Predicting methane production fluxes from the kinetics of methanogenesis enzymes

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Methanogens produce methane from acetate, H_2, and other products of organic matter degradation, driving the biogeochemical cycling of carbon (Thauer et al., 2008). Predicting methane production fluxes is a key step to understanding methanogens and the dynamics of methane production in natural environments. Current approaches compute methane fluxes using the Monod equation (Jin et al., 2013). Here we develop a new kinetic model for methanogenesis pathways, and apply the model to predict the kinetics of methanogenesis by *Methanosarcia barkeri*.

Our kinetic model accounts for 19 enzymes and 8 coenzymes in the methanogenesis network of *M. barkeri*, tracks the fluxes of carbon and energy using the reversible Michaelis-Menten kinetics, and simulates the expression of the enzymes using nonlinear optimization. The modelling output includes the optimized enzyme concentrations for maximum ATP production fluxes, metabolite concentrations, methanogenesis rates, and their responses to substrate availability in the environment. These predictions match well with previous laboratory observations, including the *in vitro* enzyme activities in crude cell extracts, and the kinetics of methanogenesis by *M. barkeri* and its mutants.

These results demonstrate that methane fluxes can be computed from the thermodynamics and kinetics of individual enzymes. By predicting the expression of methanogenesis enzymes, the new method also offers the potential for investigating methanogen metabolism and its interaction with environmental conditions. For example, the results suggest that more proteins are allocated to enzymes of less catalytic power, and enzyme expression does respond notably to the availability of energy sources.

References

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