Thermodynamic network model for predicting effects of substrate addition and other perturbations on subsurface microbial communities

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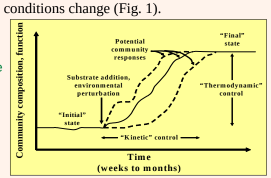
Goal and Hypothesis

The overall goal of this project is to develop and test a thermodynamic network model for predicting the effects of substrate additions and environmental perturbations on microbial growth, community composition and system geochemistry.

The hypothesis is that a thermodynamic analysis of the energy-yielding growth reactions performed by defined groups of microorganisms can be used to make quantitative and testable predictions of the change in microbial community composition that will occur when a substrate is added to the subsurface or when environmental conditions change (Fig. 1).

Fig. 1. Community response to substrate addition and environmental perturbation.



Assumptions

- Community consists of 39 *microbial groups*, each with a defined metabolism, growth equation, and biomass yield (Table 1).
- Groups that can obtain the most energy from a growth substrate in a particular *'thermodynamic niche'* grow.
- Growth is predicted using equilibrium thermodynamics

Simulation Methodology

- Simulations were performed for laboratory and field experiments at the Oak Ridge FRC, Old Rifle, and Hanford 100H
- Equilibrium reaction paths computed using The Geochemist's Workbench to predict the effects of ethanol, acetate, or lactate additions on microbial growth, geochemistry, and mobility of U, Tc, V, and Cr.
- "Batch" and "flush" simulations compared to experimental data.
- Initial geochemistry matched to initial conditions in each experiment (Table 2)

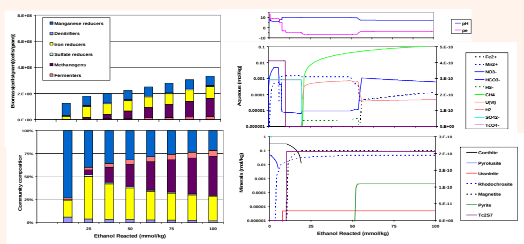
Table 2 – Site Geochemistry Data

Units (mmol)/(kg H_2O)	FRC Area1	FRC Area2	Old Rifle	Hanford 100H
React	200mM Ethanol	150mM Ethanol	150 mM NaCH3COO	100mM NaLactate
pH	3.3	6.4	7.3	7.8
O_2(aq)	0.113	0.066	0.017	0.130
NO_3^-	100	1.21	0.05	3.00
Fe^{+++} (as Geothite)	0.36	0.31	0.12	0.23
SO_4^{2-}	0.43	0.83	6.4	0.73
MnO_4^{2-} (as pyrolusite)	0.022	0.048	0.010	0.003
UO_2^{++}	0.0014	0.0049	0.00053	
CrO_4^{2-}				0.0029
TcO_4^-	1.8E-05	4.1E-07		
$VO_2(OH)_2^-$			0.0154	
Al^{3+}	12	6.0E-05		
Ca^{++}	18.5	3.5	5.3	1.5
Cl^-	7.9	0.65	3.96	0.80
HCO_3^-	0.001	0.090	0.090	0.090
K^+	0.98	0.12	0.20	0.16
Mg^{++}	8.3	1.1	5.4	
Na^+	23	1.1	8.3	0.87
NH_4^+	1.00E-03	1.00E-03	1.00E-03	1.00E-03
Ni^{++}	0.22		0.0026	

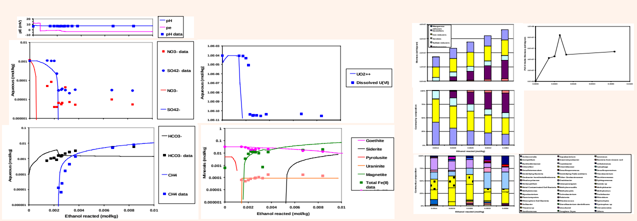
Table 1 Microbial Growth Equations

Microbial Group	Acceptor Half-Reaction	Donor Half-Reaction	YDx	ΔG (kJ/mol)	logK	Growth Equations															
1	O_2/CO_2	Ethanol/CO_2	0.56	3318	-581	-4.9	H^+	-7.5	H_2O	-3.9	HCO_3^-	1	NH_4^+	8.4	O_2(aq)	4.5	ethanol				
2		Acetate/CO_2	0.41	2731	-478	-2.1	H^+	-3.0	H_2O	-7.2	HCO_3^-	1	NH_4^+	7.2	O_2(aq)	6.1	CH_3COO^-				
3		Lactate/CO_2	0.56	1522	-267	-2.0	H^+	-3.0	H_2O	-4.1	HCO_3^-	1	NH_4^+	4.1	O_2(aq)	3.0	lactate				
4		Ethanol/Acetate	0.14	5309	-930	-13.4	H^+	-20.4	H_2O	5	HCO_3^-	1	NH_4^+	12.4	O_2(aq)	-17.4	CH_3COO^-	17.4	ethanol		
5		Lactate/Acetate	0.14	2900	-508	-7.6	H^+	-3.0	H_2O	-6.6	HCO_3^-	1	NH_4^+	6.6	O_2(aq)	-11.6	CH_3COO^-	11.6	lactate		
6		H_2/H^+	0.13	7082	-1241	4	H^+	38.6	H_2(aq)	-41.6	H_2O	5	HCO_3^-	1	NH_4^+	14.3	O_2(aq)				
7		CH_4/CO_2	0.55	5019	-879	-5.0	H^+	-12.0	H_2O	-4.0	HCO_3^-	1.0	NH_4^+	13.0	O_2(aq)	9.0	CH_4(aq)				
8	NO_3^-/N_2	Ethanol/CO_2	0.27	9037	-1583	3.7	H^+	-21.4	H_2O	-13.5	HCO_3^-	-9.1	N_2(aq)	1	NH_4^+	18.2	NO_3^-	9.25	ethanol		
9		Acetate/CO_2	0.41	2605	-456	3.7	H^+	-5.9	H_2O	-7.2	HCO_3^-	-2.9	N_2(aq)	1	NH_4^+	5.8	NO_3^-	6.1	CH_3COO^-		
10		Lactate/CO_2	0.27	5313	-931	2.5	H^+	-8.4	H_2O	-13.4	HCO_3^-	-5.4	N_2(aq)	1	NH_4^+	10.7	NO_3^-	6.1	lactate		
11		Ethanol/Acetate	0.29	1344	-236	-1.7	H^+	-13.0	H_2O	5.0	HCO_3^-	-1.4	N_2(aq)	1	NH_4^+	2.9	NO_3^-	-8.6	CH_3COO^-	8.6	ethanol
12		Lactate/Acetate	0.06	10232	-1793	-5.7	H^+	-12.5	H_2O	-23.7	HCO_3^-	-9.5	N_2(aq)	1	NH_4^+	18.9	NO_3^-	-28.7	CH_3COO^-	28.7	lactate
13		H_2/H^+	0.17	4805	-842	12.0	H^+	30.0	H_2(aq)	-37.0	H_2O	5	HCO_3^-	-4.0	N_2(aq)	1	NH_4^+	8.0	NO_3^-		
14	Fe^{3+}/Fe^{2+}	Acetate/CO_2	0.12	8153	-1428	-150.2	Fe^{2+}	150.2	Fe^{3+}	-167.4	H^+	72.1	H_2O	-37.5	HCO_3^-	1	NH_4^+	21.3	CH_3COO^-		
15		Ethanol/Acetate	0.13	3393	-594	-57.7	Fe^{2+}	57.7	Fe^{3+}	-73.1	H^+	6.4	H_2O	5.0	HCO_3^-	1	NH_4^+	-19.4	CH_3COO^-	19.4	ethanol
16		Lactate/Acetate	0.13	1992	-349	-32.2	Fe^{2+}	32.2	Fe^{3+}	-41.2	H^+	13.1	H_2O	-8.0	HCO_3^-	1.0	NH_4^+	-13.0	CH_3COO^-	13.0	lactate
17		H_2/H^+	0.07	8593	-1505	-114.8	Fe^{2+}	114.8	Fe^{3+}	-110.8	H^+	67.4	H2(aq)	-13	H_2O	5	HCO_3^-	1	NH_4^+		
18	SO_4^{2-}/HS^-	Acetate/CO_2	0.10	787	-138	1.5	H^+	-3.0	H_2O	-44.9	HCO_3^-	-22.5	HS^-	1	NH_4^+	22.5	SO_4^{2-}	25.0	CH_3COO^-		
19		Ethanol/Acetate	0.04	2692	-472	-31.8	H^+	-69.5	H_2O	5.0	HCO_3^-	-30.8	HS^-	1	NH_4^+	30.8	SO_4^{2-}	-66.5	CH_3COO^-	66.5	ethanol
20		Lactate/Acetate	0.04	2214	-388	-20.3	H^+	-3.0	H_2O	-38.5	HCO_3^-	-19.3	HS^-	1	NH_4^+	19.3	SO_4^{2-}	-43.5	CH_3COO^-	43.5	lactate
21		H_2/H^+	0.07	3415	-598	21.4	H^+	79.6	H_2(aq)	-82.6	H_2O	5.0	HCO_3^-	-17.4	HS^-	1.0	NH_4^+	17.4	SO_4^{2-}		
22	MnO_4^{2-}/Mn^{2+}	Acetate/CO_2	0.12	22342	-3914	134.0	H^+	-78.7	H_2O	-37.9	HCO_3^-	-37.9	Mn^{2+}	37.9	MnO_4^{2-}	1.0	NH_4^+	21.4	CH_3COO^-		
23		Ethanol/Acetate	0.29	2128	-373	10.1	H^+	-19.1	H_2O	5	HCO_3^-	-3.7	Mn^{2+}	3.7	MnO_4^{2-}	1.0	NH_4^+	-8.7	CH_3COO^-	8.7	ethanol
24		Lactate/Acetate	0.06	14923	-2614	70.1	H^+	-50.4	H_2O	-23.7	HCO_3^-	-23.7	Mn^{2+}	23.7	MnO_4^{2-}	1.0	NH_4^+	-28.7	CH_3COO^-	28.7	lactate
25		H_2/H^+	0.15	8061	-1412	51.7	H^+	33.9	H_2(aq)	-60.7	H_2O	5.0	HCO_3^-	-11.93	Mn^{2+}	11.9	MnO_4^{2-}	1	NH_4^+		
26	CO_2/CH_4	Acetate/CO_2	0.02	1194	-209	1.5	H^+	98.2	H_2O	-101.2	HCO_3^-	1.0	NH_4^+	103.7	CH_3COO^-	-101.2	CH_4(aq)				
27		H_2/H^+	0.02	12926	-2265	84.9	H^+	333.5	H_2(aq)	-255.6	H_2O	85.9	HCO_3^-	1	NH_4^+	-80.9	CH_4(aq)				
28	H^+/H_2	Acetate/CO_2	0.11	-1616	283	-7.7	H^+	33.7	H_2O	-18.4	HCO_3^-	1	NH_4^+	-36.7	H_2(aq)	11.7	CH_3COO^-				
29		Ethanol/Acetate	0.01	-24671	4322	-496	H^+	487	H_2O	5	HCO_3^-	1	NH_4^+	-990	H_2(aq)	-500	CH_3COO^-	500	ethanol		
30		Lactate/Acetate	0.06	-1282	225	-33.7	H^+	-65.4	H_2(aq)	62.4	H_2O	-32.7	HCO_3^-	1	NH_4^+	-37.7	CH_3COO^-	37.7	lactate		
31	$UO_2^{2+}/U^{(IV)}$	Acetate/CO_2	0.22	-58	-230	66.4	H^+	-40.1	H_2O	-18.5	HCO_3^-	1	NH_4^+	11.8	CH_3COO^-	-37.1	$U^{(IV)}$	37.1	UO_2^{2+}		
32		Ethanol/Acetate	0.19	-49	-125	23.5	H^+	-32.5	H_2O	5	HCO_3^-	1	NH_4^+	-13.2	CH_3COO^-	13.2	ethanol	-16.4	$U^{(IV)}$	16.4	UO_2^{2+}
33		H_2/H^+	0.12	-166	-244	37.4	H^+	26.7	H_2(aq)	-46.4	H_2O	5	HCO_3^-	1.0	NH_4^+	-16.7	$U^{(IV)}$	16.7	UO_2^{2+}		
34	CrO_4^{2-}/Cr^{3+}	Acetate/CO_2	0.32	5196	-910	67.9	H^+	-38.9	H_2O	-10.8	HCO_3^-	1	NH_4^+	7.9	CH_3COO^-	14.4	CrO_4^{2-}	-14.4	Cr^{3+}		
35		Lactate/Acetate	0.06	12577	-2203	130.7	H^+	-80.5	H_2O	-23.2	HCO_3^-	1	NH_4^+	-28.2	CH_3COO^-	28.2	lactate	31.0	CrO_4^{2-}	-31.0	Cr^{3+}
36		H_2/H^+	0.12	9588	-1680	113.1	H^+	42.7	H_2(aq)	5.0	HCO_3^-	1	NH_4^+	-100.3	H_2O	21.8	CrO_4^{2-}	-21.8	Cr^{3+}		
37	TCO_4^-/TcO^{2+}	Acetate/CO_2	0.07	12162	-2131	245.2	H^+	-142.3	H_2O	-69.6	HCO_3^-	1	NH_4^+	37.3	CH_3COO^-	92.8	TcO_4^-	-92.8	TcO^{2+}		
38		Ethanol/Acetate	0.06	7625	-1336	115.2	H^+	-124.2	H_2O	5.0	HCO_3^-	1	NH_4^+	-43.7	CH3COO-	43.7	ethanol	51.6	TcO_4^-	-51.6	TcO^{2+}
39		H_2/H^+	0.04	7346	-1287	120.0	H^+	68.0	H_2(aq)	-129.0	H_2O	5	HCO_3^-	1	NH_4^+	38.7	TcO_4^-	-38.7	TcO^{2+}		

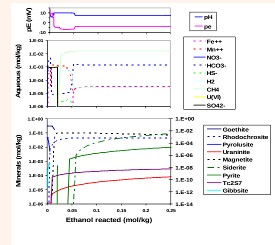
Batch Simulation - FRC Area 2

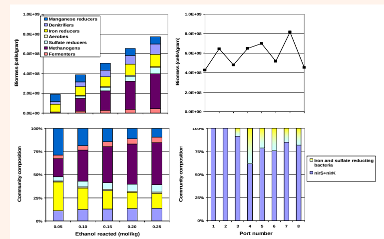


• Simulations reproduced many features of laboratory microcosm experiment by Mohanty et al.

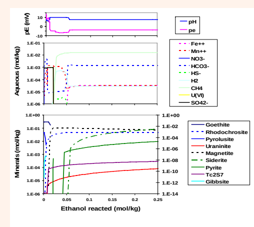


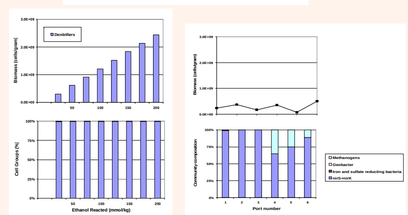
Flush Simulation - FRC Area 2



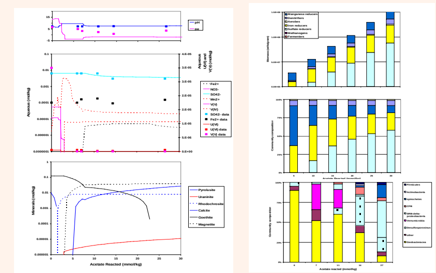


Flush Simulation FRC Area 1

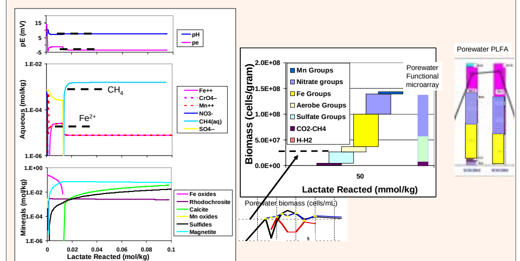




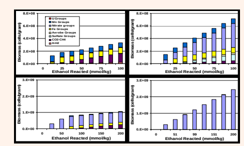
Flush Simulations Old Rifle



Flush Simulations Hanford 100H



An Interesting Observation …



Predicted biomass and community composition are very different for batch and flush simulations and provide some insight into the difficulty of transferring the results of laboratory microcosm experiments to the field

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