
Probabilistic Metabolic Modeling Identifies Key Microbiome Members in a Biomethanation Reactor That Reduces CO₂ into Pure Methane

Andrew Freiburger¹, Heather Nielsen², Daniel Morrow², Keith Tyo³, George Wells⁴ and Christopher S. Henry¹, (1)Data Science and Learning Division, Argonne National Laboratory, Lemont, IL, (2)Northwestern University, Evanston, IL, (3)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (4)Civil and Environmental Engineering, Northwestern University, Evanston, IL

Abstract Text:

Technologies that upcycle anthropogenic waste (i.e. landfill, sewage, industrial process gases and liquids) improve economies, public health, and environmental protection. Anaerobic digestion of anthropogenic waste produces biogas (40% CO₂, 60% CH₄), which can be refined through methanogenesis in a biomethanation reactor with H₂ feed into ≥95% pure CH₄. Hydrogenotrophic methanogens are a key microbial community for this process, but they compete with other biomethanation community members and are dynamically affected by the varying organic and inorganic carbon sources, which creates uncertainties and inefficiencies in full-scale biomethanation operations.

To gain a better understanding of the relationship between feed parameters, biomethanation communities, and the employed metabolic pathways that lead this carbon reduction, data from a lab-scale biomethanation reactor was processed and integrated into a new pipeline that leverages metabolic modeling (through linear optimization augmented with ML) to elucidate the active pathways and ecological roles of each community member. This pipeline **a)** matches the 16S RNA sequences to their closest hits in a database of reference genomes; **b)** assembles the union of metabolic functions associated with the reference genomes of all closest hits; **c)** reconstructs a genome-scale metabolic model (GEM) from each of these union of metabolic functions, which best captures the metabolism of the organism from which the 16S came; **d)** assembles these GEMs into a single compartmentalized community model (cGEM) with the experimentally observed member abundances; and **e)** simulates the cGEM via the Flux Balance Analysis algorithm over the experimental media.

The results from the above pipeline identify the critical members and pathways that reduce carbon from nothing more than 16S RNA sequences and media information, thereby opens the possibility for stably optimizing the purity and yield of biomethane from this system towards a circular bioeconomy. This pipeline has broad implications for automating the process for gleaning basic understanding of microbial communities from simple experimental measurements, and will be implemented into a KBase Application with point-and-click functionality that further streamlines this pipeline and accelerates bioinformatics research.

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Submitter's E-mail Address:

afreiburger@anl.gov

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First Presenting Author**Presenting Author**

Andrew Freiburger

Email: afreiburger@anl.gov -- Will not be published

Argonne National Laboratory
Data Science and Learning Division
Lemont IL
USA

Second Author

Heather Nielsen

Email: heathernielsen2026@u.northwestern.edu -- Will not be published

Northwestern University
Evanston IL
USA

Third Author

Daniel Morrow

Email: DanielMorrow2025@u.northwestern.edu -- Will not be published

Northwestern University
Evanston IL
USA

Fourth Author

Keith Tyo

Email: k-tyo@northwestern.edu -- Will not be published

Northwestern University
Department of Chemical and Biological Engineering
Evanston IL
USA

Fifth Author

George Wells

Email: george.wells@northwestern.edu -- Will not be published

Northwestern University

Civil and Environmental Engineering

Evanston IL

USA

Sixth Author

Christopher S. Henry

Email: cshenry@anl.gov

Argonne National Laboratory

Data Science and Learning Division

Scientist

Lemont IL

USA