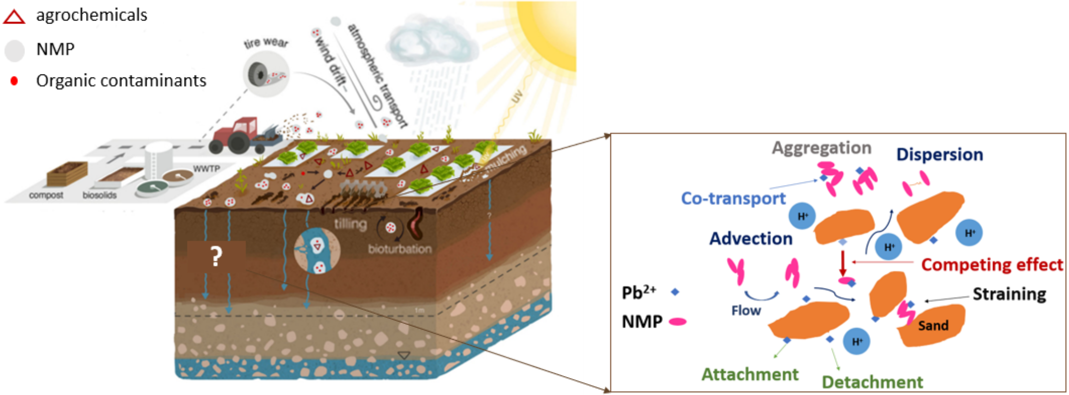
Introduction and Motivation

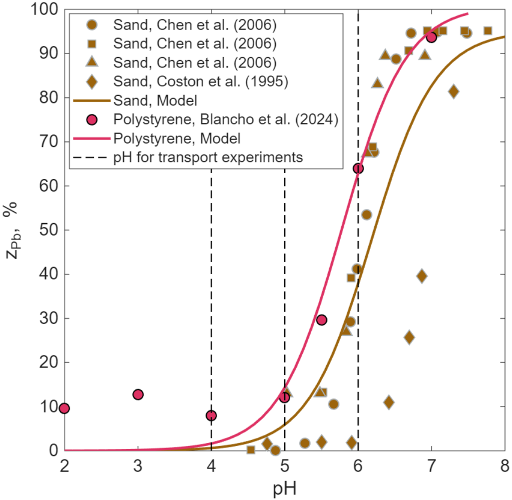


Modified after: Castan et al. (2021) Commun Earth Environ, 2. 193.
Li et al. (2025) Earth-Science Reviews, , 264. 105108.; Kang et al. (2025) Science of The Total Environment, 960. 178298.; Jeon & Kim (2024) Trends in Environmental Analytical Chemistry, 44. e00246.; Moeck et al. (2023) Grundwasser - Zeitschrift der Fachsektion Hydrogeologie, 28. 23-35.; Ren et al. (2021) Journal of Hazardous Materials, 419. 126455.

Research Hypothesis and Approach

Our hypothesis: nano-plastic particles enrich themselves with metals during transport, facilitating metal mobilization and metal-enriched plastic accumulation as metals screen repulsive forces favoring attachment.

Approach: We performed column-flood experiments with Pb^{2+}, polystyrene (PS), and sand at constant pH, and developed a reactive transport model to gain insights into transport mechanisms.

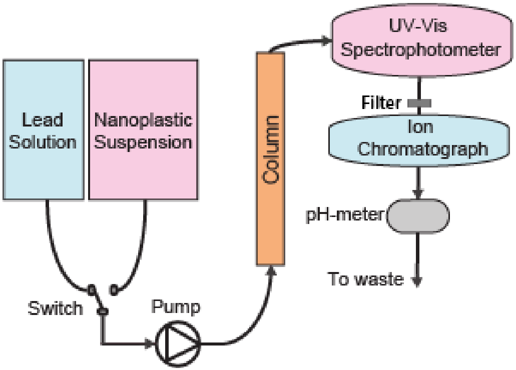


Experiments and Set-up

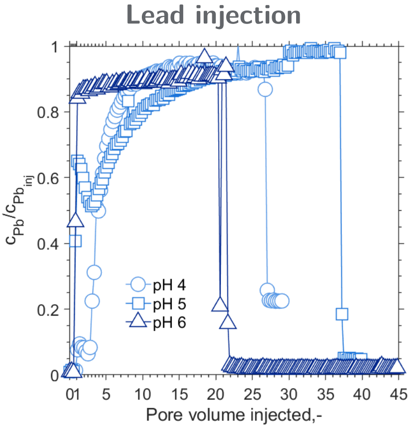
Conditions and Procedure:

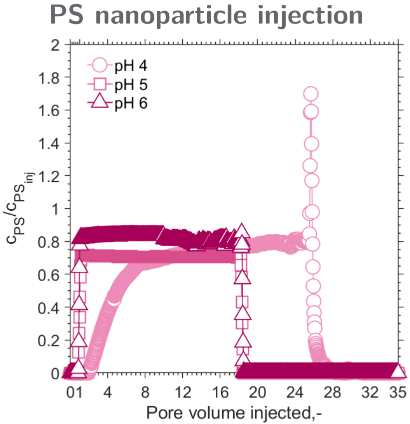
- Diba chromatographic column of 2.5 cm diameter and 30 cm length.
- Quartz sand, size 210–300 μm.
- Polystyrene (PS) nano-particles, size 600 nm, $c_{inj} = 0.05$ mg/mL.
- $Pb(NO_3)_2$: 9.65×10^{-5} mol/kg.
- pH: 4, 5, and 6.
- $n \sim 0.5$.
- Flow rate (Q): 0.7–1.4 mL/min.
- **Type I**: Single component injection experiments.
- **Type II**: Multi-component injection experiments.

Column-flood System:



Results - Type I: Single Component Injection





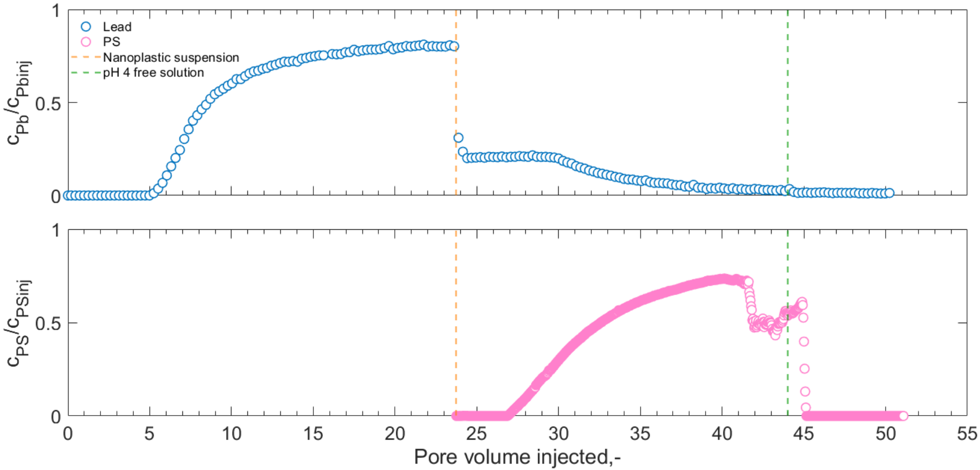
SiO^- preferentially adsorbs Pb^{2+} rather than $PbOH^+$ or $Pb(OH)_2^\circ$ near pH 6.

PS particle mobility increases with pH due to electrostatic repulsion between negatively charged particles and sand surfaces.

Pore volume injected (PV, -): $PV = Q \cdot t/V_v$, with t time and V_v the void volume.

Results - Type II: Multi-component Injection

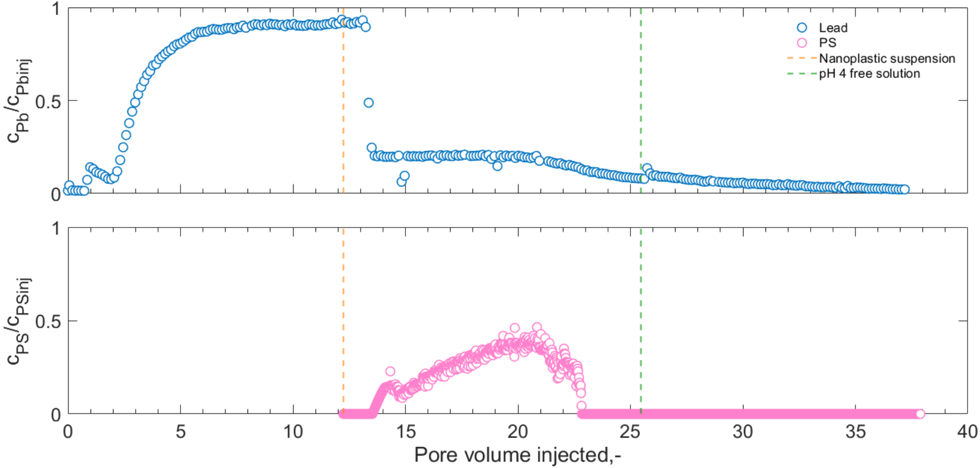
Q = 1.4 mL/min; Damköhler Number (Da = $k_{att}L/v$): Da = 7.9



In the presence of PS particles, Pb^{2+} acts as a charge screening agent, reducing electrostatic repulsion between particles and sand, promoting the co-transport of Pb^{2+} and PS through the porous medium.

Results - Type II: Multi-component Injection

Q = 0.7 mL/min; Da = 15



At lower flow rates, charge-screened PS nanoparticles have more residence time relative to the attachment timescale, so they are more retained due to attachment.

Governing Equations

One dimensional (1D) reactive transport model for Pb^{2+}, H^{+}, and nano-plastic particles under the assumptions of incompressible fluid, isothermal conditions, local equilibrium, and constant velocity:

$$\frac{\partial(c_i + \nu z_i + c_n z_{i,n}/\rho_w)}{\partial t} + v\frac{\partial(c_i + c_n z_{i,n}/\rho_w)}{\partial x} - D\frac{\partial^2(c_i + c_n z_{i,n}/\rho_w)}{\partial x^2} = 0,$$

$$\frac{\partial c_n}{\partial t} + \frac{\rho}{n}\left(\frac{dS_{att}}{dt} + \frac{dS_{str}}{dt}\right) + v\frac{\partial c_n}{\partial x} - D\frac{\partial^2 c_n}{\partial x^2} = 0,$$

for $t > 0$ and $0 < x < L$, where:

-c_i and c_n are the solute and particle concentrations with *i* either Pb^{2+} or H^{+}.

-z_i and $z_{i,n}$ are the adsorbed concentrations on sand and on the particles.

-S_{att} and S_{str} are the retained particle concentrations due to attachment/detachment and straining processes.

-ρ and n are the porous medium density and the porosity, respectively.

Constitutive Equations

Surface complexation reactions and adsorption isotherms:

$$\mathrm{X^- + H^+ \longleftrightarrow XH},$$
$$\mathrm{X^- + Pb^{2+} \longleftrightarrow XPb^+},$$

where $\mathrm{X^-}$ is the silanol group (-$\mathrm{SiO^-}$) for sand and the carboxylate group (-$\mathrm{COO^-}$) for polystyrene (PS) particles.
Site balance equation:

$$Z_t = \{\mathrm{X^-}\} + \{\mathrm{XH}\} + \{\mathrm{XPb^+}\}.$$

Competitive adsorption isotherms:

$$z_{Pb} = \frac{c_{Pb} K_{Pb} Z_t}{1 + c_H K_H + c_{Pb} K_{Pb}}, \quad z_H = \frac{c_H K_H Z_t}{1 + c_H K_H + c_{Pb} K_{Pb}}$$

PS has a lower $p\mathrm{K}_H$ than sand, meaning -COOH becomes active at lower pH than -$\mathrm{SiO^-}$ and it is at low pH where the competition is higher.

Constitutive Equations

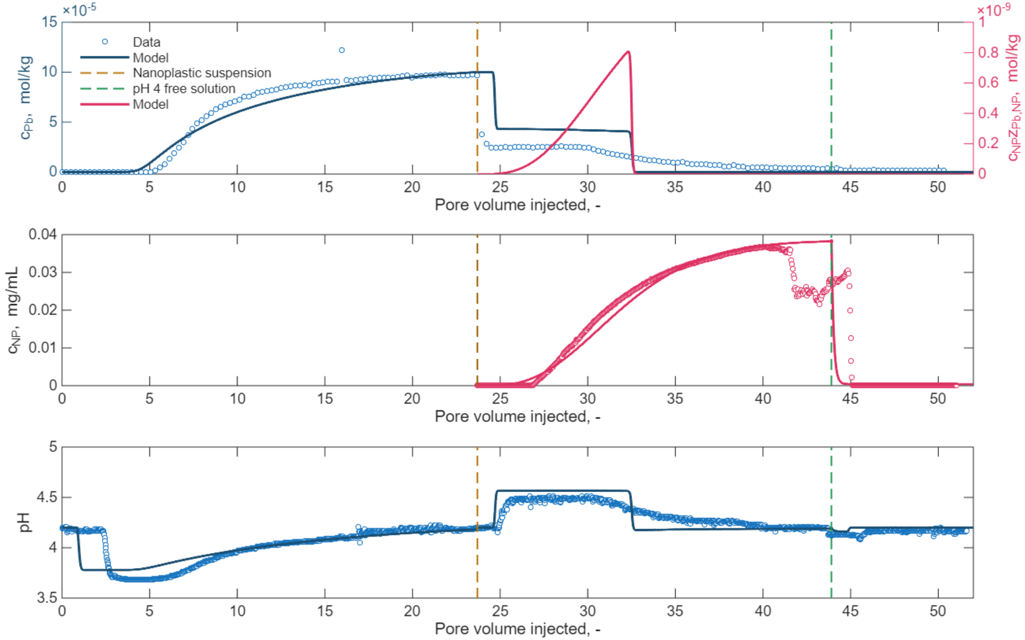
Attachment/detachment and straining processes:

$$\frac{\rho}{n}\frac{dS_{att}}{dt} = k_{att}c_n - \frac{\rho}{n}k_{det}S_{att},$$
$$\frac{\rho}{n}\frac{dS_{str}}{dt} = k_{str}\left(1 - \frac{S_{str}}{S_{max}}\right),$$

where:

- k_{att} and k_{str} represent the attachment and straining coefficients, 1/s;
- k_{det} is the detachment coefficient, 1/s;
- S_{max} is the maximum concentration on the attachment sites, g/kg.

Multi-component Injection - Data and Model at pH 4



Summary and Conclusions

- **Nano-plastic particles** could act as contaminant vectors facilitating the co-transport of inorganic and organic pollutants and accumulation in soil.
- We studied this phenomenon using polystyrene **nano-plastics and lead in sand** and perform column-flood tests and reactive transport modeling.
- **At pH 4**, where Pb^{2+} adsorbs preferentially onto plastics, the particles enrich themselves with the metal, which, by screening their negatively charged surface, favors their retention by attachment within the medium.
- Future work will focus on accounting for **the coupled mechanism of metal-nanoplastic co-transport and surface-charge evolution** to better describe metal-laden nanoplastic migration, accumulation, and displacement.

Back-up Slides

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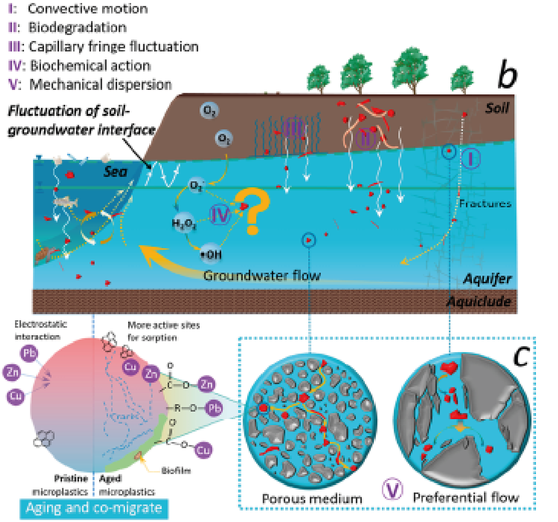

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