frontiers | Frontiers in Ecology and Evolution

TYPE Editorial
PUBLISHED 21 September 2022
DOI 10.3389/fevo.2022.994090

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OPEN ACCESS

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SPECIALTY SECTION
This article was submitted to Models in Ecology and Evolution, a section of the journal Frontiers in Ecology and Evolution

RECEIVED 14 July 2022
ACCEPTED 06 September 2022
PUBLISHED 21 September 2022

CITATION
Thullner M, Brodie EL, Meile C and Pagel H (2022) Editorial: Modeling the link between microbial ecology and biogeochemical process dynamics. *Front. Ecol. Evol.* 10:994090. doi: 10.3389/fevo.2022.994090

Editorial: Modeling the link between microbial ecology and biogeochemical process dynamics

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KEYWORDS

numerical modeling, reactive transport, microbial ecosystem service, microbial degradation, biogeochemical reactions

Editorial on the Research Topic
Modeling the link between microbial ecology and biogeochemical process dynamics

Reactions carried out by microorganisms determine the fate of many compounds in terrestrial, marine and freshwater environments. The rates of these biogeochemical processes, e.g., nutrient recycling or the degradation of natural and anthropogenic compounds, depend on the properties of the involved chemical compounds, as well as the abundance, functional traits, and activity of the microbial community catalyzing these processes. This "microbial ecosystem service" is controlled by biogeochemical interactions between microorganisms and their abiotic (micro)environment in combination with ecological interactions between microorganisms within the community. All these interactions shape the genetic potential of the microbial community and their production of enzymes which determine degradation pathways and reaction rates in environmental systems. Many systems exhibit strong spatial and temporal variations, challenging a quantitative prediction of microbial activity and biogeochemical process rates.

Numerical models and other theoretical approaches have become established means for understanding and quantifying biogeochemical processes in natural and engineered systems. Since the complex interplay of factors affecting microbially controlled reactions is typically only partially known, these models are often highly simplified representations of *in situ* conditions which limits their predictive power. However, in recent years microbial methods have improved tremendously, producing data that yield novel insight into the composition of microbial communities, their ability to provide specific ecosystem services and their ecological behavior in different environments. This progress has led to increasingly sophisticated concepts linking the rate of biogeochemical processes to the dynamic behavior of (parts of) the microbial community (Song et al., 2014; Pagel et al., 2016; Meile and Scheibe, 2018; Thullner and Regnier, 2019).

The ongoing development of microbiological methods and the growing knowledge they provide thus prompts a continuous development of new modeling concepts describing the dynamics of microbial communities and of the biogeochemical processes they control.

This Research Topic presents a collection of novel approaches allowing for a link between the description of microbial ecology and biogeochemical process dynamics. Improved molecular microbiology methods, in particular the various omics techniques, provide a large number of indicators for the ability of a community to promote specific biogeochemical processes. The paper by Störiko et al. investigates whether complex modeling concepts tying these indicators to the associate process rates provide a benefit in accuracy compared to simple Monod-type modeling concepts. Their results indicate that the tested complex modeling concepts allow for a better process understanding, while their ability to reproduce measured substrate turnover is comparable to what can be achieved with the simple Monod approach.

Microbial growth and activity are controlled by various constraints, which requires concepts to consider them in a model approach. The paper by Chakrawal et al. focuses on the stoichiometry and bioenergetics of microbial growth. Their model simulates microbial carbon, nitrogen and energy turnover and allows quantification of the impact of coupled mass and energy fluxes on microbial growth. The authors use this approach to determine which degradation pathways dominate under different environmental conditions. The paper by Chavez Rodriguez et al. addresses bioavailability limitations on microbial degradation kinetics by combining rate expressions for substrate mass transfer across bacterial cell membranes, sorption and microbial degradation. This allows determining to what extent microbial degradation activity is limited by substrate bioavailability or if other factors are responsible for a compound to persist.

Microorganisms may use different strategies to deal with changing environmental conditions that affect their growth and activity. The paper by Manzoni et al. uses a modeling approach to investigate the effect of two different intracellular storage strategies (reserve storage vs. surplus storage) on the ability of the microorganisms to respond to reoccurring substrate and nutrient limitations. Their results show that the benefit of intracellular storage depends on the chosen storage strategy and that storage is most relevant for large variations in substrate and nutrient supply. Strategies to optimize growth performance and stress tolerance vary between different microbial community members. The paper by Wang and Allison studies the extent to which the legacy of past soil disturbances affects the functional composition of microbial communities and litter decomposition rates in response to temperature and precipitation shifts. Using a trait-based approach, the results of the study show that climate-driven legacy affects the degradation efficiency of the community and that interactions between community traits and environmental factors must be considered to predict microbial degradation. Acclimation represents an additional strategy by which microorganisms respond to environmental perturbation. In the paper by Wu et al. this effect is considered in a modeling approach in which microorganisms adjust the allocation of intracellular resources to adapt to substrate and energy availability and optimize their competitive fitness. The approach also allows for a better extrapolation of laboratory findings to conditions in the field.

By representing microbial interactions, modeling supports the testing and development of ecological theories. Xenophontos et al. model a two-species community consisting of a substrate degrading species and a cheater species assimilating a portion of the microbial resources released during substrate degradation. Their results show that despite the cheater species not contributing to the degradation process, stable coexistence of the two species is possible and such a two-species community is more resistant to extinction caused by invaders.

This collection of articles highlights advanced modeling concepts linking microbial ecological theory, molecular microbial ecology, and biogeochemical process dynamics. It demonstrates that mechanistic representations of (i) coupled mass and energy flows, (ii) physiological and structural adaptation processes of microbial communities, (iii) regulation and optimal control principles of microbial metabolism in models, improve our understanding of biogeochemical processes and the potential for their quantitative prediction in environmental systems. The studies in this Research Topic clearly show that improved process understanding and its reflection in models is only achievable by tightly integrating experiments and models and advocate further progress in model-data fusion through iterative cycling of experiments, model-based data interpretation, and optimal design of experiments (Siade et al., 2021).

Author contributions

MT wrote the draft of the manuscript. EB, CM, and HP edited and commented on the draft. All authors contributed to the article and approved the submitted version.

Funding

MT was supported by the Collaborative Research Centre AquaDiva of the Friedrich Schiller University Jena, funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – SFB 1076 – project number 218627073. CM was supported by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research, Genomic Sciences Program under Award Number DE-SC0020373. HP was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) within the priority program 2322 “SoilSystems” (project TraiMErgy, STR 481/12-1).

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