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From Single Reactions to Multicomponent Systems: A Thermodynamic–Kinetic Framework for Redox Reaction Networks

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Understanding environmental reaction systems has traditionally relied on the behavior of individual reactions characterized in controlled experiments. In natural environments, however, numerous abiotic and microbially mediated reactions proceed simultaneously and interactively, including processes that may remain unrecognized or overlooked, forming complex multicomponent systems. Such systems often exhibit emergent behaviors that cannot be inferred from analyses based on limited reaction sets alone. Bridging this gap between isolated reaction behavior and system-level environmental dynamics remains a central challenge in biogeochemistry and microbial ecology.

Recent advances in computational approaches now enable comprehensive exploration of large reaction spaces and provide a pathway toward predictive analysis of complex environmental processes. However, explicitly modeling the vast number of potential reactions and their interactions still requires substantial manual effort, particularly in constructing and implementing internally consistent reaction sets. This human cost currently limits the systematic application of multicomponent reaction models.

In this presentation, I introduce a thermodynamic–kinetic modeling framework designed to address this limitation by semi-automatically constructing and implementing reaction sets that include both abiotic and microbially mediated processes. The framework integrates reaction thermodynamics and kinetic rate formulations, including formulations for microbial metabolisms, to evaluate the feasibility and progression of multiple reactions under given physicochemical conditions. By coupling Gibbs free energy calculations with kinetic constraints, the model quantifies how competing and cooperating reactions collectively shape system-level behavior [1,2].

This reaction-set–centric approach enables systematic exploration of how environmental shifts or changes in microbial functional composition reorganize effective reaction networks and thereby alter observable system dynamics. I will present recent applications to environmental time-series and controlled incubation datasets, demonstrating that reaction progress and microbial metabolic expression can be interpreted as cumulative outcomes of multiple interacting reactions constrained by both thermodynamics and kinetics.

[1] Seto, M. et al. (2025) Thermodynamics underpinning the microbial community-level nitrogen energy metabolism, Environmental Microbiology, 27(2), e70055

[2] Seto, M. and Kondoh, M. (2023) Microbial redox cycling enhances ecosystem thermodynamic efficiency and productivity, Ecology Letters, 26(10), 1714-1725.