

Integrating Genomics and Thermodynamics to Explore the Subsurface Microbial Impacts on Hydrogen Dynamics

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Our new modeling framework paves the way for predicting microbial and hydrogen interactions in the deep subsurface by unprecedented data integration.

Background & Motivation

- Hydrogen is a highly energy-dense, zero-carbon fuel whose conventional production from methane is both costly and CO₂-intensive.
- Deep, mineral-hosted H₂, for example, from forsterite-water reactions in the Midcontinent Rift beneath Nebraska and Lincoln (Fig. 1), offers a clean, geologically stored alternative; if tapped, it could significantly bolster Nebraska's energy economy and drive regional development.
- Microbial processes in the deep subsurface significantly affects H₂ availability and dynamics, but little is known about their interactions.

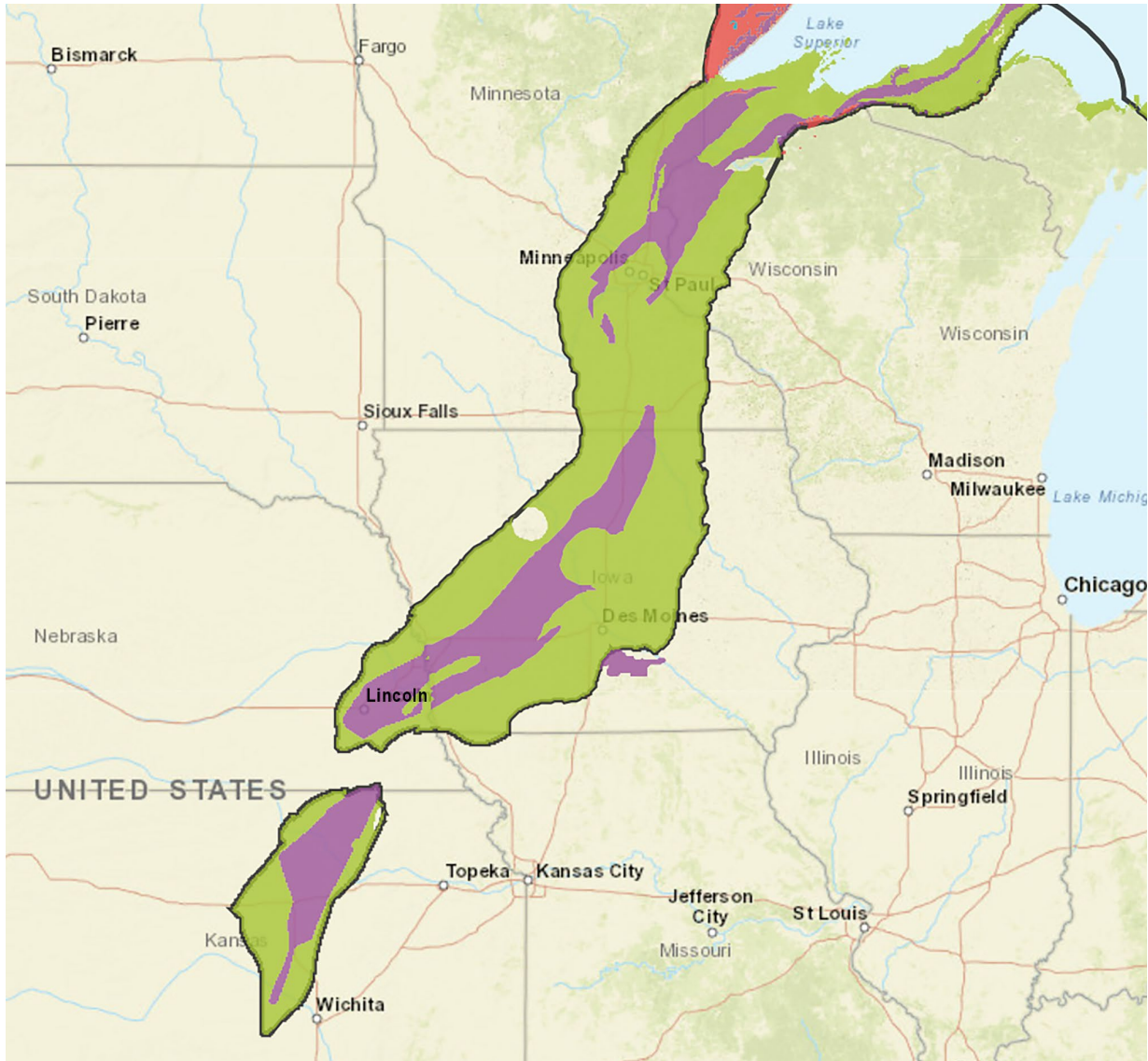


Figure 1: Map of the Midcontinent Rift showing forsterite-rich zones beneath Nebraska and Lincoln [1].

Objectives & Approach

- We use computational models to understand how microbes produce and consume the underground H₂ and identify metabolic byproducts (such as organic acids) that could potentially affect reservoir integrity and cause hydrogen loss.
- Traditional modeling approaches are ineffective, partly due to a number of kinetics parameters, the identification of which requires substantial amount of experimental data.
- This issues becomes even more serious for microorganisms such as those in the subsurface that are not culturable in experimental lab settings.
- We addressed this issue by minimizing the number of parameters based on genomics and thermodynamic analysis [2]. We theoretically estimate crucial kinetic parameters (growth rate, substrate uptake rate) directly from microbial genomic data. Specifically, we utilize genomic indicators like Codon Usage Bias (CUB) as proxies for microbial growth using tools as gRodon/Phydon, then use thermodynamic information to get metabolic rates. The workflow of our modeling approach is shown in Figure 2.

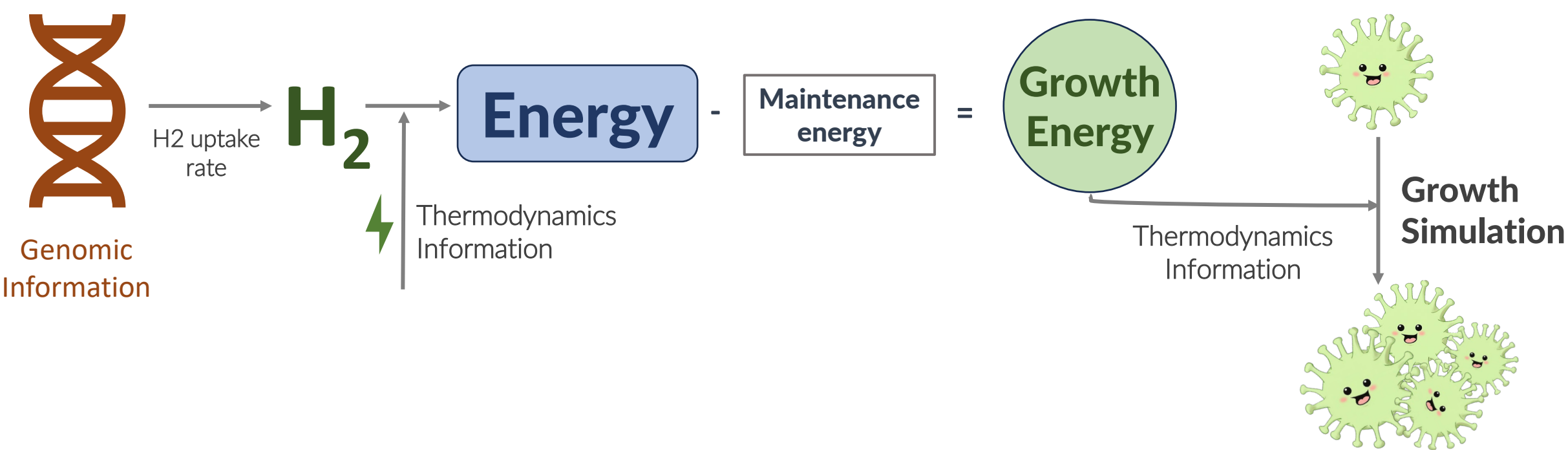


Figure 2: Workflow of incorporating thermodynamics and kinetic parameters to model a dynamic microbial community.

- We developed a dynamic microbial community model focused on H₂ and CO₂ metabolism, incorporating three most abundant organisms that were studied in an experiment [3]: two H₂-consuming autotrophs (*Methanobacterium* sp. and *Acetoanaerobium noterae*) and the heterotroph *Pseudomonas stutzeri* (Fig. 2).

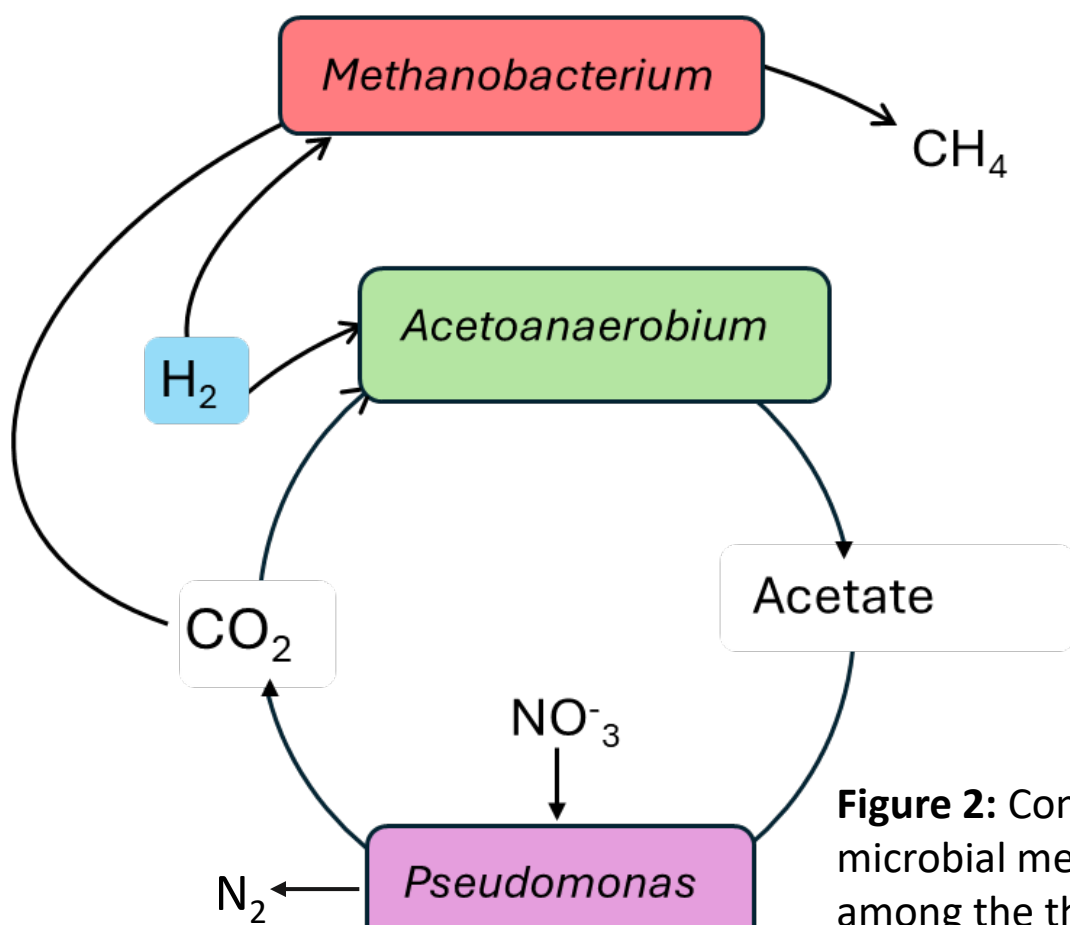


Figure 2: Conceptualization of microbial metabolic interactions among the three species.

Results

Microbial growth traits and energy use characterized by the identified model parameters

Despite *Acetoanaerobium* having a higher maximum growth rate, its lower energy yield compared to *Methanobacterium* means actual growth can be slower when energy availability is limited. Maintenance energy requirements (m_e) are similar across all three microbial species (Table 1).

Table 1: Key parameters in the three-member microbial community model

Species	max growth rate (h ⁻¹)	max substrate utilization rate (mol-X h ⁻¹ g-biomass ⁻¹)	Energy yield (mol ATP /substrate consumed)	maintenance energy (kJ h ⁻¹ g-biomass ⁻¹)
Methanobacterium sp.	0.042	0.041	0.75	0.08
A. Noterae	0.201	0.0056	1.11	0.05
P. Stutzeri	0.19	0.009	19.1	0.056

Our model is more consistent with the experimental data, compared to traditional kinetic models

Our model addresses traditional Monod kinetics limitations by incorporating thermodynamic constraints, reflecting realistic energy yields. It also illustrates how a species can support others' growth through its metabolic byproducts even while maintaining itself. For instance, *P. stutzeri* can grow using acetate produced by *A. noterae*, despite *A. noterae* itself only maintaining its biomass (Fig. 3B).

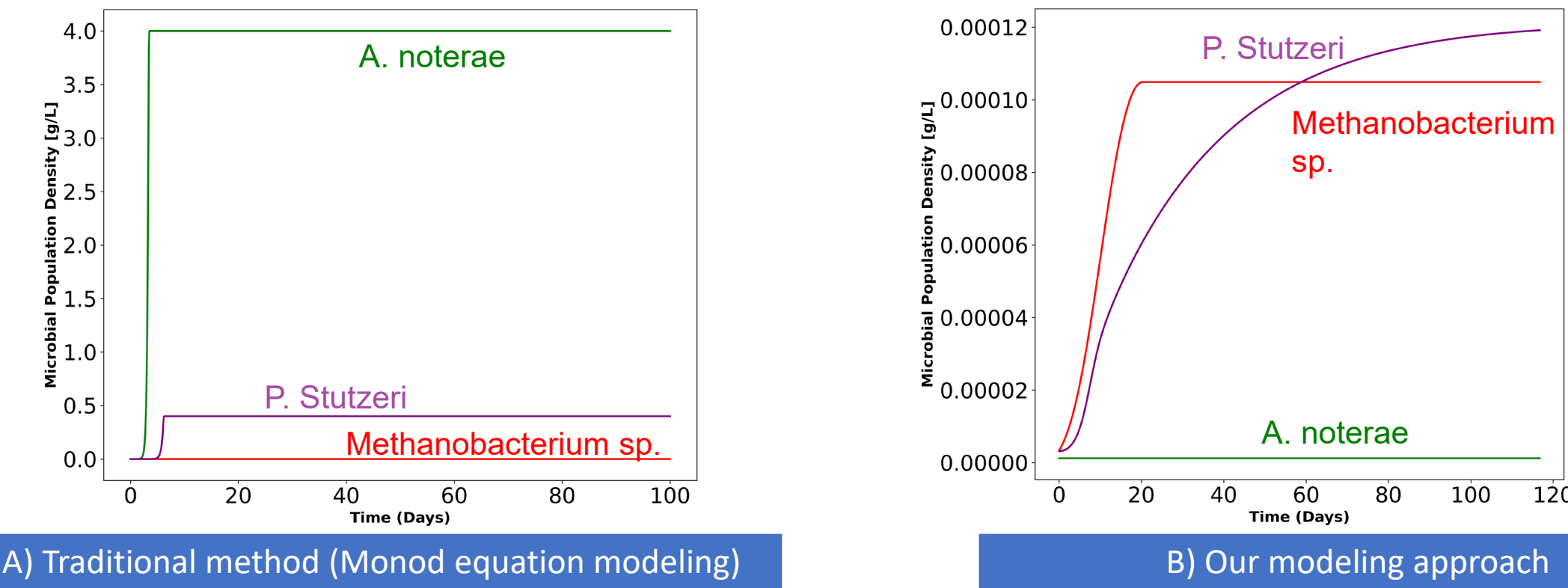


Figure 3: Traditional model vs our model simulation results for microbial dynamics

H₂ consumption significantly exceeds CO₂ consumption, and acetate remains low

Our model shows H₂ is consumed at a significantly higher rate than CO₂, and acetate concentration does not increase significantly due to its consumption by *Pseudomonas* (Fig. 4), similar to the findings in the methanogenesis paper [3].

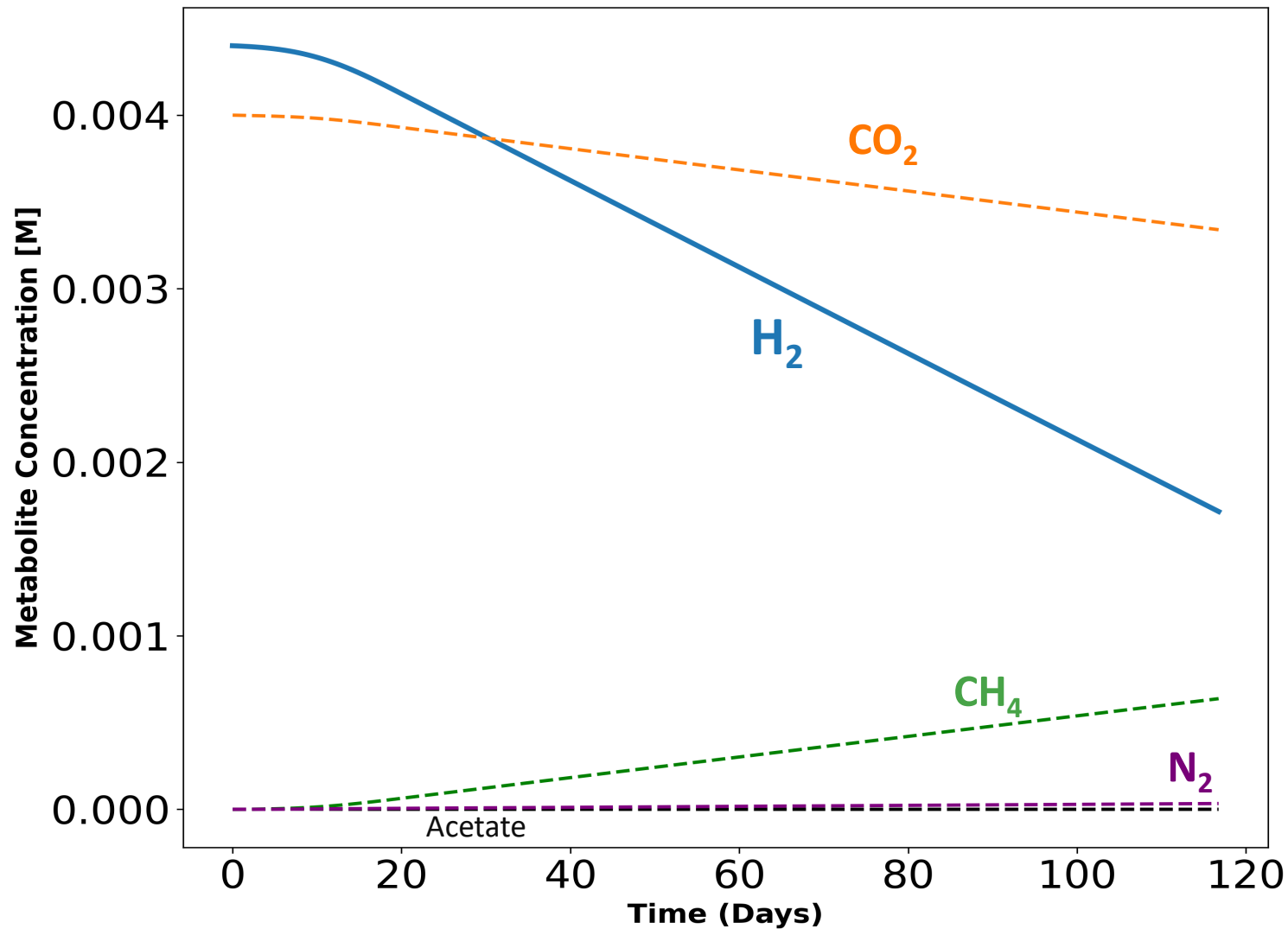


Figure 4: Our model simulation results for metabolite dynamics, especially H₂

Conclusions and Path Forward

- Our integrated genomics and thermodynamics model effectively addresses the challenge of parameterization in microbial growth models.
- The model clearly illustrates how microbial interactions significantly influence hydrogen dynamics in subsurface environments and has broad applicability in general microbial community modeling.
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Reference

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Acknowledgement

This work was supported by the Nebraska Public Power District through the Nebraska Center for Energy Sciences Research at the University of Nebraska-Lincoln.

