

## Integrating bioenergetics into biogeochemical reaction-path modeling

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Predicting accurately the kinetics of microbial metabolisms in natural environments is essential for both geomicrobial and geochemical applications. Because of the limited energy availability in the environment, these predictive capabilities require a rigorous account on how the available energy controls the rates of microbial metabolisms. Currently, several theoretical models are available for this purpose. The question remains: which model better describes the impact of bioenergetics on microbial kinetics?

Here, these models were tested by applying to both redox enzymes (i.e., NADH dehydrogenase, terminal oxidase, etc.) and cellular respiration. The results suggest that, among various models, the thermodynamic potential factor

$$F_T = 1 - \exp[(\Delta G + \Delta G_C)/\chi RT]$$

describes adequately the dependence of reaction rates on the available energy (i.e.,  $\Delta G$ ) in the environment. Here  $\Delta G_C$  represents the energy saved by microbial catabolism,  $\chi$  is the number of times the rate determining steps occur in the metabolism,  $R$  is the gas constant, and  $T$  is the absolute temperature.

To demonstrate how the thermodynamic factor can help elucidate biogeochemical processes in the environment, a metabolic network model was constructed for the degradation of natural organic matter (NOM) in the environment. In this model, NOM is fermented to acetate and  $H_2$ , which are then oxidized by acetotrophic and hydrogentrophic sulfate reduction, and acetoclastic and hydrogentrophic methanogenesis. This model was then applied to predict the distribution and rates of biogeochemical processes in the sediments of Lake Washington, USA. The model accounting for the thermodynamic control predicts that sulfate concentrations decreased with sediment depth, but remained constant ( $\sim 15 \mu\text{molal}$ ) at depths beyond 15 cm. At the same time, acetate,  $H_2$ , and methane concentrations increased steadily with depth. However, models without an accurate description of the thermodynamic control predict dramatically different results. Significantly, sulfate would be consumed rapidly and its concentrations decrease to zero at sediment depths below 10 cm.

[1] Jin & Bethke (2005) *Geochim. Cosmochim. Acta* **69** 1133–1143. [2] Jin & Bethke (2007) *Amer J of Sci* **307** 643–677.

## Assessment of impact of land cover change on Mississippi River basin hydrology with satellite data

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The land cover change in the Mississippi River (MR) basin and its impact on the basin-scale hydrology were quantitatively assessed using the Global Inventory Modeling and Mapping Studies (GIMMS) normalized difference vegetation index (NDVI) data. Four levels of the vegetation changes in the basin were established based on the annually averaged NDVI values from 1982 to 2003. Roughly one-third of the MR basin suffered severe or slight vegetation degradation, mostly in the upper MR basin, including Iowa, Wisconsin, and Minnesota. The main cause for the deteriorating vegetation coverage in the MR basin is the conversion of perennial vegetation to annual crops.

The large-scale land cover change in the MR basin may significantly affect the basin hydrology, especially the allocation of the main components, e.g., precipitation (P), streamflow (Q), and evapotranspiration (ET), of the basin-scale water cycle. More precipitation has been routed into the MR since 1938 because vegetation degradation have reduced the amount of ET in the basin: the ratio of ET over P decreased 9% from 78% in 1938 to 69% in 2003 while the ratio of Q over P increased 9% from 22% in 1938 to 31% in 2003. The increase in Q is mainly in the baseflow (BF) which increased 76 mm from 117 mm in 1938 to 193 mm in 2003. The ratio of BF over Q increased 9% from 68% in 1938 to 77% in 2003 while the ratio of overland flow (OF) over Q decreased 9% from 32% in 1938 to 23% in 2003. This means that more water has been routed into the river through subsurface because of the land cover change.

There is an inverse relationship between the NDVI and Q or BF in the basin since the NDVI decreases as Q or BF decreases. Such inverse relationship doesn't exist for the NDVI and OF.