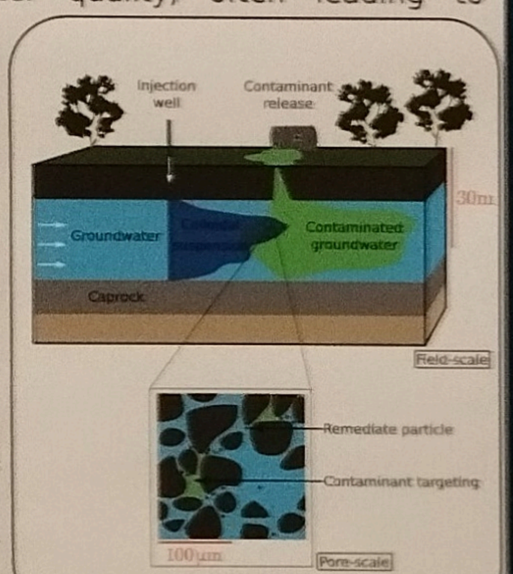
Diffusiophoresis in porous media for groundwater remediation

Florian Cajot[1], Cyprien Soulaine[1] and Sophie Roman[1]
florian.cajot@univ-orleans.fr, cyprien.soulaine@cnrs-orleans.fr, sophie.roman@univ-orleans.fr
[1]ISTO, UMR 7327, Orléans, France

A novel approach considers the concentration gradient generated by pollutants to drive particles toward contaminated zones for remediation.
This particle transport driven by **concentration gradients** is known as **diffusiophoresis**.
This phenomenon remains poorly studied in porous media, and existing models are largely limited to simplified cases.
A key question is how to incorporate diffusiophoresis into transport mechanisms within porous media.
We propose a model and OpenFOAM simulations to study particle movement in porous media under solute concentration gradients.
This will help improve understanding of how to model diffusiophoresis in dead-end pores and porous media.

1) Introduction

The presence of pollutants in soils and subsurface geological formations poses a serious threat to groundwater quality, often leading to contaminantion that renders the resource unusable. Effective remediation requires strategies capable of reaching the most isolated zones within the porous matrix. One approach is to use particles as decontaminants. In this context, we explore **diffusiophoresis**—the directed movement of particles under solute concentration gradients—as a promising mechanism to enhance particle transport in contaminated porous media. In particular how can diffusiophoresis be effectively incorporated into models of transport particle movement in complex porous media during groundwater remediation?

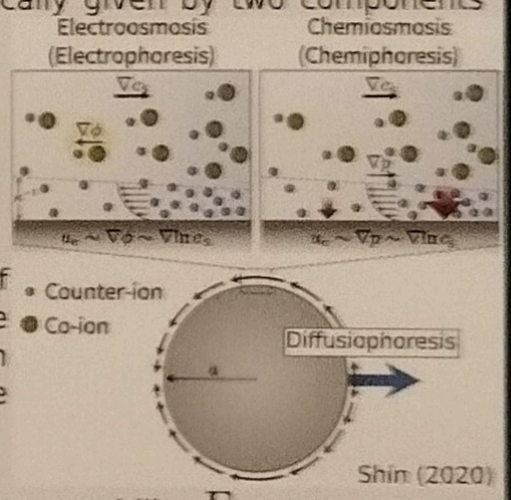


2) Modelling

Diffusiophoresis

Diffusiophoresis refers to the motion of microscopic colloidal particles driven by local solute concentration gradients, as first described by Derjaguin et al. (1947). For instance, trapped NAPL (Non-Aqueous Phase Liquid) within porous media can release chemical compounds, creating local concentration gradients that influence the movement of colloidal particles.

The phoretic motion of particle are physically given by two components Velegol et al. (2016)



➡ **Electrophoresis** is the migration of **charged particles** suspended in a solution of fluid under the influence of a **local electric field**, which exerts a force on the surface of the charged particle.

➡ **Chemiphoresis** is the movement of particles induced by a solute concentration gradient that generates an **osmotic pressure gradient** along the particle surface.

The phoretic motion is proportional to a mobility Γ_d and a solute concentration C_s ➡ $\mathbf{u}_{dp} = \Gamma_d \nabla \ln C_s$

Governing equation of fluid velocity

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla \frac{p}{\rho_w} + \nu \Delta \mathbf{u} - \frac{\nu}{k} \mathbf{u}$$

$\mathbf{u}$: fluid velocity — ν : kinematic viscosity
p : pressure — k : permeability

Governing equation of particle concentration

$$\partial_t C_p + \nabla \cdot ([\mathbf{u} + \mathbf{u}_{dp}] C_p) = D_p \Delta C_p$$

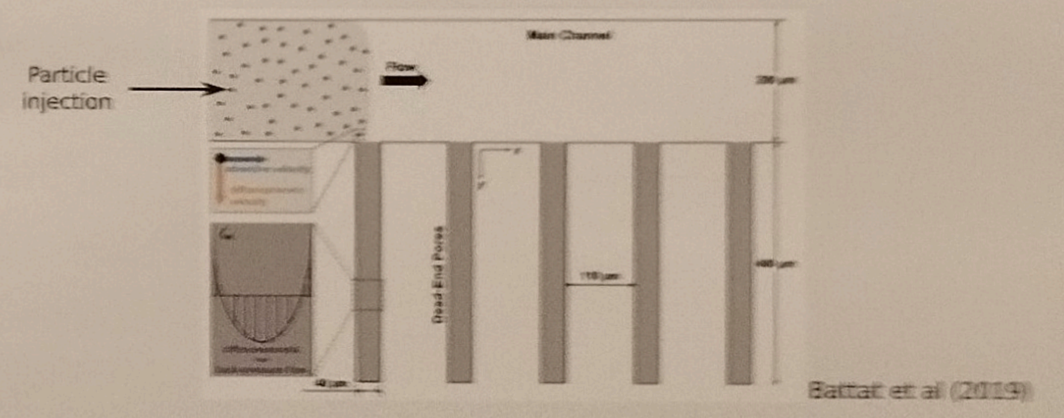
$$\boldsymbol{n} \cdot \nabla C_p = 0 \quad \text{(Boundary condition)}$$

C_p: particle concentration D_p: particle diffusivity

3) Modelling results

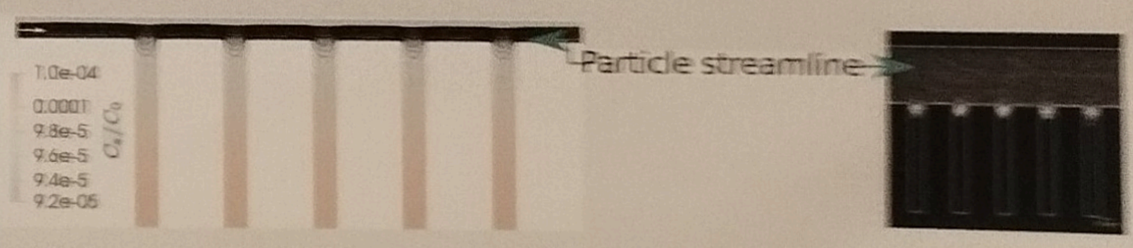
Comparison with literature experiment

Experimental set-up :



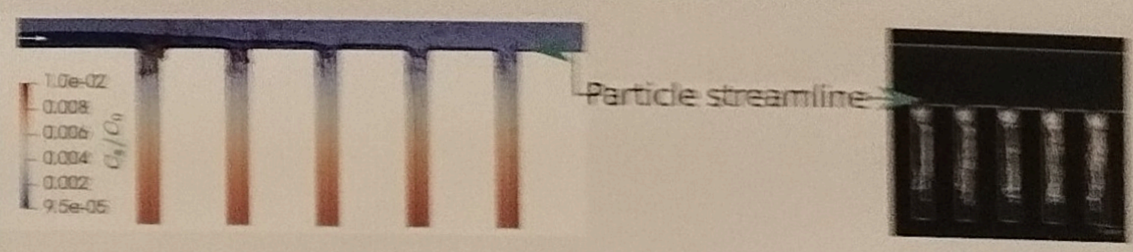
We compare our OpenFOAM simulations with experimental results from the literature under two conditions: (i) without a concentration gradient and (ii) with a concentration gradient.

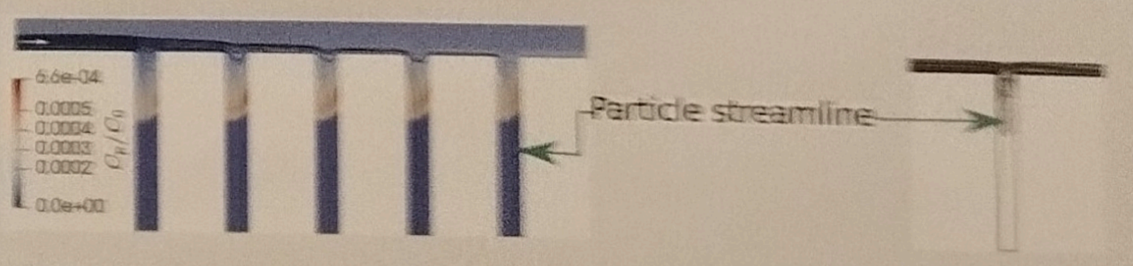
No solute concentration gradient



➡ Particle enter only at the entrance of the dead-end pores

Solute concentration gradient in dead-end pore





➡ Particle goes in the dead-end pores under the influence of the solute concentration gradient

The model capture diffusiophoresis in presence of solute concentration gradient

4) Conclusion

This modelling framework highlights the influence of solute concentration gradients on particle migration within dead-end pores via diffusiophoresis.

This approach may be extended to more complex porous media, including systems with reactive substrates, and validated through laboratory experiments. Furthermore, it provides a foundation for upscaling to the continuum scale by incorporating thermodynamic principles, such as free energy [Cajot et al 2025a,b].

References

Battat et al, (2019). Particle entrainment in dead-end pores by diffusiophoresis.
Cajot et al, (2025a). A free energy based model for water transfer in amphiphilic soils.
Cajot et al, (2025b). Model of drop infiltration into a thin amphiphilic porous medium.
Derjaguin et al, (1947). Kinetic Phenomena in the boundary layers of liquids 1. the capillary osmosis.
Shin, (2020). Diffusiophoretic separation of colloids in microfluidic flows.
Velegol et al, (2016). Origins of concentration gradients fordiffusiophoresis.

Acknowledgement

This work is funded by the European Union (ERC, TRACE-it, 101039854).