# Understanding the Relationship Between Key Water Parameters and the Behaviour of Sulfolane in Groundwater

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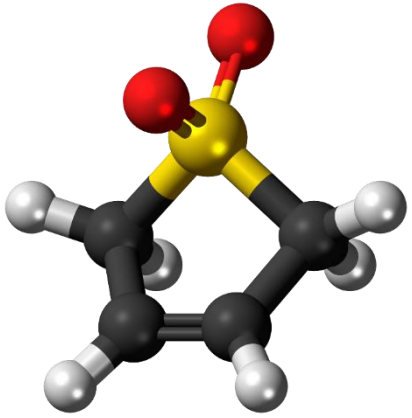
# Agenda

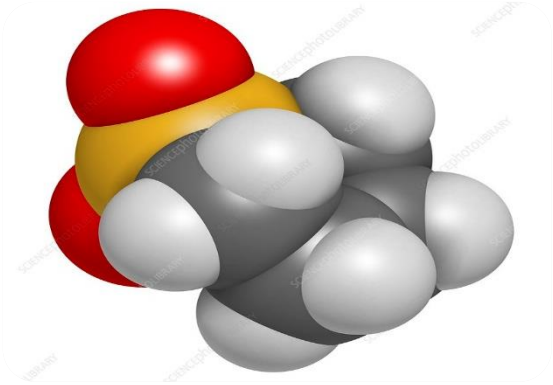
1. Background
2. Properties of Sulfolane
3. Experimental Design
4. Conclusion

# Why are we doing anything?

The study of Sulfolane's behaviour when interacting with other water parameters is poorly documented. General parameters such as chemical oxygen demand (COD) and sulfate (SO42-) are typically used as indicators for the presence of Sulfolane.



# Properties of Sulfolane



## Polar

High dipole moment of 4.69 debye.

## Very Stable

Very stable even at high temperatures in air; decomposition rate of 0.009% at 200°C.

## Sheen

Sulfolane-containing water would have an inorganic layer of sheen on top of the water.

## Dense

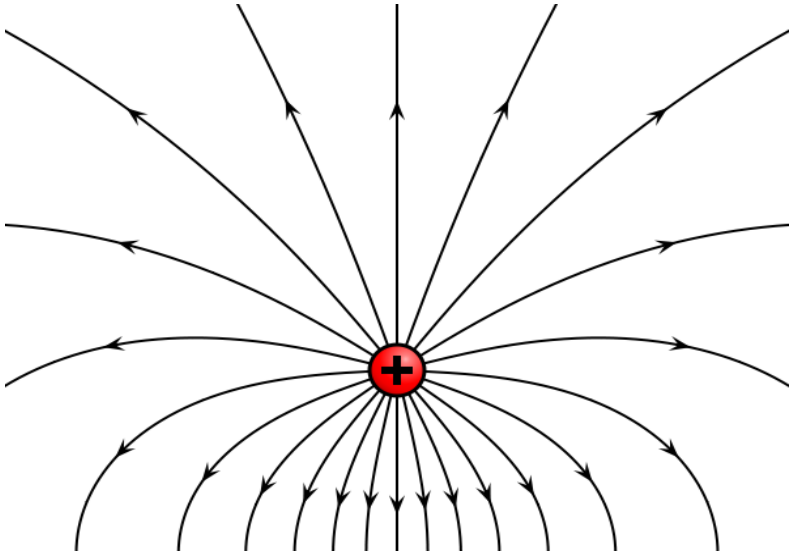
Density of 1.26 g/cm$^3$.

# Sulfolane properties – degradation rate comparisons

| Hydrocarbons | Sulfolane | Chloride |
| --- | --- | --- |
| • Degrades at a fast rate<br>• Rate of degradation = 0.3-4% per day | • Degrades slowly by aeration<br>• Rate of degradation = 0.009% /h at 200°C | • Salt doesn't degrade |

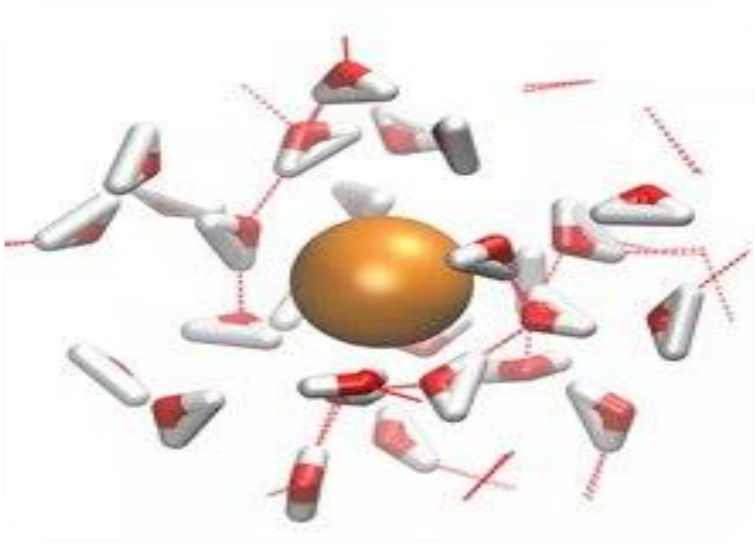
- Sulfolane does not readily degrade, but can in certain conditions.

# Properties of Sulfolane Continued



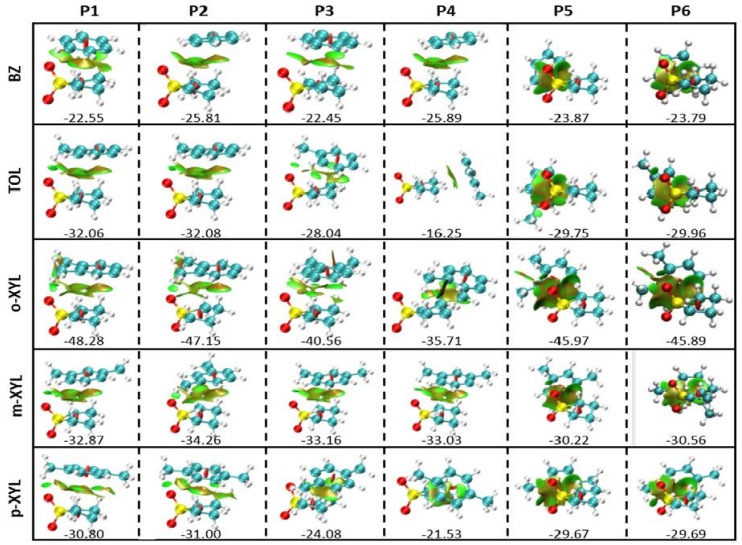
## Elevated Relative Permitivity

Sulfolane has a high relative permittivity of 43.4 @ 30 °C.



## Strong Solvation

Sulfolane can have strong solvation of cations which leads to increasing nucleophilicity (electron donating) of the less solvated anion.

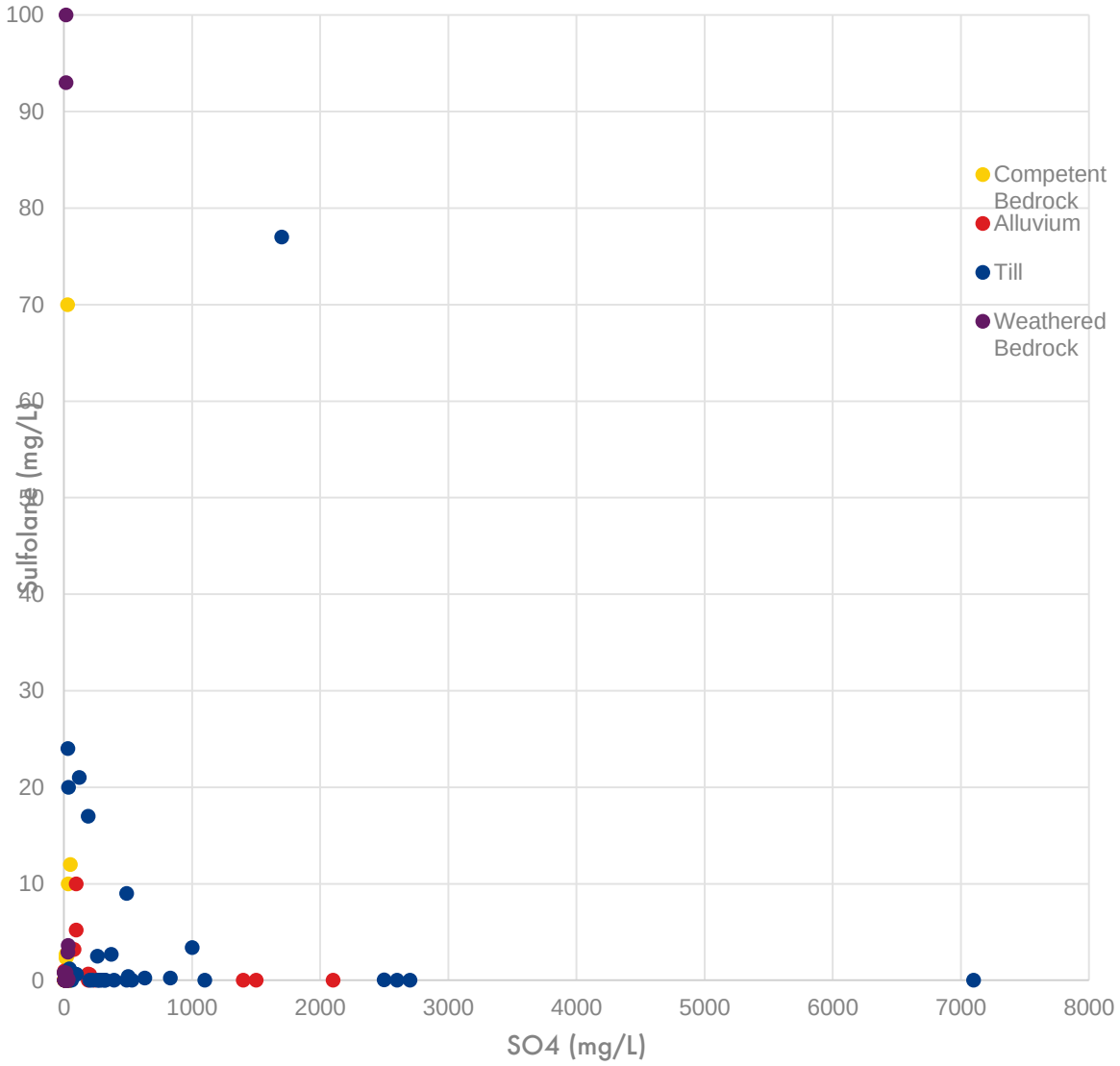



## Reaction with BTX

Strong reactivity with BTX has been identified.

# Data Correlation - Cross-plots

- Often the relation between COD and Sulfolane are used as evidence of presence and/or degradation of Sulfolane.
- The cross-plot can present linear patterns, logarithmic patterns, or no pattern at all. Example shown on the right: $SO_4$ vs Sulfolane



# Importance of Experimental Designs

**Distilled (DI) Water**

- To establish baseline.

**Synthetic Groundwater**

- To simulate site conditions focusing on inorganics.

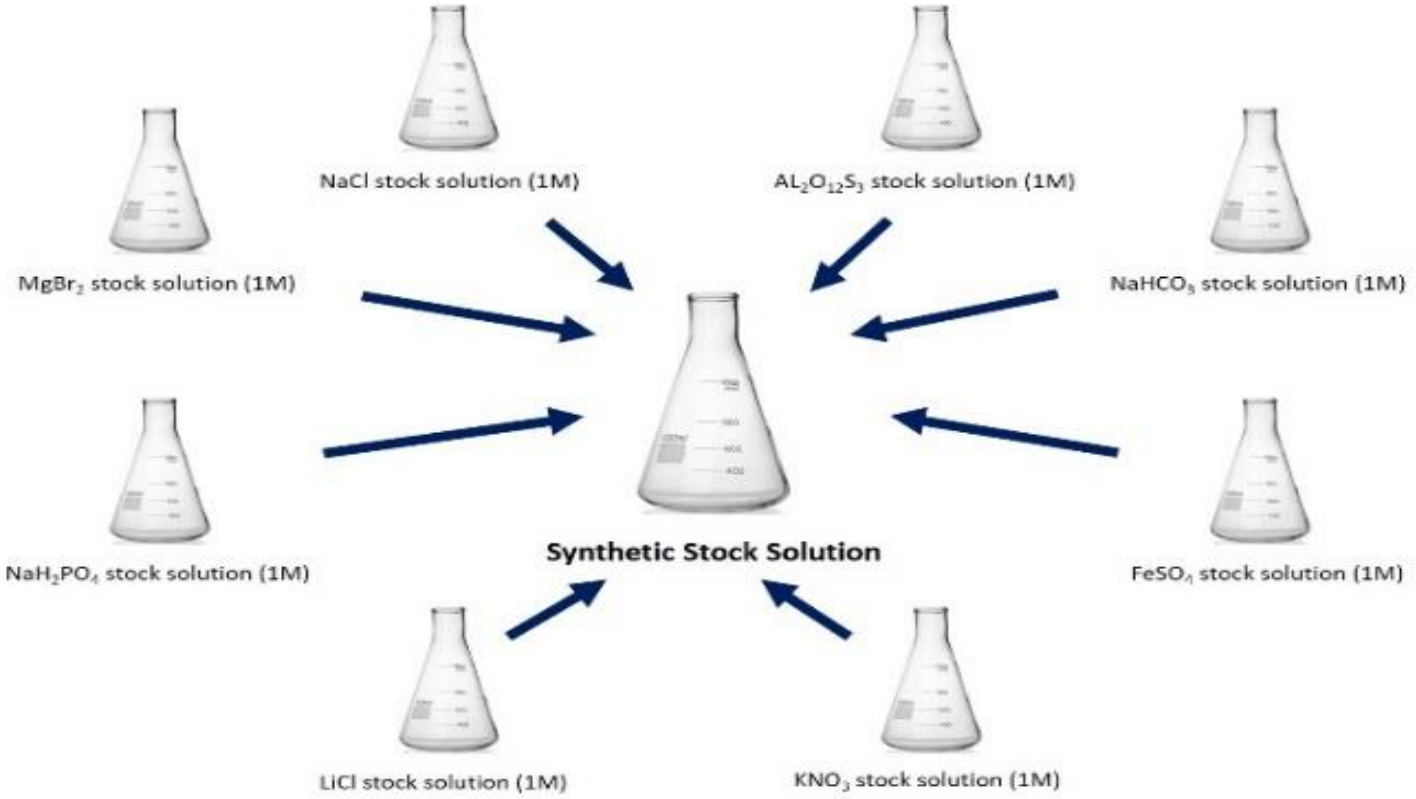
**Environmental Groundwater**

- Actual site conditions focusing on organics.

Increasing Matrix Complexity

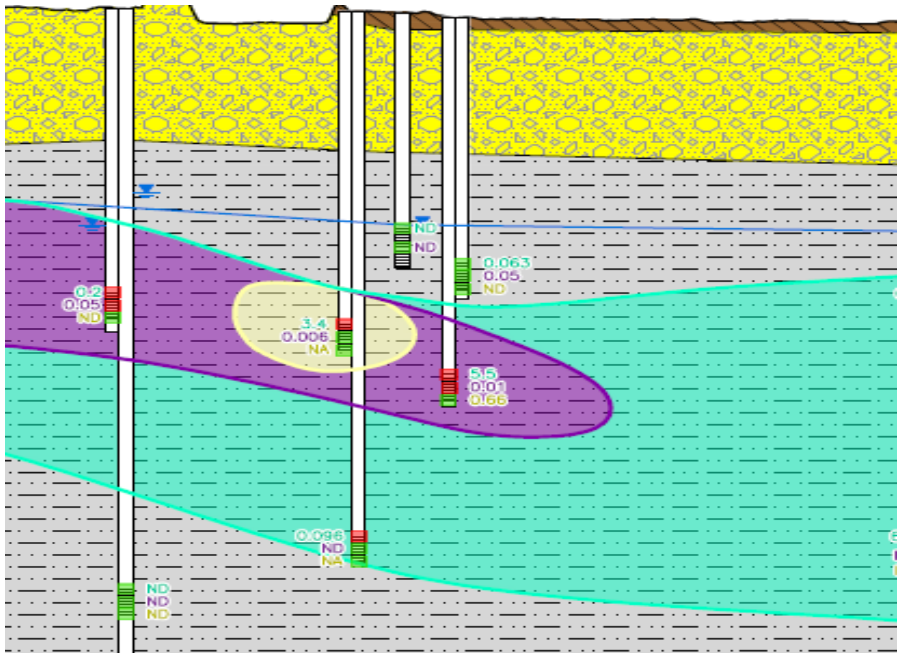
# Experimental Design Idea – synthetic groundwater

Using the major cation and anion analysis data from each site as a reference, calculations are made for each ion's concentration to recreate the on-site condition of inorganics in the lab.



# Experiment – Hydrocarbon Interactions

- Sulfolane was developed to remove aromatics from aliphatics, so how does this impact groundwater?
- Does interaction with hydrocarbons affect density effect of Sulfolane?
- Does it impact analysis
- First phase of bench scale experiments were performed with Sulfolane-BTEX mixtures with different treatments in order to determine the interactions under different conditions.
- Second phase of experiments are in progress.



# Conclusion

- Results to date indicate that co-contaminants can impact Sulfolane behaviour in groundwater.
- Based on these results site-specific evaluation of potential interactions is warranted.

## Take Away Message

- What is the cost of not designing investigation and remediation activities to account for the variability in Sulfolane behaviour?

# Questions and Answers