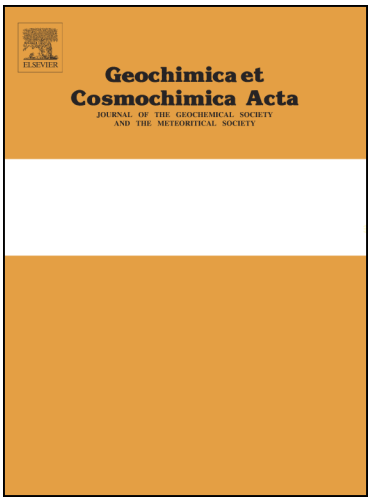

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Benjamin Shapiro, Tori M. Hoehler, Qusheng Jin

PII: S0016-7037(18)30502-7
DOI: https://doi.org/10.1016/j.gca.2018.08.047
Reference: GCA 10920

To appear in: *Geochimica et Cosmochimica Acta*

Received Date: 17 September 2017
Accepted Date: 30 August 2018

Please cite this article as: Shapiro, B., Hoehler, T.M., Jin, Q., Integrating genome-scale metabolic models into the prediction of microbial kinetics in natural environments, *Geochimica et Cosmochimica Acta* (2018), doi: https://doi.org/10.1016/j.gca.2018.08.047

Integrating genome-scale metabolic models into the prediction of microbial kinetics in natural environments

Benjamin Shapiro[1], Tori M. Hoehler[2], and Qusheng Jin[1,*]

[1]Department of Earth Sciences, University of Oregon, Eugene, OR 97403, USA

[2]NASA Ames Research Center, Mail Stop 239-4, Moffett Field, CA 94035, USA

[*]Corresponding author. qjin@uoregon.edu. Phone: (541) 346-4999.

Abstract

We propose a new method to predict microbial metabolic rates in natural environments using genome-scale metabolic models. This method is a hybrid of existing approaches, i.e., rate laws and flux balance analysis (FBA). It accounts for the availabilities of chemical energy and growth nutrients in the environment, and applies FBA independently to the respiration and biosynthesis pathways of genome-scale metabolic models. We illustrate the new method by modeling the metabolism of a representative methanogen – *Methanosarcina barkeri* – in laboratory reactors and in pristine and biostimulated aquifers. The laboratory application demonstrates that the hybrid method predicts the rates of individual biochemical reactions within overall cell metabolism and tracks, explicitly, cellular fluxes of carbon and energy. The aquifer applications reveal that the growth of methanogens in natural systems can be limited by multiple factors, including energy sources and growth nutrients, and that the limitations are subject to Liebig's Law of the Minimum. These results highlight the improvements of the new method in biogeochemical reaction modeling, including its applicability to diverse environments, from eutrophic to oligotrophic.

Keywords: genome-scale metabolic model, biogeochemical reaction modeling, microbial kinetics, flux balance analysis, nutrient limitation, methanogenesis