Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.38048

The limits of predictability: When can microbial activities in the environment be predicted from cell-level thermodynamics and kinetics?

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The chemistry of natural waters is shaped by a network of biogeochemical reactions that reflect the metabolic activities of functionally distinct microbial populations competing for resources. As metabolic capacities are constrained by the genetically determined cellular machinery and the physical and chemical conditions, theoretically, cell-level kinetics may be predicted from the rate-limiting factors for the given pathway, under given conditions. Interactions of microbial populations then might predict the net biogeochemical outcomes, and the shifts in their patterns across environments. Recent efforts suggest that such modeling may indeed be possible, at least in stable systems dominated by a relatively small number of microbial pathways, such as the anoxic strata of meromictic lakes [1]. They may also be useful for exploring experimentally inaccessible systems, such as early oceans [2]. The approach reproduces, for example, the dominance patterns of anaerobic pathways such as iron reduction, sulfate reduction, and methanogenesis, in sediments versus water column, and between freshwater and marine environments. Several knowledge gaps, however, need to be addressed to improve model transferability across a wider range of environments. A well-recognized discrepancy, for example, exists between the values of microbial parameters, such as Monod constants or cell-specific reaction rates, that are measured in lab studies versus natural waters. Several conceptual advances may improve energetics-based modeling, including refinements in parameters such as the amount of energy dissipated by cells during biosynthesis and the thresholds imposed by the energy conservation into ATP during catabolism. Describing the actively growing populations in surface waters and the less active biomass in deep subsurface within the same approach would require a better understanding of maintenance rates, under different growth regimes. We will provide examples for common respiratory and fermentative pathways in anoxic environments and highlight the under-appreciated role of physical transport in shaping biogeochemical distributions.

[1] Hawkins V. M., Sheik C. S. & Katsev, S. (2025) Understanding Ferruginous Versus Euxinic Conditions by Simulating Microbial Conditions in Meromictic Lakes. *Geobiology*, *23*(5), e70037.

[2] Katsev S. & Halevy I. (2025) Combined thermodynamic-kinetic-competitive controls on anaerobic respiration pathways and the chemistry of natural waters. *Earth ArXiv*, https://doi.org/10.31223/X53X79