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This document describes fully the assumptions made in constructing the numerical model of reactive transport in sediments beneath Lake Washington shown in Figure 4 of Jin and Bethke, "Cellular energy conservation and the rate of microbial sulfate reduction," and contains the input file used to run the simulation.

The transport of a reacting component A — which might be sulfate (SO_4^{2-}), dioxygen (O_2), sulfide (H_2S and HS^-), or methane (CH_4) — can be described by the equation

$$\frac{d[A]}{dt} = D_S \frac{\partial^2[A]}{\partial x^2} + \frac{r_A}{\phi} \quad \text{(S1)}$$

(Berner, 1980). Here, concentration [A] is carried in mol cm^{-3} fluid, D_S is the diffusion coefficient (cm^2 s^{-1}), x is the sediment depth (cm), r_A is the rate (mol cm^{-3} s^{-1}) at which A is added to (positive) or removed from (negative) the pore fluid by microbial reaction, expressed per cm^3 of fluid-saturated sediment, and ϕ is sediment porosity.

We considered a sediment column 36 cm deep, divided into 36 nodal blocks. We took temperature in the lake-bottom sediments to be 10°C, set porosity to 0.9, and fixed pH to 7 (Kuivila and Murray, 1984; Quay et al., 1986). We set a diffusion coefficient of 6×10^{-6} cm^2 s^{-1} (Kuivila and Murray, 1984) and fixed the concentration profile of bicarbonate to that reported by Kuivila et al. (1989). We assumed throughout the column an initial biomass concentration of 10^{-3} mg kg^{-1} for each group of microorganism; the population of each group was free to grow over the course of the simulation. We set very small initial concentrations for the reacting species and applied an upper boundary condition of 100 μmolal O_2 concentration, 105 μmolal sulfate, 50 μmolal acetate, and near-zero sulfide and methane. The rate of acetate production, estimated by fitting results of the modeling to the concentration profile observed for acetate (Kuivila et al., 1989, their Fig. 3C), was 3.0×10^{-15} mol cm^{-3} s^{-1} or $r = 3.3\times10^{-12}$ molal s^{-1}. Table DR1 lists the values assumed in the simulation for the kinetic parameters, and the data sources.

TABLE DR1. Data used to evaluate kinetic rate laws in reactive transport model.

	Aerobic respiration	Sulfate reduction	Methanogenesis
k, mol·mg^{-1}·s^{-1}	10^{-9} [(a)]	10^{-9} [(b)]	10^{-9} [(b)]
K_D, molal	5.0×10^{-5} [(a)]	5.0×10^{-6} [(b)]	2.0×10^{-3} [(b)]
K_A, molal	10^{-7} [(c)]	6.8×10^{-5} [(b)]	—[(d)]
ΔG_C, kJ·(mol acetate)$^{-1}$	360.0 [(e)]	46.75 [(f)]	22.5 [(b)]
χ	8 [(g)]	5 [(b)]	2 [(b)]
Y, mg·(mol acetate)$^{-1}$	2.0×10^4 [(a)]	4.3×10^3 [(b)]	2.0×10^3 [(b)]
D, s^{-1} [(h)]	10^{-8}	10^{-8}	10^{-8}

[(a)]Logan et al. (2001); [(b)]Widdel (1988) and Bethke et al. (2008); [(c)]Button (1985); [(d)]Acetate serves as electron donor as well as acceptor and hence the $m_A/(K_A+m_A)$ term does not appear in the rate law; [(e)]Assuming one ATP is synthesized per electron

transferred; [f]This study; [g]Estimated as the number of protons translocated per acetate oxidized; [h]Schmidt (1992).

We solved for the apparent steady-state distribution of pore water chemistry and microbial activity in the sediment column by running the reactive transport simulation forward from arbitrary initial conditions for 500 years, well past the point at which the results stabilized, at about 100 years.

The simulations were run using program X1t of The Geochemist's Workbench® software package, version 7.0.4, with the following input data:

```
# Input data for the reactive transport simulation of
# microbial activity in Lake Washington sediments.

# Load chemical species considered.

data = thermo.dat
decouple ALL

# Properties of the sediment column.

time end         = 500 years
length           =  36 cm
left             = inlet
right            = outlet
Nx               =  36
Porosity         =   0.9
diffusion_coef   =   6e-6
discharge        =   0
dispersivity     =   0
temperature      =  10

# Time weighting.

Theta            =   1

# Aqueous composition at sediment/water interface.

scope = inlet
   pH            =    7
   Na+           = 3000     umolal
   Cl-           = 3000     umolal
   SO4--         =  105     umolal
   O2(aq)        =  100     umolal
   CH3COO-       =   50     umolal
   HCO3-         =     .8   umolal
   HS-           =     .1   umolal
   CH4(aq)       =     .1   umolal
   balance on Na+

# Initial conditions.

scope initial = inlet
   O2(aq)        =     .1   umolal
   SO4--         =     .1   umolal
   CH3COO-       =     .1   umolal
   HCO3-         = eqn "1.0 + 5.5 * Xposition / (Xposition + 16)" mmolal

fix pH
fix activity HCO3-
```

```
#  Acetate source, from fermentation of organic matter.

react 3.0e-15 mol/cm3sec of NaCH3COO

#  Microbial metabolisms.  Note that the negative product of ATP_energy
#  and ATP_number is the energy conserved, as given in the article.

#  (1) Aerobic acetate oxidizers.

kinetic microbe-ARB \
   rxn = "CH3COO-  + 2*O2(aq)  -> 2*HCO3-  + H+", \
   biomass = .001, rate_con = 1e-9, KA = 1e-7, KD = 5e-5, \
   mpower(CH3COO-) = 1, mpowerD(CH3COO-) = 1, \
   mpower(O2(aq))  = 1, mpowerA(O2(aq))  = 1, \
   ATP_energy = -45, ATP_number = 8, order1 = 1/8, \
   growth_yield = 20000, decay_con = 1e-8

#  (2) Sulfate reducers.

kinetic microbe-SRB \
   rxn = "CH3COO-  + SO4--  -> 2*HCO3-  + HS-", \
   biomass = .001, rate_con = 1e-9, KA = 6.8e-5, KD = 5.0e-6, \
   mpower(CH3COO-) = 1, mpowerD(CH3COO-) = 1, \
   mpower(SO4--)   = 1, mpowerA(SO4--)   = 1, \
   ATP_energy = -46.75, ATP_number = 1, order1 = 1/5, \
   growth_yield = 4300, decay_con = 1e-8

#  (3) Acetotrophic methanogens.

kinetic microbe-ACM \
   rxn = "CH3COO-  + H2O  -> CH4(aq)  + HCO3-", \
   biomass = .001, rate_con = 1e-9, KA = 0, KD = 2.0e-3, \
   mpower(CH3COO-) = 1, mpowerD(CH3COO-) = 1, \
   ATP_energy = -45, ATP_number = 0.5, order1 = 1/2, \
   growth_yield = 2000, decay_con = 1e-8

#  Initiate the calculation.

go

#  To repeat the simulation neglecting the thermodynamic control
#  on sulfate reduction, issue the commands:
```

(*cont'd*)

```
kinetic microbe-SRB order2 = 0
go
```

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