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Genome-Informed Thermodynamic Modeling Identifies Potential Drivers of Microbial Community and H2 Dynamics in the Deep Subsurface Environment

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Hydrogen (H_2) in the deep subsurface is a promising clean energy resource, but microbial activity can strongly change how much H_2 remains available over time. To study these dynamics, we developed a genome-informed thermodynamic model that does not rely on traditional, data-fitted growth parameters, which are difficult to obtain for subsurface microbes that are hard to culture, isolate, and test across many substrates. Instead, we use genomic traits and reaction energetics to estimate growth parameters and ATP yields, and couple this to mineral dissolution and gas–liquid exchange in a carbonate-buffered H_2 enrichment. The model represents four key microbes found in deep subsurface: the methanogen *Methanobacterium* sp., the acetogen *Acetoanaerobium noterae*, the heterotroph *Pseudomonas stutzeri*, and the sulfate-reducing H_2 oxidizer *Nitratidesulfovibrio* sp. We tested two known pathways for *Acetoanaerobium noterae* (Stickland fermentation of amino acids and hydrogenotrophic acetogenesis from H_2 and CO_2) by simulating each to see which one can realistically support its growth under the experimental conditions. By accounting for energy yields based on substrate supply, the model indicated that necromass-derived amino acids at the low cell densities in the experiment cannot sustain measurable growth, whereas hydrogenotrophic acetogenesis produced biomass trends consistent with the data. We then applied the model to the unexplained growth of *Pseudomonas stutzeri* in bottles designed to be anoxic, where its electron acceptor was not obvious from the media alone. We hypothesized that small amounts of O_2 were inadvertently entering the bottles during each sampling event, and model simulations showed that adding such realistic O_2 pulses (about 0.085 mL O_2 at STP, roughly 10 µmol per sampling time) was sufficient to explain the observed *Pseudomonas stutzeri* growth. This shows that even very small O_2 intrusions can alter community structure in nominally anoxic systems and potentially confound interpretations of hydrogen-driven experiments. Finally, we used the model to explore how carbonate dissolution controls community structure: when $CaCO_3$ dissolution released CO_2 slowly, *Nitratidesulfovibrio* sp. became the main H2 consumer, whereas faster or earlier CO_2 supply allowed *Methanobacterium* and *Acetoanaerobium noterae* to dominate and reproduced the experimental community and gas trends.