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Kinetics of Anaerobic Methane Oxidation: A Metabolism-based Modeling Approach

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Anaerobic oxidation of methane coupled to sulfate reduction is crucial in preventing methane, a potent greenhouse gas, from escaping to Earth's atmosphere. As methane diffuses upward from deeper marine sediments, ANaerobic MEthanotrophic (ANME) archaea capture these molecules and form a consortium with Sulfate Reducing Bacteria (SRB) in order to transfer electrons from methane oxidation to the reduction of sulfate. Current models assume that ANME uses the pathway of "reverse methanogenesis" to oxidize methane and transfer electrons to SRB that carries canonical sulfate reduction pathway [1]. This hypothesis can be tested with the consortium in laboratory settings, but the consortium cultivation has remained challenging.

Here we test this hypothesis by building a metabolic model for the consortium of ANME and SRB. Our model includes two metabolic networks: one accounts for the enzymes and coenzymes in the network of reverse methanogenesis, and the other includes those in sulfate reduction network. We track the fluxes of carbon, sulfur, and energy through the two networks using reversible Michaelis-Menten kinetics, and simulate the expression of the enzymes using optimization. Modelling outputs include optimal enzyme levels, metabolite concentrations, and rates of methane oxidation and sulfate reduction.

We applied the metabolic model and simulated the metabolisms of the consortium by using *in situ* concentrations of methane and sulfate. The simulated rates of methane oxidation and sulfate reduction match well with previous field observations [2]. These results support that the "reverse methanogenesis" pathway combined with canonical sulfate reduction is a feasible mechanism. Furthermore, the results shed new light on how the limited chemical energy released by anaerobic methane oxidation is shared between the two members of the consortium. Thus, our model provides a framework for understanding biological processes that have so far escaped laboratory cultivation.

[1] McGlynn, S. E., et al. (2015). *Nature*, *526*(7574), 531–535.

[2] Nauhaus, K., et al. (2005). *Environmental Microbiology*, *7*(1), 98–106.