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Reversible Degradation of Diclofenac under Biotic, Denitrifying Redox Conditions: Geochemical Model and Uncertainty Quantification

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Drinking water resources and the associated delicate aquatic ecosystem are threatened by several contaminants. A growing emphasis is nowadays given to Pharmaceuticals, such as antibiotics and analgesics. Amongst these, Diclofenac poses major concerns due to its persistent nature and frequent detection in groundwater. Despite some evidences of its biodegradability under reducing conditions, Diclofenac attenuation is often interpreted through geochemical models which are too simplified, thus potentially biasing the actual extent of its degradation. In this context, we suggest a modelling framework based on the conceptualization of the molecular mechanisms of Diclofenac biodegradation which we then embed in a stochastic context. The latter enables one to quantify predictive uncertainty. Reference environmental conditions (biotic and denitrifying) are taken from a set of batch experiments that evidence the occurrence of a reversible degradation pathway (Barbieri et al., 2012), a feature that is fully captured by our model. The latter is then calibrated through a Maximum Likelihood approach, assisted by modern sensitivity analyses. Our results fully embed uncertainty quantification and support the recalcitrance of Diclofenac in groundwater.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

Barbieri, M., Carrera, J., Ayora, C., Sanchez-Vila, X., Licha, T., Noodler, K., Osorio, V., P_erez, S., Koock-Schulmeyer, M., de Alda, M.L., et al., 2012. Formation of diclofenac and sulfamethoxazole reversible transformation products in aquifer material under denitrifying conditions: batch experiments. Science of the Total Environment 426, 256-263.

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Primary authors: Mrs CERESA, Laura (Politecnico di Milano - Department of Civil and Environmental Engineering); Prof. GUADAGNINI, Alberto (Politecnico di Milano); RIVA, Monica (Politecnico di Milano); PORTA, Giovanni (Politecnico di Milano)

Presenter: Mrs CERESA, Laura (Politecnico di Milano - Department of Civil and Environmental Engineering)

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