Syngas Biomethanation: metabolic modeling to improve methane production

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The biological conversion of syngas (H_2, CO, CO_2) into methane presents an attractive route for sustainable bioenergy production. Trickle bed reactors (TBRs) offer a promising configuration for syngas biomethanation by enabling biofilm formation, which enhances the process stability. However, process efficiency remains constrained by mass transfer limitations and thermodynamic bottlenecks influencing microbial interactions and metabolic pathways. The reactor environment facilitates key metabolic pathways, including hydrogenotrophic and acetoclastic methanogenesis, carboxydotrophic hydrogenogenesis, and syntrophic acetate oxidation. The interplay of these pathways is governed by the availability of syngas constituents, gas-liquid mass transfer, and diffusive transport within the biofilm. Notably, hydrogen accumulation was found to impose thermodynamic constraints that hinder CO conversion, thereby affecting microbial consortia composition. In this study, we focus on genome-scale metabolic modeling to elucidate the role of microbial communities in syngas biomethanation, particularly the impact of the microorganism interactions within the reactor to optimize methane conversion. By integrating metabolic modeling with reactor performance data, we establish a framework for optimizing reactor operation through targeted interventions in gas composition control and biofilm structure management.

Samples were collected from the central part of the reactor to analyze the microbial community involved in methanation. A genome-centric metagenomics approach was used to reconstruct and characterize key microbial members. Metabolic models were developed at both single-species and community levels to explore cooperation and competition dynamics, with a focus on cross-feeding mechanisms and the impact of key species on biogas upgrading. Additionally, a pairwise analysis of microbial models was conducted to assess the impact of specific interactions on methane production and biomass growth. Finally, in silico simulations were performed to evaluate bioaugmentation strategies for optimizing syngas-to-methane conversion.

Biochemical data indicated that even slight changes in the gas retention time or liquid recirculation rates impacted the microbial community, drastically changing the total amount of methane converted. Using genome-scale metabolic modelling of the community, we managed to accurately simulate the interactions between species, predicting similar values of methane produced (Figure 1). Cross-feeding interactions, particularly the transfer of hydrogen, formate, and acetate between syntrophic partners, played a crucial role in sustaining methane production. By integrating metabolic modeling with reactor performance data, we established a framework for optimizing reactor operation through targeted interventions in gas composition and biofilm structure. Pairwise metabolic simulations revealed key metabolic exchanges driving methanogenesis under different reactor conditions. Simulating optimal conditions for both microbial growth and methanogenesis allowed us to identify a set of microbial species that could enhance reactor performance (Figure 2). By augmenting the in silico community with these selected species pairs, we achieved a significant improvement in methane production from syngas.

This study underscores the critical role of metabolic modeling in understanding and optimizing microbial community dynamics in syngas biomethanation reactors. The insights gained contribute to the broader application of microbial metabolic modeling in engineered bioprocesses aimed at sustainable bioenergy production. Future work will refine the community models with experimental validation and expanded kinetic parameters to improve predictive accuracy.

Table 1. Biochemical parameters of the reactions involved in the study.

Steady state samples	Syngas quality index (SQI)	Gas retention time (h)	Liquid recirculation rate (mL/min)	Trace elements
High GRT - Low SQI	**1.2**	3.0	20.0	No
High GRT	**2.7**	3.0	20.0	No
Low GRT	2.7	**1.0**	20.0	No
Low GRT - High LRR	2.7	1.0	**280.0**	No
Low GRT - Trace elements	2.7	1.0	20.0	**Yes**

Figure 1. Comparison of the measured and simulated methane production for the different reactor conditions.

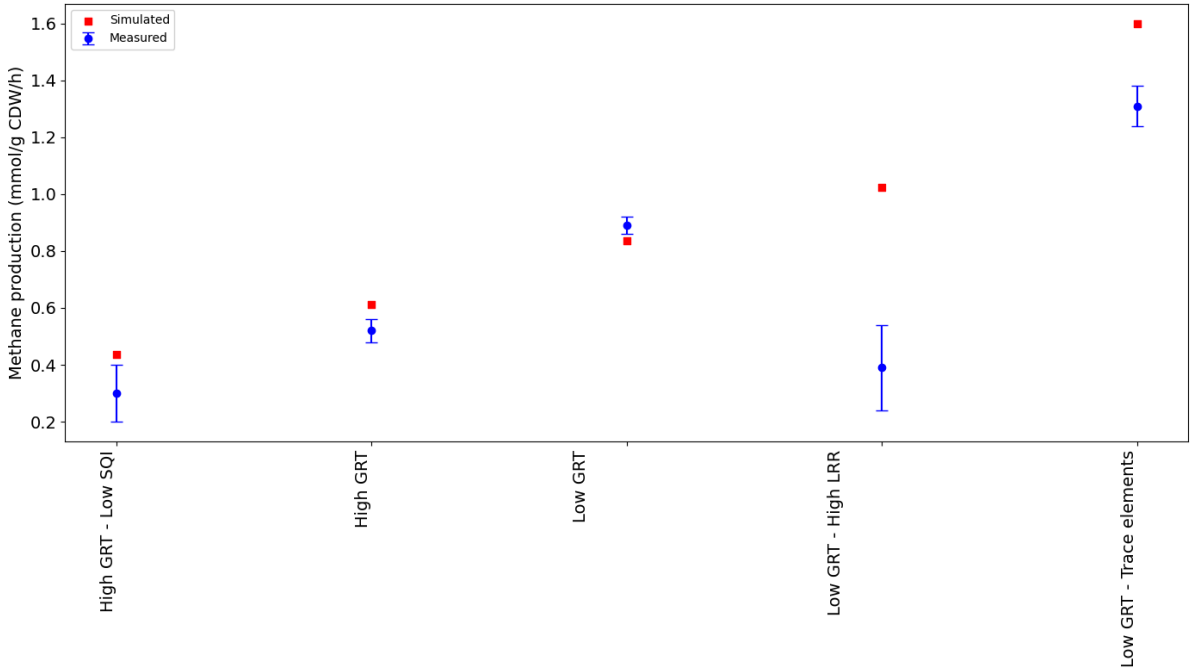

Figure 2. Pairwise metabolic modelling of species highlighting potential microbial dependencies and/or syntrophic relationships.