Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.35123

Advances in modeling redox-dynamic environments: Some things I picked up over the years

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In this talk, I will review some new concepts and method developments that have lately made their way into the predictive modeling of contaminant and nutrient cycling in redox-dynamic environments. This review is based on my own journey and therefore overtly biased and far from exhaustive. Focus will be on incorporating process-based understanding into numerical models, not on the current progress in computational capabilities stimulated by the artificial intelligence revolution. The following are the main topics I will briefly touch on. (1) The energy content and, hence, the reducing power, of natural organic matter can be quantified by coupling molecular characterization methods to bioenergetic theory. (2) Reactive transport modeling helps framing the information content of environmental omics data, especially across temporally dynamic redox gradients. (3) Recent modeling advances call for more attention on the role of reactive oxygen species in subsurface biogeochemistry. The take-home message is that, until we can measure everything everywhere, knowledge-driven modeling remains an essential tool to overcome the inherent temporal and spatial data gaps in environmental research.