# Special Issue: Microbial Community Modeling: Prediction of Microbial Interactions and Community Dynamics

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## Editorial Special Issue: Microbial Community Modeling: Prediction of Microbial Interactions and Community Dynamics

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Microbial communities are networks of species, the interaction structure of which dynamically reorganizes in a varying environment. Even in a static condition, community dynamics are often difficult to predict due to highly nonlinear interspecies interactions. Understanding the fundamental principles of microbial interactions is therefore key for predicting and harnessing community function and properties. As extensively reviewed previously, mathematical models and computational methods that can predictively link interactions to community behaviors are indispensable tools for achieving this goal [1].

This Special Issue of Processes collects eleven papers from lead scientists and researchers active in the area, under the topic "Microbial Community Modeling: Prediction of Microbial Interactions and Community Dynamics". The collected papers cover various topics of interest: (1) two review/opinion papers discussing recent advances in biofilm modeling [2] and specific issues for successful collaboration between experimentalists and theorists [3]; (2) one paper on the dynamics of complex environmental communities [4]; (3) six papers dealing with fundamental aspects of microbial interactions and stability in model communities [5–10]; and (4) two papers on the development and utilization of microbial consortia for biotechnology applications [11,12].

The paper by Graham and Stegen [4] serves as a good example to show how mathematical modeling and simulation techniques can be useful for addressing fundamental ecological questions, for example, compositional and functional shifts in environmental communities under the influence of deterministic (such as selection) versus stochastic (such as dispersal) processes. Their model reveals that, under given postulates, dispersal can increase the proportion of maladapted taxa, which in turn decreases community-performed biogeochemical function.

Understanding microbial interactions in ecological communities can be greatly facilitated by studying model consortia of tractable complexity. Based on a relatively simple metabolic network structure, El Moustaid et al. [8] develop a dynamic model of a phototroph-heterotroph consortium to provide new insights into the role of oxygenic phototroph reactions in interspecies metabolic coupling. The study by Beck et al. [5] addresses more complex aspects of phototrophy, such as metabolic acclimation to stresses of irradiance,  $O_2$  and nutrients, through a comprehensive pathway analysis of the developed genome-scale metabolic network of a cyanobacterium. Their prediction of the shifts in growth efficiency, photosystem utilization and photorespiration is consistent with the experimental data.

Microbial interactions can significantly affect stability in communities (such as coexistence and resistance to invasion). For a nitrifying consortium composed of two ammonia-oxidizing bacteria and two nitrite-oxidizing bacteria growing in a chemostat, Dumont et al. [7] show that interspecies interactions enable the coexistence of the four species on two limiting nutrients. Henson and Phalak [9] investigate the effect of interspecies interactions on stability in a more mechanistic way by developing

a genome-scale community metabolic network model. For a model community composed of three species that represent Bacteriodetes, Firmicutes and Proteobactera in the gut microbiome, they identify four essential cross-feeding relationships enabling the coexistence of the three species. Moejes et al. [10] investigate the effect of culture media on community dynamics and stability. For a community composed of one microalgae and four bacterial species, they reveal that the community growth is more stable in minimal media than in complex media, as indicated by an accelerated culture crash in the latter. The developed dynamic model may serve as a monitoring tool with industrial applications, for example, for predicting harvesting time before a crash occurs. In the case study of a bioaugmented sand filter community, Daly et al. [6] extends the discussion to a spatially heterogeneous environment. Using an individual-based model accounting for interspecies competition (both deterministic and non-deterministic), they reproduce experimentally observed community dynamics and, further, reveal that community diversity (particularly evenness) promotes stability.

Examples showing the direct application of mathematical models for practical applications include the work by Wilken et al. [12] and by Capodaglio et al. [11] With an aim toward constructing consortia converting lignocellulose to valuable bioproducts, Wilken et al. use dynamic flux balance analysis to screen fermenting bacterial partners to pair with a given anaerobic fungus that possesses cellulolytic machinery. Consequently, they identify two candidate organisms found in the rumen microbiome. Capodaglio et al. provide a mathematical model for microbial fuel cells, which are drawing increased attention due to the capability of simultaneous waste treatment and energy recovery. Their work presents a microbial community model as a key component for reliable simulations of such complex systems.

The need to develop reliable mathematical models of microbial communities for both fundamental and applied science will keep increasing. A mechanistic understanding of interspecies interaction principles and the link to community function and properties will remain a key issue for predictive modeling. State-of the-art examples of microbial community modeling presented in this Special Issue may serve as valuable references for future research in this direction.

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