Measuring diffusion of trichloroethylene breakdown products in polyvinylalginate

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The Problem

Trichloroethylene-Contaminated Sites

Figure 1. Map of TCE-, DCE-, and VC-contaminated sites
Legend:
Trichloroethylene (TCE)
1,2-cis-dichloroethylene (DCE)
Vinyl Chloride (VC)
Courtesy of toxmap.nlm.nih.gov, October 2018

Chlorinated solvents, including trichloroethylene (TCE), are present in approximately 60% of Superfund sites as a persistent groundwater pollutant.

Bioremediation using natural microorganisms is an appealing strategy for TCE degradation, but the metabolism of TCE produces both protons (which inhibit microbe growth) and increasingly toxic compounds until the final step[1], often causing more harm than good.

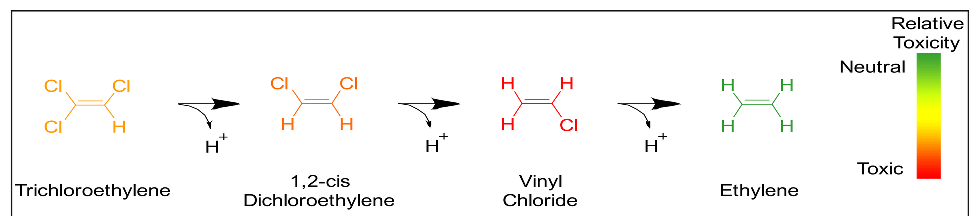


Figure 2. Abridged metabolic pathway of TCE breakdown

Our Solution

Biobeads

Encapsulating microorganisms inside of polymer membrane beads can protect them and control the diffusion rate, enabling them to survive the remediation process.

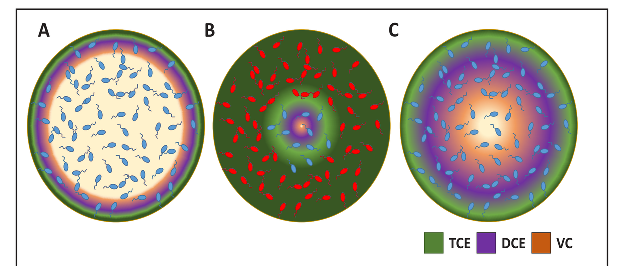


Figure 3. Idealized diffusion model for microorganism-encapsulating biobeads.

Previous work[2] has demonstrated that a calcium alginate polyvinylalcohol copolymer hydrogel (hereafter called polyvinylalginate or PVA) possesses many properties for biobead formation, but no data exist for diffusivity of TCE and its breakdown products within this compound.

This research sought to characterize the diffusion rates of TCE and its breakdown products within PVA membranes.

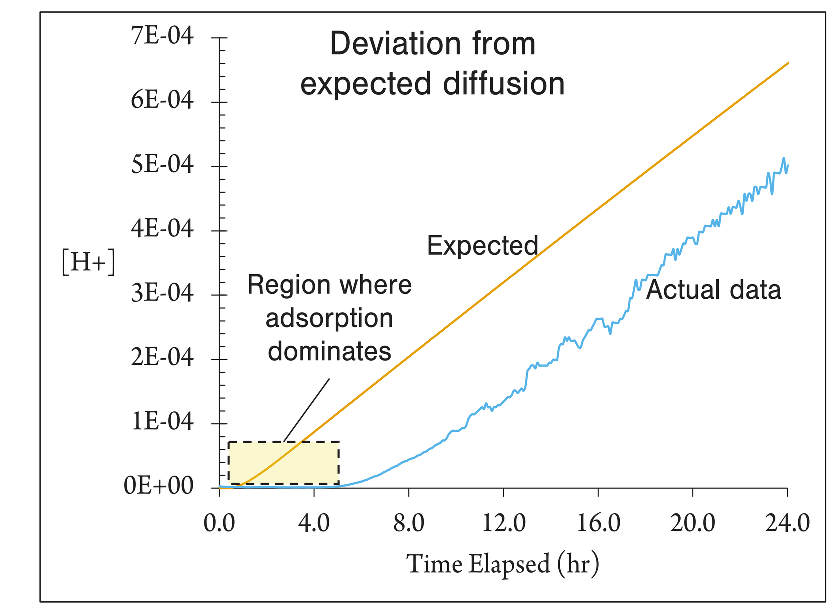
Future Work

Numerical Solutions

The selection of the linear graph indicating constant diffusion time is somewhat arbitrary. We are currently working on a computer program to numerically solve Fick's 1st and 2nd laws simultaneously for this system and more accurately determine the diffusivity.

Adsorption

For H^+, the lag period before diffusion begins suggests proton adsorption in the membrane. This merits more study.



The Experiment

The Diaphragm Cell Method

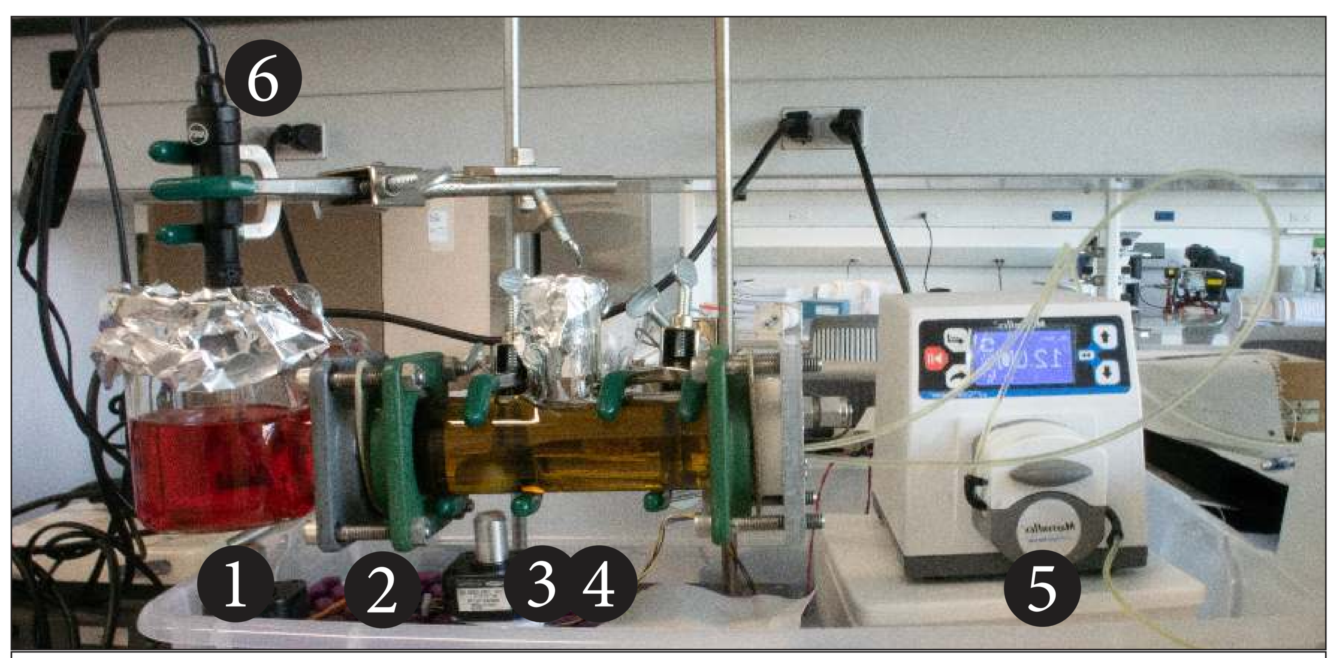


Figure 4. Diaphragm cell for H+ diffusion using pH indicator dye. Similar experiments were conducted in an air-tight system for the highly volatile chlorinated solvents.

❶ Chlorinated solvent/H^+ source with high concentration
❷ Molecules diffuse through PVA membrane
❸ Initially low concentration in sink increases due to diffusion
❹ Sink changes absorbence based on the concentration
❺ Well-mixed solution is pumped to spectrophotometer, which reads said absorbence
❻ For H^+ experiments, the pH probe can also measure H^+ concentration directly

Results

Effective Diffusion Coefficients

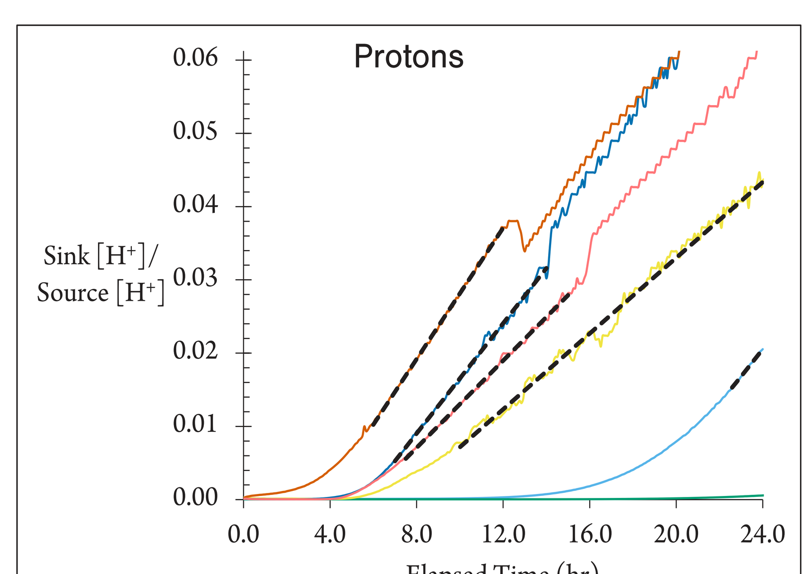
Compound	Diffusion in PVA (x 10⁶ cm²/s)	Diffusion in Water (x 10⁶ cm²/s)
Trichloroethey-lene (TCE)	12.4 ± 1.64	8.16 ± 0.06[3]
1,2-cis-dichloro-elthylene (DCE)	7.83 ± 0.54	11.2[4*]
Vinyl Chloride (VC)	4.68 ± 4.14	13[4*]
Protons	14.1 ± 1.6	70[4*]

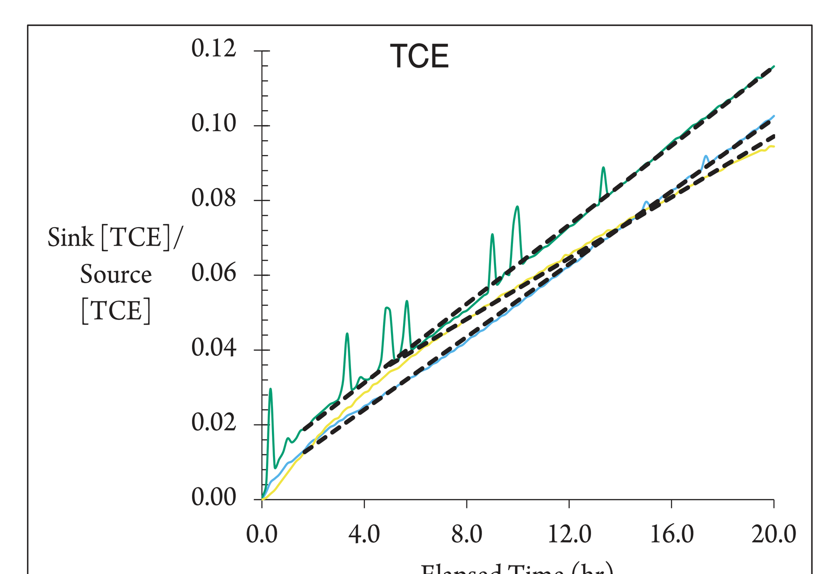
**Diffusivity determined by empirical correlation*

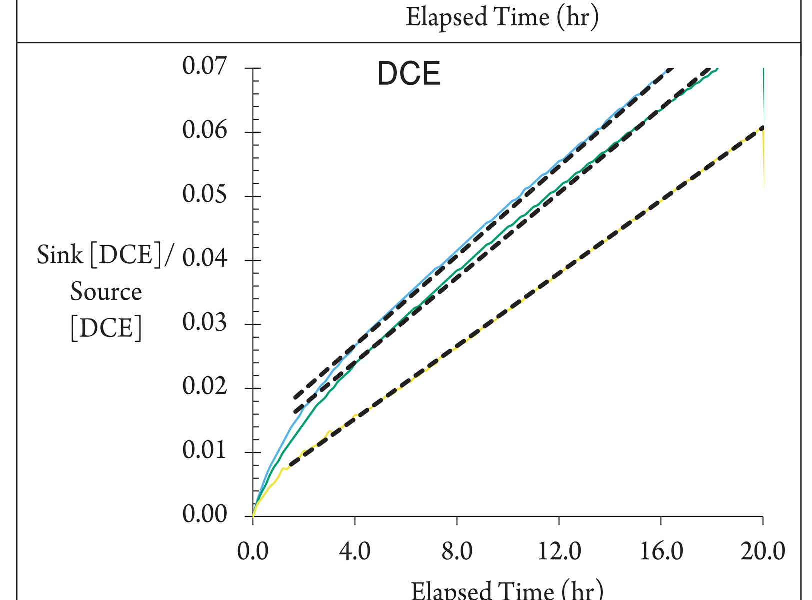
The diffusion coefficients were found using the equation

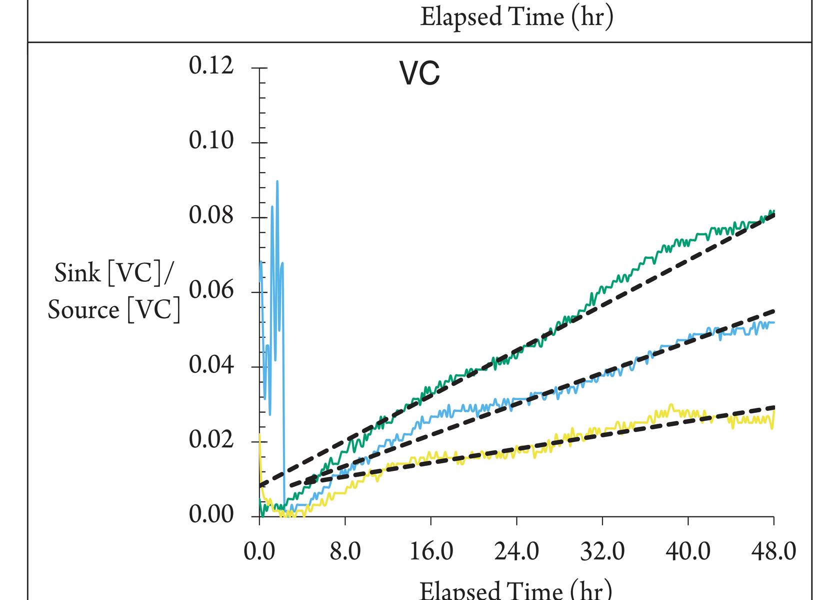
$$D_{ab} = \frac{mLV}{AC_0}$$

Where:
D_{ab} = Diffusivity
m = Slope of linear diffusion plot
L = Length across membrane
V = Volume of sink
A = Cross-sectional area of membrane
C_0 = Initial concentration in source









Discussion & Conclusion

The diffusivity of all compounds in PVA is less than in water.

The diffusivity of protons leaving the membrane is greater than that of TCE entering.

The adsorption of protons into the membrane would also allow it to act as a buffer.

These observed properties of polyvinylalginate suggest that it is suitable for encapsulation of microorganisms undertaking bioremediation of trichloroethylene.

Acknowledgments

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