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Center for Environmental Kinetics Analysis

CEKA

Building a Kinetics Database for DMRB Activity.

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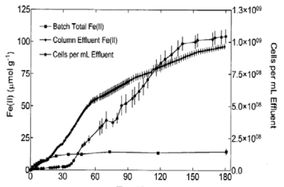
DMRB Kinetics

Over the past two decades, numerous studies have produced high quality information on the rates at which bacteria can reduce metal oxides. The prototypical study—such as the one depicted to the right—focuses on only a few of the myriad variables affecting the rate. This approach allows for effective dissection of the mechanisms underlying DMRB activity, but, it also produces disjoint information that must be synthesized if we hope to predict the behavior of bacteria at the systems level.

Meta-data describing experimental conditions reside in the text.

Column and batch reactors. The flowthrough column reactors (Omnifit, Ltd.; 1.6 ml, total volume) were wet packed inside an anaerobic chamber with 2.2 g of synthetic goethite-coated sand and ca. 1-ml of culture medium containing ca. 5×10^8 cells ml^{-1} of the groundwater Fe(III)-reducing bacterium *Shewanella putrefaciens* strain CN32 (3). The final water content of the columns was ca. 40% (vol/vol). After an overnight equilibration period, the columns were flushed continuously (6-h residence time) in down-flow mode with a PIPES (piperazine-*N*,*N*′-bis(2-ethanesulfonic acid)-buffered (10 mM, pH 6.8) artificial groundwater medium (1) containing 10 mM sodium lactate as a carbon and energy

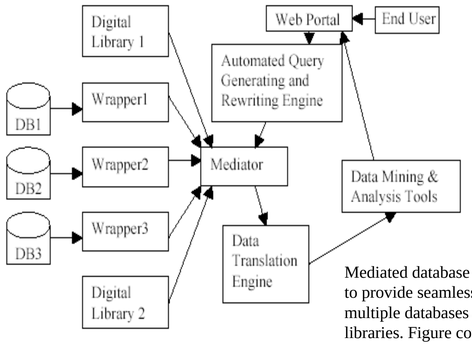
Rate-data reside in tables and time series



Roden et al. Appl. Env. Microbiol. 2000

Databases for Synthesizing DMRB Kinetics

Recent advances in information technology for storing, organizing, and searching large quantities of data make databases an ideal tool for synthesizing rates of DMRB activity. Below is a schematic depicting the architecture of a database that has been developed through Penn State's Center for Environmental Kinetics Analysis (CEKA) and is currently being beta-tested by researchers working on the kinetics of bacteria mediated reactions at scales ranging from the molecular to the field.

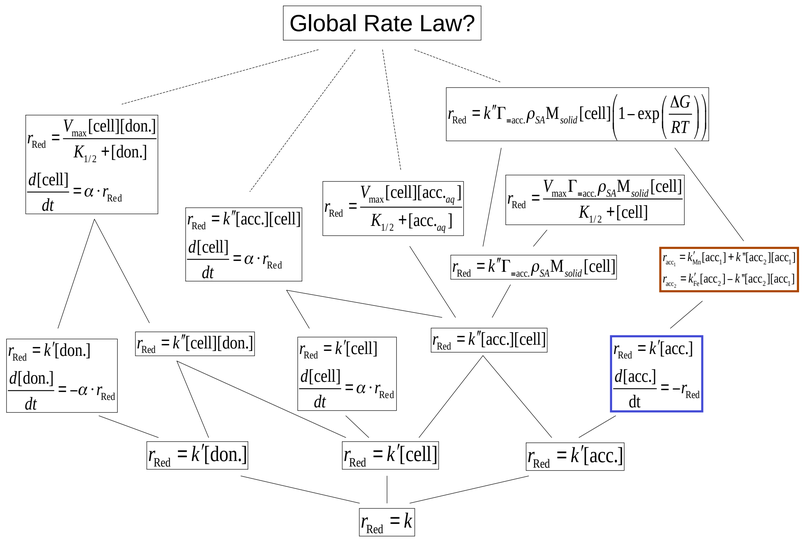


Mediated database architecture used to provide seamless access to multiple databases and digital libraries. Figure courtesy of P. Mitra

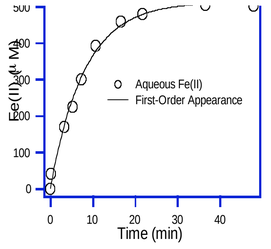
Ultimately, this database—and databases for a number of abiotic processes—will be made web-accessible, along with tools for advanced data analysis (multivariate fitting, data-mining, etc.) and predictive modeling.

Organizing DMRB Rate Data

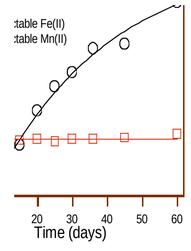
Although the chemical processes underlying the activity of dissimilatory metal reducing bacteria are complex, it is usually possible to describe rate data using simple equations. These pseudo rate formulations can be organized as a partially ordered set (POSET) under the relationship that greater elements (i.e., rate laws) converge to lesser elements in some asymptotic limit. By organizing published DMRB rate data according to this POSET we hope to generate a single, global, rate formulation that can be used both to predict the behavior of DMRBs in the field and to make inferences about underlying enzymatic mechanisms.



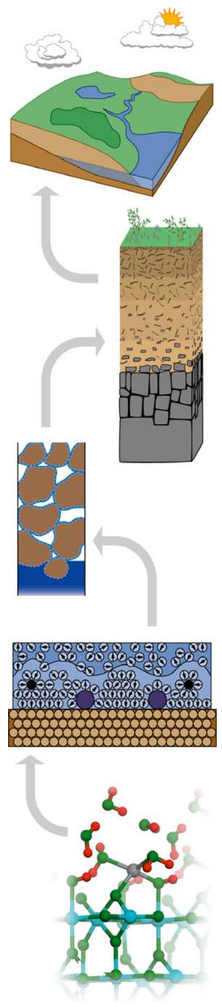
Rate laws organized into a POSET can be used to systematically analyze the results of individual experiments by finding the "smallest" element(s) of the set that accurately capture the primary features of the data. Examples of this type of analysis for iron reduction and mixed iron/manganese reduction are shown below. This procedure will also enable us to automatically identify holes in our knowledge and machine learning algorithms may even allow us (partially) to automate the process of rate law development.



First-order fitting of CN32 + Fe-citrate data in Lui et al. Bioeng. Biotechnol. (2002)

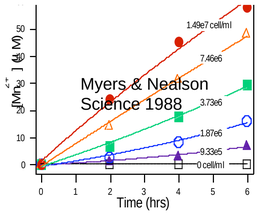


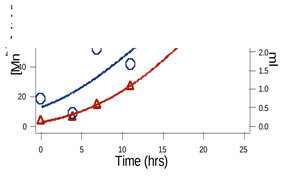
Multi-acceptor fitting of CN32 + FRC-saprolite data from Fredrickson et al. GCA (2004)

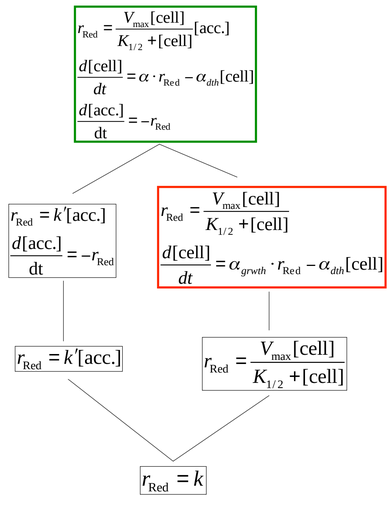


Generating Hypotheses from Database

Compiling and synthesizing DMRB rate data allows us to readily identify gaps in our understanding and to develop hypotheses that can form the basis for filling the gaps. Shown below is an example of such an analysis.



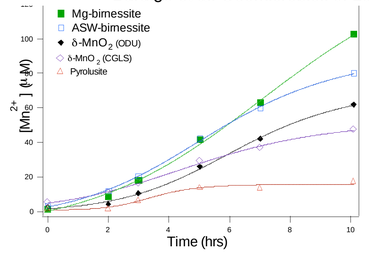




Compiled manganese reduction time series data were analyzed with the simplified POSET shown above. Global analysis of the Myers and Nealson data (left) using the coupled Monod/growth-death model (red box) gives an expression for population dynamics that can be exported to the Burdige et al. data (below). Fitting the Burdige et al. data with a simplified version of the maximal element (green box) indicates that the trend in reactivities that would be obtained in a zero-order treatment may be opposite from reality and that the principle difference between the various Mn phases may not be the reactivity, *per se*, but rather the amount of bioavailable Mn(IV). Predictive modeling of cell concentration provides a means of testing these hypotheses since the relative sizes and locations of the maxima could be compared to time series biomass data.

$$r_{Red} = k[cell][acc.]$$
$$\frac{d[cell]}{dt} = 3.98\times10^{5} \cdot r_{Red} - 0.637 \cdot [cell]$$
$$\frac{d[acc.]}{dt} = -r_{Red}$$

Burdige et al. Geomicrobiol. J. 1992



Future Directions: Field Up-Scaling

The synthesized laboratory data and global rate formulations contained in our database will provide an excellent means for understanding discrepancies between field and lab determined rates. A promising approach is the development of scaling laws for field data on the basis of lab determined mechanisms such as the analysis shown to the right for FRC push-pull rate data.

Donor limited rate with laboratory determined population dynamics

$$r = k[cell][don.] \qquad \frac{d[don.]}{dt} = -\beta \cdot r \qquad \frac{d[cell]}{dt} = \alpha_{grth} \cdot r - \alpha_{dth}[cell]$$

Scaling law for successive donor amendments at fixed time intervals

$$\frac{d[cell]}{dt} = \frac{\alpha_{grth} \cdot r - \alpha_{dth}[cell]}{-\beta \cdot r} \cdot \frac{d[don.]}{dt}$$

$$\frac{r_{N+1} - r_N}{k \cdot [don.]^{init}} = \frac{1}{k[don.]^{init}}\left(\frac{\alpha_{grth}}{\beta}\left([don.]^{init} - [don.]_N^{final}\right) + \frac{\alpha_{dth}}{\beta k}\ln\left(\frac{[don.]_N^{final}}{[don.]^{init}}\right)\right)$$

The above scaling law takes the form of the Istok et al. FRC rate data (i.e., concave up) only if cell death (α_{dth}) is negligible over the time scale of the amendment interval. Since most lab data indicate that death occurs on the order of tens of hours, this indicates that a major piece of the lab/field discrepancy are the mechanisms by which microorganisms evolve at the colony level.

Istok et al. ES&T 2004