

Mechanistic Modeling of Dynamic Cellular Regulation Leads to Accurate Simulation of Biological Denitrification Process

Objectives

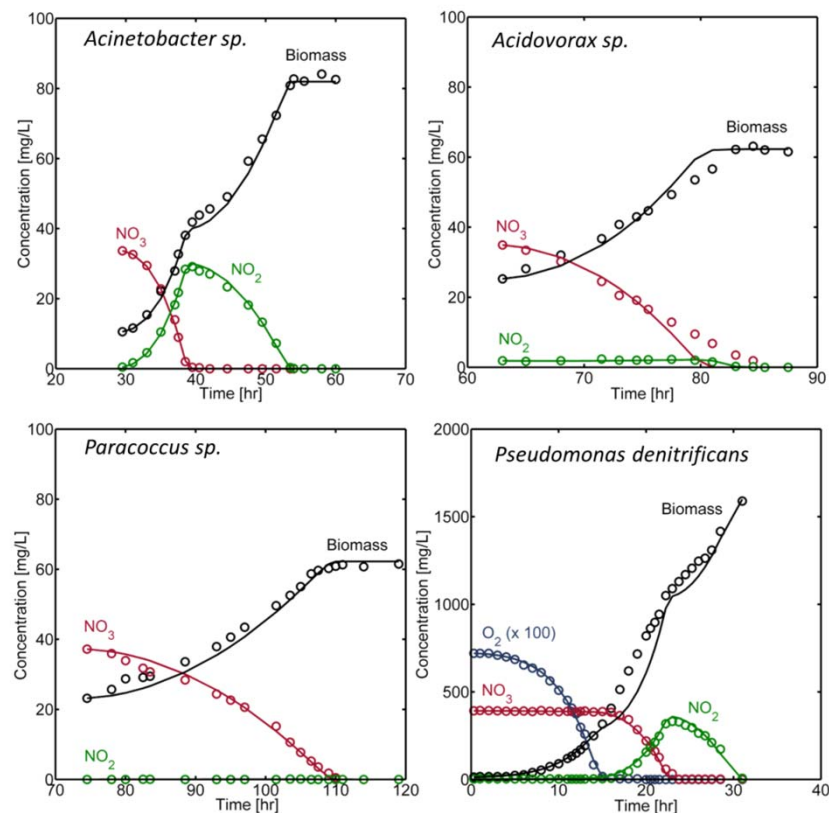
- Develop a high-fidelity dynamic metabolic model that enables an accurate prediction of complex bacterial growth patterns observed in denitrification process.

Approach and Results

- Constructed a dynamic metabolic model based on the cybernetic approach that accounts for cellular regulation based on the optimal control theory.
- Accurately simulated complex bacterial growth dynamics with fewer parameters compared to empirical inhibition-based kinetic models.
- Through a systematic comparative analysis, identified the key elements of regulation required for ensuring reliable model prediction.

Significance and Impact

- Along with other systems approaches in development, the current work provides a general modeling platform that is readily applicable to predict microbial community dynamics beyond the simulation of single bacterial growth.



Simulation of diverse bacterial growth patterns on multiple electron acceptors sequentially generated through denitrification process

Song, HS, and Liu, C. (2015) Dynamic Metabolic Modeling of Denitrifying Bacterial Growth: The Cybernetic Approach. *Industrial & Engineering Chemistry Research*, **54** (42):10221–10227. doi:10.1021/acs.iecr.5b01615.