

# Transport of Organic Molecules in environment: insights from retardation in sedimentary rocks.

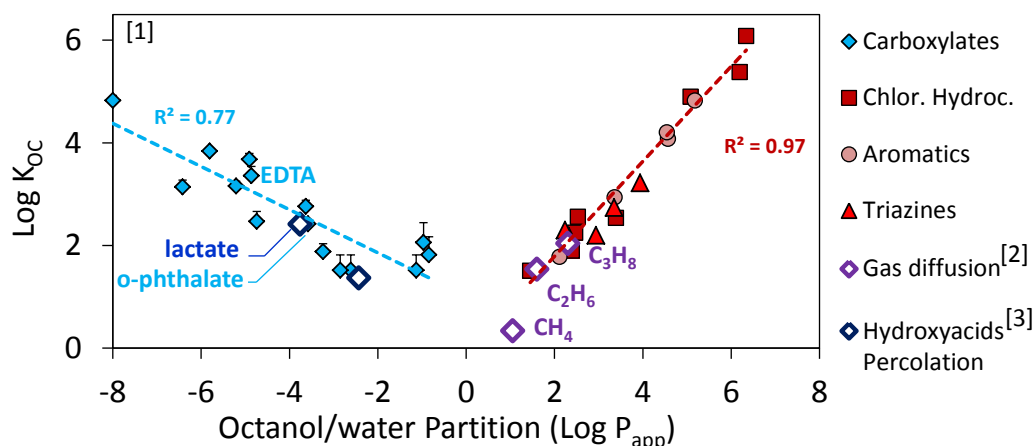
Dagnelie Romain V.H.<sup>1</sup>, Robinet J.-C.<sup>2</sup>

<sup>1</sup> Den-SERVICE d'Etude du Comportement des Radionucléides (SECR), CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France.

<sup>2</sup> Andra, R&D Division, parc de la Croix Blanche, 92298, Châtenay-Malabry, France

E-mail contact: [romain.dagnelie@cea.fr](mailto:romain.dagnelie@cea.fr)

Organic molecules are widely studied in environmental sciences, marine chemistry, soil- and geo-sciences. Among them, anthropogenic organic matter (AOM) can be potentially released from hazardous waste and migrate through geological rock formation or soils. AOM refers to a wide range of compounds, including both ionic and neutral molecules, polar and apolar molecules. The ionic polar molecules are highly soluble in water and more mobile in soils and rocks. The neutral (poly)aromatic compounds are less soluble, often absorbed by soil organic matter, but also more resistant against (bio)degradation. For all these compounds, adsorption or absorption processes can slow down their migration in environmental conditions. Consequently, understanding retardation phenomena of soluble organic matter in rocks and soils is crucial for safety assessments of waste storage, decontamination processes, ore extraction and remediation of soils.



**Figure 1: Correlation between octanol/water partition coefficient and adsorption of organic molecules.** For comparison, data on ions (blue) were divided by content of N.O.M. content of COx clay rock (0.6%).

A considerable effort has been made for 20 years to study migration phenomena in clay-rich geological barriers in the context of radioactive waste storage. Recent studies emphasized the adsorption of organic molecules on clayrocks<sup>[1]</sup>. One of our main findings is the correlation between adsorption and hydrophilicity of adsorbates, which highlights the role of various minerals as main sorbing phases (Figure 1). Hydrophobic molecules (red dots,  $\log(P_{APP}) > 1$ ) are absorbed by natural organic matter, whereas hydrophilic anions (blue dots,  $\log(P_{APP}) < -1$ ) are mainly adsorbed on oxides or clay minerals. These sorption data are strengthened by various migration experiments, e.g. *in-situ* diffusion of dissolved gas<sup>[2]</sup>, or percolation of hydroxyacids in compacted clays<sup>[3]</sup>. One of the main remaining issue is the discrepancy between adsorption data measured by batch experiments and retardation factors measured by diffusion experiments on highly compacted rocks<sup>[4]</sup>. Potential origins of these discrepancies, such as the “anionic exclusion” effect, will be discussed. The outcomes will be also discussed on a more general level, dealing with industrial processes and fate of organic molecules in the environment.

## References

- [1] Rasamimanana, S., Lefèvre G., Dagnelie, R.V.H.. *Adsorption of polar organic molecules on sediments: Case-study on Callovian-Oxfordian claystone*. Chemosphere 191 (2017) 296-303.
- [2] Vinsot, A., Anthony, C., Appelo, J. et al. *Natural gas extraction and artificial gas injection experiments in Opalinus Clay, Mont Terri rock laboratory (Switzerland)*. Swiss JGeosci 110 (2017) 375-390.
- [3] Chen, Y., Glaus, M. A. Van Loon, L. R., Mäder, U. *Transport of low molecular weight organic compounds in compacted illite and kaolinite*. Chemosphere 198 (2018) 226-237.
- [4] Dagnelie, R., Descotes, M., Pointeau, I., et al. *Sorption and diffusion of organic acids through clayrock: Comparison with inorganic anions*. Journal of hydrology 511 (2014) 619-627.