Thermodynamic efficiency of microbial energy transformation – a genome-scale metabolic modeling perspective

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Microbes save the energy available in the environment by making ATPs, and then use the ATPs to power the synthesis and maintenance of biomass. The ratio of the conserved energy to the available energy gives the efficiency of microbial energy transformation, a parameter that determines the significance and impact of microbial metabolisms in the environment. Evaluating the thermodynamic efficiency requires *a prior* the ATP yield of microbial catabolism, which is not available for most microbial processes. Here we apply a genome-scale metabolic modeling framework to predict the thermodynamic efficiency of microbial process, and how the efficiency may respond to variations of environmental conditions.

We simulate microbial energy transformation using genome-scale metabolic models. We break these models into submodels of catabolism and biosynthesis, and simulate the catabolic submodels using kinetic modeling and the biosynthesis submodels using stoichiometric modeling. The stoichiometric modeling gives the flux ratios of ATP, redox cofactors, and carbon sources consumed by cell growth. The kinetic modeling predicts the fluxes of ATP production at given environmental conditions and metabolic objectives. By integrating the two submodels, we can compute the energy fluxes from the environment to the ATP pool and then to biomass, and how the energy fluxes respond to the perturbations of the environment.

We applied the modeling framework to evaluate the thermodynamic efficiency of acetoclastic methanogenesis – a common anaerobic process in natural environment. Specifically, we simulate the metabolism of Methanosarcina barkeri growing on acetate. The results show that the energy fluxes driven by the metabolism depends on acetate concentrations in the environment, but the thermodynamic efficiency remains relatively stable, around 50%. This efficiency falls below previous theoretical estimations, but is consistent with laboratory observations. Our results demonstrate the feasibility of the thermodynamic assessment by combining environmental conditions and metabolic models, and how genome-scale metabolic models may help better understand the occurrence and significance of microbial processes in natural environments.