

# Modellierung (Model-Output)

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 Reading data base.  
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SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END
SOLUTION 1 lakustrine water
      units  ppm
pH      7.2
pe     -7.8
density 1.011
temp    8.0
Ca             50
Mg             10
Na             40
K              10
Si             10
Cl             50
Alkalinity    400 as HCO3
S              20
SAVE solution 1
END
  
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 Beginning of initial solution calculations.  
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Initial solution 1. lakustrine water

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	6.559e-03	6.559e-03
Ca	1.248e-03	1.248e-03
Cl	1.411e-03	1.411e-03
K	2.559e-04	2.559e-04
Mg	4.116e-04	4.116e-04
Na	1.741e-03	1.741e-03
S	2.083e-04	2.083e-04
Si	1.665e-04	1.665e-04

-----Description of solution-----

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pH = 7.200
pe = -7.800
Activity of water = 1.000
Ionic strength = 8.158e-03
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 7.562e-03
Total CO2 (mol/kg) = 7.562e-03
Temperature (deg C) = 8.000
Electrical balance (eq) = -2.654e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -20.22
Iterations = 9
Total H = 1.110432e+02
Total O = 5.552845e+01
  
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-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	6.846e-08	6.310e-08	-7.165	-7.200	-0.035
OH-	4.252e-08	3.872e-08	-7.371	-7.412	-0.041
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000
C (4)	7.562e-03				
HCO3-	6.366e-03	5.824e-03	-2.196	-2.235	-0.039
CO2	1.117e-03	1.119e-03	-2.952	-2.951	0.001
CaHCO3+	4.679e-05	4.281e-05	-4.330	-4.368	-0.039
MgHCO3+	1.969e-05	1.796e-05	-4.706	-4.746	-0.040
NaHCO3	5.181e-06	5.190e-06	-5.286	-5.285	0.001

	CO3-2	4.039e-06	2.829e-06	-5.394	-5.548	-0.155
	CaCO3	3.203e-06	3.209e-06	-5.494	-5.494	0.001
	MgCO3	5.713e-07	5.724e-07	-6.243	-6.242	0.001
	NaCO3-	3.686e-08	3.363e-08	-7.433	-7.473	-0.040
Ca		1.248e-03				
	Ca+2	1.198e-03	8.387e-04	-2.921	-3.076	-0.155
	CaHCO3+	4.679e-05	4.281e-05	-4.330	-4.368	-0.039
	CaCO3	3.203e-06	3.209e-06	-5.494	-5.494	0.001
	CaOH+	2.417e-09	2.205e-09	-8.617	-8.657	-0.040
	CaSO4	1.647e-39	1.651e-39	-38.783	-38.782	0.001
Cl		1.411e-03				
	Cl-	1.411e-03	1.285e-03	-2.850	-2.891	-0.041
H(0)		2.338e-02				
	H2	1.169e-02	1.171e-02	-1.932	-1.931	0.001
K		2.559e-04				
	K+	2.559e-04	2.331e-04	-3.592	-3.632	-0.041
	KOH	1.278e-11	1.280e-11	-10.893	-10.893	0.001
	KSO4-	0.000e+00	0.000e+00	-40.775	-40.815	-0.040
Mg		4.116e-04				
	Mg+2	3.913e-04	2.753e-04	-3.407	-3.560	-0.153
	MgHCO3+	1.969e-05	1.796e-05	-4.706	-4.746	-0.040
	MgCO3	5.713e-07	5.724e-07	-6.243	-6.242	0.001
	MgOH+	3.408e-09	3.109e-09	-8.467	-8.507	-0.040
	MgSO4	4.726e-40	4.735e-40	-39.325	-39.325	0.001
Na		1.741e-03				
	Na+	1.736e-03	1.585e-03	-2.761	-2.800	-0.039
	NaHCO3	5.181e-06	5.190e-06	-5.286	-5.285	0.001
	NaCO3-	3.686e-08	3.363e-08	-7.433	-7.473	-0.040
	NaOH	1.656e-10	1.659e-10	-9.781	-9.780	0.001
	NaSO4-	0.000e+00	0.000e+00	-40.043	-40.083	-0.040
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-94.455	-94.454	0.001
S(-2)		2.083e-04				
	HS-	1.057e-04	9.623e-05	-3.976	-4.017	-0.041
	H2S	1.027e-04	1.028e-04	-3.989	-3.988	0.001
	S-2	7.679e-11	5.358e-11	-10.115	-10.271	-0.156
S(6)		1.886e-38				
	SO4-2	1.674e-38	1.167e-38	-37.776	-37.933	-0.157
	CaSO4	1.647e-39	1.651e-39	-38.783	-38.782	0.001
	MgSO4	4.726e-40	4.735e-40	-39.325	-39.325	0.001
	NaSO4-	0.000e+00	0.000e+00	-40.043	-40.083	-0.040
	KSO4-	0.000e+00	0.000e+00	-40.775	-40.815	-0.040
	HSO4-	0.000e+00	0.000e+00	-43.254	-43.294	-0.040
Si		1.665e-04				
	H4SiO4	1.663e-04	1.666e-04	-3.779	-3.778	0.001
	H3SiO4-	2.200e-07	2.007e-07	-6.658	-6.698	-0.040
	H2SiO4-2	9.169e-14	6.350e-14	-13.038	-13.197	-0.160

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-36.67	-4.69	31.98	CaSO4
Aragonite	-0.38	-8.62	-8.25	CaCO3
Calcite	-0.22	-8.62	-8.40	CaCO3
Chalcedony	-0.02	-3.78	-3.76	SiO2
Chrysotile	-9.47	24.96	34.43	Mg3Si2O5(OH)4
CO2(g)	-1.71	-19.95	-18.24	CO2
Dolomite	-1.06	-17.73	-16.67	CaMg(CO3)2
Gypsum	-36.41	-4.69	31.72	CaSO4:2H2O
H2(g)	1.27	1.20	-0.07	H2
H2O(g)	-1.98	-0.00	1.98	H2O
H2S(g)	-3.18	-11.22	-8.04	H2S
O2(g)	-91.71	-2.40	89.31	O2
Quartz	0.46	-3.78	-4.24	SiO2
Sepiolite	-5.89	10.35	16.23	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.31	10.35	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-0.92	-3.78	-2.86	SiO2
Sulfur	-10.49	-12.42	-1.93	S
Talc	-6.05	17.41	23.45	Mg3Si4O10(OH)2

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End of simulation.  
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Reading input data for simulation 2.  
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SOLUTION 2 Seawater  
units ppm

pH 8.2  
 pe 5.9  
 density 1.023  
 temp 16.0  
 Ca 460  
 Mg 1480  
 Na 11090  
 K 430  
 Si 2.58  
 Cl 22109.0  
 Alkalinity 100 as HCO3  
 S 3000.0

END

-----  
 Beginning of initial solution calculations.  
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Initial solution 2. Seawater

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.705e-03	1.705e-03
Ca	1.194e-02	1.194e-02
Cl	6.487e-01	6.487e-01
K	1.144e-02	1.144e-02
Mg	6.332e-02	6.332e-02
Na	5.018e-01	5.018e-01
S	3.249e-02	3.249e-02
Si	4.467e-05	4.467e-05

-----Description of solution-----

pH = 8.200  
 pe = 5.900  
 Activity of water = 0.979  
 Ionic strength = 7.475e-01  
 Mass of water (kg) = 1.000e+00  
 Total carbon (mol/kg) = 1.593e-03  
 Total CO2 (mol/kg) = 1.593e-03  
 Temperature (deg C) = 16.000  
 Electrical balance (eq) = -5.162e-02  
 Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.88  
 Iterations = 7  
 Total H = 1.110141e+02  
 Total O = 5.564111e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.256e-06	7.602e-07	-5.901	-6.119	-0.218
H+	8.365e-09	6.310e-09	-8.078	-8.200	-0.122
H2O	5.551e+01	9.787e-01	1.744	-0.009	0.000
C (4)	1.593e-03				
HCO3-	1.123e-03	7.563e-04	-2.950	-3.121	-0.172
MgHCO3+	1.851e-04	1.403e-04	-3.733	-3.853	-0.120
NaHCO3	1.262e-04	1.499e-04	-3.899	-3.824	0.075
MgCO3	5.250e-05	6.236e-05	-4.280	-4.205	0.075
CaHCO3+	3.273e-05	2.204e-05	-4.485	-4.657	-0.172
NaCO3-	2.485e-05	1.884e-05	-4.605	-4.725	-0.120
CO3-2	2.231e-05	4.585e-06	-4.652	-5.339	-0.687
CaCO3	1.508e-05	1.791e-05	-4.822	-4.747	0.075
CO2	1.057e-05	1.256e-05	-4.976	-4.901	0.075
Ca	1.194e-02				
Ca+2	1.064e-02	2.698e-03	-1.973	-2.569	-0.596
CaSO4	1.247e-03	1.481e-03	-2.904	-2.829	0.075
CaHCO3+	3.273e-05	2.204e-05	-4.485	-4.657	-0.172
CaCO3	1.508e-05	1.791e-05	-4.822	-4.747	0.075
CaOH+	9.161e-08	6.946e-08	-7.038	-7.158	-0.120
Cl	6.487e-01				
Cl-	6.487e-01	4.028e-01	-0.188	-0.395	-0.207
H (0)	7.689e-32				
H2	3.845e-32	4.567e-32	-31.415	-31.340	0.075
K	1.144e-02				
K+	1.127e-02	6.995e-03	-1.948	-2.155	-0.207
KSO4-	1.741e-04	1.320e-04	-3.759	-3.879	-0.120

Mg	KOH	3.167e-09	3.762e-09	-8.499	-8.425	0.075	
	Mg+2	6.332e-02	5.545e-02	1.636e-02	-1.256	-1.786	-0.530
	MgSO4	7.630e-03	9.064e-03	-2.117	-2.043	0.075	
	MgHCO3+	1.851e-04	1.403e-04	-3.733	-3.853	-0.120	
	MgCO3	5.250e-05	6.236e-05	-4.280	-4.205	0.075	
	MgOH+	5.257e-06	3.986e-06	-5.279	-5.399	-0.120	
Na	Na+	5.018e-01	4.951e-01	3.524e-01	-0.305	-0.453	-0.148
	NaSO4-	6.590e-03	4.997e-03	-2.181	-2.301	-0.120	
	NaHCO3	1.262e-04	1.499e-04	-3.899	-3.824	0.075	
	NaCO3-	2.485e-05	1.884e-05	-4.605	-4.725	-0.120	
	NaOH	3.040e-07	3.611e-07	-6.517	-6.442	0.075	
	O(0)	2.834e-33	1.417e-33	1.683e-33	-32.849	-32.774	0.075
S(-2)	O2	0.000e+00	0.000e+00	0.000e+00	-88.245	-88.463	-0.218
	HS-	0.000e+00	0.000e+00	0.000e+00	-89.623	-89.548	0.075
	H2S	0.000e+00	0.000e+00	0.000e+00	-92.738	-93.457	-0.719
S(6)	S-2	3.249e-02	1.684e-02	3.001e-03	-1.774	-2.523	-0.749
	SO4-2	7.630e-03	9.064e-03	-2.117	-2.043	0.075	
	MgSO4	6.590e-03	4.997e-03	-2.181	-2.301	-0.120	
	NaSO4-	1.247e-03	1.481e-03	-2.904	-2.829	0.075	
	CaSO4	1.741e-04	1.320e-04	-3.759	-3.879	-0.120	
	KSO4-	2.010e-09	1.524e-09	-8.697	-8.817	-0.120	
	HSO4-	4.467e-05	4.352e-05	5.170e-05	-4.361	-4.287	0.075
Si	H4SiO4	1.143e-06	8.667e-07	-5.942	-6.062	-0.120	
	H3SiO4-	1.523e-11	5.034e-12	-10.817	-11.298	-0.481	
	H2SiO4-2						

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-0.76	-5.09	-4.34	CaSO4
Aragonite	0.38	-7.91	-8.28	CaCO3
Calcite	0.53	-7.91	-8.43	CaCO3
Chalcedony	-0.61	-4.27	-3.66	SiO2
Chrysotile	1.91	35.26	33.35	Mg3Si2O5(OH)4
CO2(g)	-3.55	-21.73	-18.18	CO2
Dolomite	1.84	-15.03	-16.87	CaMg(CO3)2
Gypsum	-0.53	-5.11	-4.58	CaSO4:2H2O
H2(g)	-28.14	-28.20	-0.06	H2
H2O(g)	-1.76	-0.01	1.75	H2O
H2S(g)	-88.65	-131.69	-43.04	H2S
O2(g)	-29.95	56.38	86.33	O2
Quartz	-0.17	-4.27	-4.10	SiO2
Sepiolite	0.37	16.37	16.00	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-2.29	16.37	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-1.48	-4.27	-2.79	SiO2
Sulfur	-66.45	-103.49	-37.04	S
Talc	4.28	26.73	22.46	Mg3Si4O10(OH)2

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End of simulation.  
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Reading input data for simulation 3.  
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MIX 1
      1      0.1
      2      0.9
SAVE solution 3
END

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Beginning of batch-reaction calculations.  
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Reaction step 1.

Using mix 1.

Mixture 1.

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1.000e-01 Solution 1lakustrine water
9.000e-01 Solution 2Seawater

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-----Solution composition-----

Elements	Molality	Moles
C	2.189e-03	2.190e-03
Ca	1.087e-02	1.087e-02
Cl	5.840e-01	5.840e-01
K	1.032e-02	1.032e-02
Mg	5.703e-02	5.703e-02
Na	4.518e-01	4.518e-01
S	2.926e-02	2.926e-02
Si	5.685e-05	5.685e-05

-----Description of solution-----

pH	=	8.496	Charge balance
pe	=	-5.012	Adjusted to redox equilibrium
Activity of water	=	0.981	
Ionic strength	=	6.746e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	2.775e-03	
Total CO2 (mol/kg)	=	2.189e-03	
Temperature (deg C)	=	15.200	
Electrical balance (eq)	=	-4.672e-02	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-3.90	
Iterations	=	19	
Total H	=	1.110170e+02	
Total O	=	5.562985e+01	

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.297e-06	1.409e-06	-5.639	-5.851	-0.212
H+	4.212e-09	3.191e-09	-8.376	-8.496	-0.121
H2O	5.551e+01	9.808e-01	1.744	-0.008	0.000
C (-4)	5.785e-08				
CH4	5.785e-08	6.757e-08	-7.238	-7.170	0.067
C (4)	2.189e-03				
HCO3-	1.491e-03	1.012e-03	-2.827	-2.995	-0.168
MgHCO3+	2.257e-04	1.694e-04	-3.647	-3.771	-0.125
NaHCO3	1.546e-04	1.805e-04	-3.811	-3.743	0.067
MgCO3	1.235e-04	1.443e-04	-3.908	-3.841	0.067
NaCO3-	5.612e-05	4.212e-05	-4.251	-4.376	-0.125
CO3-2	5.593e-05	1.189e-05	-4.252	-4.925	-0.672
CaHCO3+	3.920e-05	2.662e-05	-4.407	-4.575	-0.168
CaCO3	3.618e-05	4.225e-05	-4.442	-4.374	0.067
CO2	7.369e-06	8.608e-06	-5.133	-5.065	0.067
Ca	1.087e-02				
Ca+2	9.688e-03	2.479e-03	-2.014	-2.606	-0.592
CaSO4	1.106e-03	1.292e-03	-2.956	-2.889	0.067
CaHCO3+	3.920e-05	2.662e-05	-4.407	-4.575	-0.168
CaCO3	3.618e-05	4.225e-05	-4.442	-4.374	0.067
CaOH+	1.685e-07	1.265e-07	-6.773	-6.898	-0.125
Cl	5.840e-01				
Cl-	5.840e-01	3.666e-01	-0.234	-0.436	-0.202
H (0)	1.338e-10				
H2	6.691e-11	7.815e-11	-10.175	-10.107	0.067
K	1.032e-02				
K+	1.017e-02	6.384e-03	-1.993	-2.195	-0.202
KSO4-	1.519e-04	1.140e-04	-3.818	-3.943	-0.125
KOH	5.824e-09	6.803e-09	-8.235	-8.167	0.067
Mg	5.703e-02				
Mg+2	5.011e-02	1.478e-02	-1.300	-1.830	-0.530
MgSO4	6.560e-03	7.663e-03	-2.183	-2.116	0.067
MgHCO3+	2.257e-04	1.694e-04	-3.647	-3.771	-0.125
MgCO3	1.235e-04	1.443e-04	-3.908	-3.841	0.067
MgOH+	8.802e-06	6.607e-06	-5.055	-5.180	-0.125
Na	4.518e-01				
Na+	4.459e-01	3.171e-01	-0.351	-0.499	-0.148
NaSO4-	5.701e-03	4.279e-03	-2.244	-2.369	-0.125
NaHCO3	1.546e-04	1.805e-04	-3.811	-3.743	0.067
NaCO3-	5.612e-05	4.212e-05	-4.251	-4.376	-0.125
NaOH	5.513e-07	6.440e-07	-6.259	-6.191	0.067
O (0)	0.000e+00				
O2	0.000e+00	0.000e+00	-75.587	-75.520	0.067
S (-2)	3.130e-04				
HS-	3.061e-04	1.878e-04	-3.514	-3.726	-0.212

	H2S	6.857e-06	8.009e-06	-5.164	-5.096	0.067
	S-2	1.793e-08	3.550e-09	-7.747	-8.450	-0.703
S (6)		2.894e-02				
	SO4-2	1.542e-02	2.871e-03	-1.812	-2.542	-0.730
	MgSO4	6.560e-03	7.663e-03	-2.183	-2.116	0.067
	NaSO4-	5.701e-03	4.279e-03	-2.244	-2.369	-0.125
	CaSO4	1.106e-03	1.292e-03	-2.956	-2.889	0.067
	KSO4-	1.519e-04	1.140e-04	-3.818	-3.943	-0.125
	HSO4-	9.668e-10	7.256e-10	-9.015	-9.139	-0.125
Si		5.685e-05				
	H4SiO4	5.415e-05	6.324e-05	-4.266	-4.199	0.067
	H3SiO4-	2.706e-06	2.031e-06	-5.568	-5.692	-0.125
	H2SiO4-2	6.936e-11	2.201e-11	-10.159	-10.657	-0.498

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-0.81	-5.15	-4.34	CaSO4
Aragonite	0.75	-7.53	-8.28	CaCO3
Calcite	0.90	-7.53	-8.43	CaCO3
CH4 (g)	-4.41	-49.76	-45.35	CH4
Chalcedony	-0.51	-4.18	-3.67	SiO2
Chrysotile	3.62	37.08	33.46	Mg3Si2O5(OH)4
CO2 (g)	-3.72	-21.91	-18.19	CO2
Dolomite	2.57	-14.29	-16.85	CaMg(CO3)2
Gypsum	-0.58	-5.16	-4.58	CaSO4:2H2O
H2 (g)	-6.91	-6.97	-0.06	H2
H2O (g)	-1.78	-0.01	1.77	H2O
H2S (g)	-4.20	-47.37	-43.17	H2S
O2 (g)	-72.71	13.92	86.62	O2
Quartz	-0.07	-4.18	-4.11	SiO2
Sepiolite	1.70	17.73	16.03	Mg2Si3O7.5OH:3H2O
Sepiolite (d)	-0.93	17.73	18.66	Mg2Si3O7.5OH:3H2O
SiO2 (a)	-1.39	-4.18	-2.80	SiO2
Sulfur	-3.25	-40.40	-37.16	S
Talc	6.17	28.72	22.55	Mg3Si4O10(OH)2

-----  
End of simulation.  
-----

-----  
Reading input data for simulation 4.  
-----

```
Mix 2
1 0.2
2 0.8
Save Solution 3
End
```

-----  
Beginning of batch-reaction calculations.  
-----

Reaction step 1.

Using mix 2.

Mixture 2.

```
2.000e-01 Solution 1lakustrine water
8.000e-01 Solution 2Seawater
```

-----Solution composition-----

Elements	Molality	Moles
C	2.786e-03	2.787e-03
Ca	9.800e-03	9.801e-03
Cl	5.192e-01	5.192e-01
K	9.202e-03	9.203e-03
Mg	5.074e-02	5.074e-02
Na	4.018e-01	4.018e-01
S	2.603e-02	2.603e-02
Si	6.904e-05	6.904e-05

-----Description of solution-----

```
pH = 8.645      Charge balance
pe = -5.206     Adjusted to redox equilibrium
Activity of water = 0.983
```

Ionic strength = 6.014e-01  
 Mass of water (kg) = 1.000e+00  
 Total alkalinity (eq/kg) = 3.844e-03  
 Total CO2 (mol/kg) = 2.786e-03  
 Temperature (deg C) = 14.400  
 Electrical balance (eq) = -4.183e-02  
 Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.92  
 Iterations = 17  
 Total H = 1.110199e+02  
 Total O = 5.561858e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.984e-06	1.858e-06	-5.525	-5.731	-0.206
H+	2.978e-09	2.267e-09	-8.526	-8.645	-0.118
H2O	5.551e+01	9.829e-01	1.744	-0.008	0.000
C(-4)	1.581e-07				
CH4	1.581e-07	1.816e-07	-6.801	-6.741	0.060
C(4)	2.786e-03				
HCO3-	1.870e-03	1.282e-03	-2.728	-2.892	-0.164
MgHCO3+	2.577e-04	1.918e-04	-3.589	-3.717	-0.128
MgCO3	1.941e-04	2.229e-04	-3.712	-3.652	0.060
NaHCO3	1.772e-04	2.035e-04	-3.752	-3.691	0.060
CO3-2	9.400e-05	2.076e-05	-4.027	-4.683	-0.656
NaCO3-	8.423e-05	6.268e-05	-4.075	-4.203	-0.128
CaCO3	5.814e-05	6.678e-05	-4.236	-4.175	0.060
CaHCO3+	4.409e-05	3.022e-05	-4.356	-4.520	-0.164
CO2	6.830e-06	7.844e-06	-5.166	-5.105	0.060
Ca	9.800e-03				
Ca+2	8.731e-03	2.265e-03	-2.059	-2.645	-0.586
CaSO4	9.665e-04	1.110e-03	-3.015	-2.955	0.060
CaCO3	5.814e-05	6.678e-05	-4.236	-4.175	0.060
CaHCO3+	4.409e-05	3.022e-05	-4.356	-4.520	-0.164
CaOH+	2.190e-07	1.630e-07	-6.660	-6.788	-0.128
Cl	5.192e-01				
Cl-	5.192e-01	3.300e-01	-0.285	-0.481	-0.197
H(0)	1.676e-10				
H2	8.380e-11	9.625e-11	-10.077	-10.017	0.060
K	9.202e-03				
K+	9.072e-03	5.767e-03	-2.042	-2.239	-0.197
KSO4-	1.298e-04	9.661e-05	-3.887	-4.015	-0.128
KOH	7.548e-09	8.669e-09	-8.122	-8.062	0.060
Mg	5.074e-02				
Mg+2	4.473e-02	1.324e-02	-1.349	-1.878	-0.529
MgSO4	5.543e-03	6.366e-03	-2.256	-2.196	0.060
MgHCO3+	2.577e-04	1.918e-04	-3.589	-3.717	-0.128
MgCO3	1.941e-04	2.229e-04	-3.712	-3.652	0.060
MgOH+	1.038e-05	7.726e-06	-4.984	-5.112	-0.128
Na	4.018e-01				
Na+	3.967e-01	2.823e-01	-0.402	-0.549	-0.148
NaSO4-	4.827e-03	3.592e-03	-2.316	-2.445	-0.128
NaHCO3	1.772e-04	2.035e-04	-3.752	-3.691	0.060
NaCO3-	8.423e-05	6.268e-05	-4.075	-4.203	-0.128
NaOH	7.040e-07	8.085e-07	-6.152	-6.092	0.060
O(0)	0.000e+00				
O2	0.000e+00	0.000e+00	-76.041	-75.981	0.060
S(-2)	6.260e-04				
HS-	6.156e-04	3.832e-04	-3.211	-3.417	-0.206
H2S	1.038e-05	1.192e-05	-4.984	-4.924	0.060
S-2	4.659e-08	9.617e-09	-7.332	-8.017	-0.685
S(6)	2.540e-02				
SO4-2	1.394e-02	2.722e-03	-1.856	-2.565	-0.709
MgSO4	5.543e-03	6.366e-03	-2.256	-2.196	0.060
NaSO4-	4.827e-03	3.592e-03	-2.316	-2.445	-0.128
CaSO4	9.665e-04	1.110e-03	-3.015	-2.955	0.060
KSO4-	1.298e-04	9.661e-05	-3.887	-4.015	-0.128
HSO4-	6.465e-10	4.811e-10	-9.189	-9.318	-0.128
Si	6.904e-05				
H4SiO4	6.467e-05	7.427e-05	-4.189	-4.129	0.060
H3SiO4-	4.371e-06	3.253e-06	-5.359	-5.488	-0.128
H2SiO4-2	1.526e-10	4.678e-11	-9.817	-10.330	-0.513

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-0.88	-5.21	-4.33	CaSO4
Aragonite	0.95	-7.33	-8.28	CaCO3
Calcite	1.10	-7.33	-8.43	CaCO3

CH4 (g)	-3.99	-49.46	-45.47	CH4
Chalcedony	-0.44	-4.11	-3.68	SiO2
Chrysotile	4.41	37.97	33.56	Mg3Si2O5(OH)4
CO2 (g)	-3.77	-21.96	-18.19	CO2
Dolomite	2.95	-13.89	-16.84	CaMg(CO3)2
Gypsum	-0.64	-5.23	-4.59	CaSO4:2H2O
H2 (g)	-6.82	-6.88	-0.06	H2
H2O (g)	-1.80	-0.01	1.79	H2O
H2S (g)	-4.04	-47.34	-43.30	H2S
O2 (g)	-73.17	13.74	86.92	O2
Quartz	0.01	-4.11	-4.13	SiO2
Sepiolite	2.39	18.44	16.05	Mg2Si3O7.5OH:3H2O
Sepiolite (d)	-0.22	18.44	18.66	Mg2Si3O7.5OH:3H2O
SiO2 (a)	-1.31	-4.11	-2.80	SiO2
Sulfur	-3.18	-40.46	-37.27	S
Talc	7.09	29.75	22.65	Mg3Si4O10(OH)2

-----  
End of simulation.  
-----

-----  
Reading input data for simulation 5.  
-----

Mix 3  
1 0.3  
2 0.7  
Save Solution 3  
End

-----  
Beginning of batch-reaction calculations.  
-----

Reaction step 1.  
Using mix 3.  
Mixture 3.

3.000e-01 Solution 1lakustrine water  
7.000e-01 Solution 2Seawater

-----Solution composition-----

Elements	Molality	Moles
C	3.383e-03	3.384e-03
Ca	8.731e-03	8.732e-03
Cl	4.545e-01	4.545e-01
K	8.084e-03	8.084e-03
Mg	4.445e-02	4.445e-02
Na	3.518e-01	3.518e-01
S	2.280e-02	2.280e-02
Si	8.122e-05	8.123e-05

-----Description of solution-----

pH = 8.749                   Charge balance  
pe = -5.334                   Adjusted to redox equilibrium  
Activity of water = 0.985  
Ionic strength = 5.280e-01  
Mass of water (kg) = 1.000e+00  
Total alkalinity (eq/kg) = 4.914e-03  
Total CO2 (mol/kg) = 3.383e-03  
Temperature (deg C) = 13.600  
Electrical balance (eq) = -3.693e-02  
Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -3.94  
Iterations = 20  
Total H = 1.110228e+02  
Total O = 5.560731e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.492e-06	2.211e-06	-5.457	-5.655	-0.199
H+	2.329e-09	1.784e-09	-8.633	-8.749	-0.116
H2O	5.551e+01	9.850e-01	1.744	-0.007	0.000
C (-4)	3.166e-07				
CH4	3.166e-07	3.575e-07	-6.499	-6.447	0.053
C (4)	3.383e-03				
HCO3-	2.264e-03	1.569e-03	-2.645	-2.804	-0.159
MgHCO3+	2.810e-04	2.077e-04	-3.551	-3.683	-0.131
MgCO3	2.632e-04	2.972e-04	-3.580	-3.527	0.053



	NaHCO3	1.936e-04	2.186e-04	-3.713	-3.660	0.053
	CO3-2	1.371e-04	3.162e-05	-3.863	-4.500	-0.637
	NaCO3-	1.085e-04	8.023e-05	-3.964	-4.096	-0.131
	CaCO3	8.103e-05	9.151e-05	-4.091	-4.039	0.053
	CaHCO3+	4.752e-05	3.293e-05	-4.323	-4.482	-0.159
	CO2	6.779e-06	7.656e-06	-5.169	-5.116	0.053
Ca		8.731e-03				
	Ca+2	7.773e-03	2.055e-03	-2.109	-2.687	-0.578
	CaSO4	8.289e-04	9.361e-04	-3.081	-3.029	0.053
	CaCO3	8.103e-05	9.151e-05	-4.091	-4.039	0.053
	CaHCO3+	4.752e-05	3.293e-05	-4.323	-4.482	-0.159
	CaOH+	2.548e-07	1.884e-07	-6.594	-6.725	-0.131
Cl		4.545e-01				
	Cl-	4.545e-01	2.930e-01	-0.342	-0.533	-0.191
H (0)		1.909e-10				
	H2	9.545e-11	1.078e-10	-10.020	-9.967	0.053
K		8.084e-03				
	K+	7.976e-03	5.142e-03	-2.098	-2.289	-0.191
	KSO4-	1.080e-04	7.982e-05	-3.967	-4.098	-0.131
	KOH	8.719e-09	9.846e-09	-8.060	-8.007	0.053
Mg		4.445e-02				
	Mg+2	3.931e-02	1.174e-02	-1.405	-1.930	-0.525
	MgSO4	4.578e-03	5.170e-03	-2.339	-2.287	0.053
	MgHCO3+	2.810e-04	2.077e-04	-3.551	-3.683	-0.131
	MgCO3	2.632e-04	2.972e-04	-3.580	-3.527	0.053
	MgOH+	1.092e-05	8.068e-06	-4.962	-5.093	-0.131
Na		3.518e-01				
	Na+	3.475e-01	2.478e-01	-0.459	-0.606	-0.147
	NaSO4-	3.974e-03	2.937e-03	-2.401	-2.532	-0.131
	NaHCO3	1.936e-04	2.186e-04	-3.713	-3.660	0.053
	NaCO3-	1.085e-04	8.023e-05	-3.964	-4.096	-0.131
	NaOH	8.005e-07	9.040e-07	-6.097	-6.044	0.053
O (0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-76.414	-76.362	0.053
S (-2)		9.389e-04				
	HS-	9.258e-04	5.861e-04	-3.033	-3.232	-0.199
	H2S	1.303e-05	1.471e-05	-4.885	-4.832	0.053
	S-2	8.145e-08	1.762e-08	-7.089	-7.754	-0.665
S (6)		2.186e-02				
	SO4-2	1.237e-02	2.550e-03	-1.908	-2.593	-0.686
	MgSO4	4.578e-03	5.170e-03	-2.339	-2.287	0.053
	NaSO4-	3.974e-03	2.937e-03	-2.401	-2.532	-0.131
	CaSO4	8.289e-04	9.361e-04	-3.081	-3.029	0.053
	KSO4-	1.080e-04	7.982e-05	-3.967	-4.098	-0.131
	HSO4-	4.722e-10	3.490e-10	-9.326	-9.457	-0.131
Si		8.122e-05				
	H4SiO4	7.504e-05	8.474e-05	-4.125	-4.072	0.053
	H3SiO4-	6.179e-06	4.568e-06	-5.209	-5.340	-0.131
	H2SiO4-2	2.636e-10	7.868e-11	-9.579	-10.104	-0.525

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-0.95	-5.28	-4.33	CaSO4
Aragonite	1.08	-7.19	-8.27	CaCO3
Calcite	1.24	-7.19	-8.42	CaCO3
CH4 (g)	-3.70	-49.30	-45.59	CH4
Chalcedony	-0.37	-4.06	-3.69	SiO2
Chrysotile	4.88	38.55	33.67	Mg3Si2O5 (OH) 4
CO2 (g)	-3.79	-21.99	-18.20	CO2
Dolomite	3.20	-13.62	-16.82	CaMg (CO3) 2
Gypsum	-0.71	-5.29	-4.59	CaSO4:2H2O
H2 (g)	-6.77	-6.83	-0.06	H2
H2O (g)	-1.82	-0.01	1.82	H2O
H2S (g)	-3.96	-47.38	-43.43	H2S
O2 (g)	-73.56	13.65	87.21	O2
Quartz	0.08	-4.06	-4.14	SiO2
Sepiolite	2.85	18.92	16.07	Mg2Si3O7.5OH:3H2O
Sepiolite (d)	0.26	18.92	18.66	Mg2Si3O7.5OH:3H2O
SiO2 (a)	-1.25	-4.06	-2.81	SiO2
Sulfur	-3.16	-40.55	-37.39	S
Talc	7.69	30.44	22.75	Mg3Si4O10 (OH) 2

-----  
End of simulation.

-----  
Reading input data for simulation 6.  
-----

Mix 4

1 0.4  
2 0.6  
Save Solution 3  
End

-----  
Beginning of batch-reaction calculations.  
-----

Reaction step 1.

Using mix 4.

Mixture 4.

4.000e-01 Solution 1lakustrine water  
6.000e-01 Solution 2Seawater

-----Solution composition-----

Elements	Molality	Moles
C	3.980e-03	3.981e-03
Ca	7.662e-03	7.663e-03
Cl	3.898e-01	3.898e-01
K	6.965e-03	6.966e-03
Mg	3.816e-02	3.816e-02
Na	3.017e-01	3.018e-01
S	1.957e-02	1.957e-02
Si	9.341e-05	9.341e-05

-----Description of solution-----

pH	=	8.835	Charge balance
pe	=	-5.436	Adjusted to redox equilibrium
Activity of water	=	0.987	
Ionic strength	=	4.544e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	5.983e-03	
Total CO2 (mol/kg)	=	3.980e-03	
Temperature (deg C)	=	12.800	
Electrical balance (eq)	=	-3.203e-02	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-3.98	
Iterations	=	15	
Total H	=	1.110257e+02	
Total O	=	5.559605e+01	

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.907e-06	2.521e-06	-5.408	-5.598	-0.190
H+	1.898e-09	1.463e-09	-8.722	-8.835	-0.113
H2O	5.551e+01	9.871e-01	1.744	-0.006	0.000
C (-4)	5.610e-07				
CH4	5.610e-07	6.228e-07	-6.251	-6.206	0.045
C (4)	3.980e-03				
HCO3-	2.676e-03	1.878e-03	-2.573	-2.726	-0.154
MgCO3	3.299e-04	3.663e-04	-3.482	-3.436	0.045
MgHCO3+	2.947e-04	2.170e-04	-3.531	-3.664	-0.133
NaHCO3	2.031e-04	2.255e-04	-3.692	-3.647	0.045
CO3-2	1.862e-04	4.513e-05	-3.730	-4.346	-0.616
NaCO3-	1.284e-04	9.450e-05	-3.892	-4.025	-0.133
CaCO3	1.050e-04	1.166e-04	-3.979	-3.933	0.045
CaHCO3+	4.954e-05	3.476e-05	-4.305	-4.459	-0.154
CO2	6.864e-06	7.621e-06	-5.163	-5.118	0.045
Ca	7.662e-03				
Ca+2	6.814e-03	1.849e-03	-2.167	-2.733	-0.566
CaSO4	6.932e-04	7.697e-04	-3.159	-3.114	0.045
CaCO3	1.050e-04	1.166e-04	-3.979	-3.933	0.045
CaHCO3+	4.954e-05	3.476e-05	-4.305	-4.459	-0.154
CaOH+	2.812e-07	2.070e-07	-6.551	-6.684	-0.133
Cl	3.898e-01				
Cl-	3.898e-01	2.555e-01	-0.409	-0.593	-0.183
H (0)	2.098e-10				
H2	1.049e-10	1.165e-10	-9.979	-9.934	0.045
K	6.965e-03				
K+	6.879e-03	4.509e-03	-2.162	-2.346	-0.183
KSO4-	8.662e-05	6.377e-05	-4.062	-4.195	-0.133
KOH	9.498e-09	1.055e-08	-8.022	-7.977	0.045
Mg	3.816e-02				
Mg+2	3.385e-02	1.026e-02	-1.470	-1.989	-0.519

	MgSO4	3.666e-03	4.071e-03	-2.436	-2.390	0.045
	MgCO3	3.299e-04	3.663e-04	-3.482	-3.436	0.045
	MgHCO3+	2.947e-04	2.170e-04	-3.531	-3.664	-0.133
	MgOH+	1.082e-05	7.966e-06	-4.966	-5.099	-0.133
Na		3.017e-01				
	Na+	2.983e-01	2.136e-01	-0.525	-0.670	-0.145
	NaSO4-	3.151e-03	2.320e-03	-2.502	-2.635	-0.133
	NaHCO3	2.031e-04	2.255e-04	-3.692	-3.647	0.045
	NaCO3-	1.284e-04	9.450e-05	-3.892	-4.025	-0.133
	NaOH	8.573e-07	9.519e-07	-6.067	-6.021	0.045
O(0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-76.758	-76.713	0.045
S(-2)		1.252e-03				
	HS-	1.236e-03	7.978e-04	-2.908	-3.098	-0.190
	H2S	1.519e-05	1.687e-05	-4.818	-4.773	0.045
	S-2	1.206e-07	2.755e-08	-6.919	-7.560	-0.641
S(6)		1.832e-02				
	SO4-2	1.072e-02	2.349e-03	-1.970	-2.629	-0.660
	MgSO4	3.666e-03	4.071e-03	-2.436	-2.390	0.045
	NaSO4-	3.151e-03	2.320e-03	-2.502	-2.635	-0.133
	CaSO4	6.932e-04	7.697e-04	-3.159	-3.114	0.045
	KSO4-	8.662e-05	6.377e-05	-4.062	-4.195	-0.133
	HSO4-	3.528e-10	2.597e-10	-9.452	-9.586	-0.133
Si		9.341e-05				
	H4SiO4	8.523e-05	9.463e-05	-4.069	-4.024	0.045
	H3SiO4-	8.175e-06	6.018e-06	-5.088	-5.221	-0.133
	H2SiO4-2	4.053e-10	1.190e-10	-9.392	-9.924	-0.532

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.03	-5.36	-4.33	CaSO4
Aragonite	1.19	-7.08	-8.27	CaCO3
Calcite	1.34	-7.08	-8.42	CaCO3
CH4(g)	-3.47	-49.19	-45.71	CH4
Chalcedony	-0.31	-4.01	-3.70	SiO2
Chrysotile	5.21	38.99	33.78	Mg3Si2O5(OH)4
CO2(g)	-3.81	-22.01	-18.20	CO2
Dolomite	3.38	-13.41	-16.79	CaMg(CO3)2
Gypsum	-0.79	-5.37	-4.59	CaSO4:2H2O
H2(g)	-6.74	-6.80	-0.06	H2
H2O(g)	-1.84	-0.01	1.84	H2O
H2S(g)	-3.91	-47.46	-43.56	H2S
O2(g)	-73.92	13.58	87.50	O2
Quartz	0.14	-4.01	-4.15	SiO2
Sepiolite	3.20	19.29	16.09	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	0.63	19.29	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-1.20	-4.01	-2.82	SiO2
Sulfur	-3.16	-40.67	-37.51	S
Talc	8.12	30.97	22.85	Mg3Si4O10(OH)2

-----  
End of simulation.

-----  
Reading input data for simulation 7.

-----  
Mix 5  
1 0.5  
2 0.5  
Save Solution 3  
End

-----  
Beginning of batch-reaction calculations.

-----  
Reaction step 1.

Using mix 5.

Mixture 5.

5.000e-01 Solution 1lakustrine water

5.000e-01 Solution 2Seawater

-----Solution composition-----

Elements	Molality	Moles
C	4.577e-03	4.577e-03
Ca	6.593e-03	6.593e-03
Cl	3.250e-01	3.251e-01
K	5.847e-03	5.848e-03
Mg	3.186e-02	3.187e-02
Na	2.517e-01	2.518e-01
S	1.635e-02	1.635e-02
Si	1.056e-04	1.056e-04

```

-----Description of solution-----
pH = 8.913          Charge balance
pe = -5.528        Adjusted to redox equilibrium
Activity of water = 0.989
Ionic strength = 3.806e-01
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 7.052e-03
Total CO2 (mol/kg) = 4.576e-03
Temperature (deg C) = 12.000
Electrical balance (eq) = -2.714e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -4.02
Iterations = 16
Total H = 1.110287e+02
Total O = 5.558478e+01

```

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.283e-06	2.826e-06	-5.368	-5.549	-0.181
H+	1.571e-09	1.221e-09	-8.804	-8.913	-0.109
H2O	5.551e+01	9.892e-01	1.744	-0.005	0.000
C (-4)	9.432e-07				
CH4	9.432e-07	1.030e-06	-6.025	-5.987	0.038
C (4)	4.576e-03				
HCO3-	3.107e-03	2.213e-03	-2.508	-2.655	-0.147
MgCO3	3.930e-04	4.290e-04	-3.406	-3.368	0.038
MgHCO3+	2.978e-04	2.190e-04	-3.526	-3.660	-0.133
CO3-2	2.426e-04	6.238e-05	-3.615	-4.205	-0.590
NaHCO3	2.047e-04	2.235e-04	-3.689	-3.651	0.038
NaCO3-	1.429e-04	1.051e-04	-3.845	-3.978	-0.133
CaCO3	1.305e-04	1.425e-04	-3.884	-3.846	0.038
CaHCO3+	5.018e-05	3.573e-05	-4.299	-4.447	-0.147
CO2	6.962e-06	7.600e-06	-5.157	-5.119	0.038
Ca	6.593e-03				
Ca+2	5.853e-03	1.646e-03	-2.233	-2.783	-0.551
CaSO4	5.593e-04	6.105e-04	-3.252	-3.214	0.038
CaCO3	1.305e-04	1.425e-04	-3.884	-3.846	0.038
CaHCO3+	5.018e-05	3.573e-05	-4.299	-4.447	-0.147
CaOH+	3.010e-07	2.214e-07	-6.521	-6.655	-0.133
Cl	3.250e-01				
Cl-	3.250e-01	2.173e-01	-0.488	-0.663	-0.175
H (0)	2.275e-10				
H2	1.137e-10	1.241e-10	-9.944	-9.906	0.038
K	5.847e-03				
K+	5.781e-03	3.865e-03	-2.238	-2.413	-0.175
KSO4-	6.602e-05	4.856e-05	-4.180	-4.314	-0.133
KOH	9.949e-09	1.086e-08	-8.002	-7.964	0.038
Mg	3.186e-02				
Mg+2	2.835e-02	8.799e-03	-1.547	-2.056	-0.508
MgSO4	2.810e-03	3.067e-03	-2.551	-2.513	0.038
MgCO3	3.930e-04	4.290e-04	-3.406	-3.368	0.038
MgHCO3+	2.978e-04	2.190e-04	-3.526	-3.660	-0.133
MgOH+	1.031e-05	7.587e-06	-4.987	-5.120	-0.133
Na	2.517e-01				
Na+	2.490e-01	1.796e-01	-0.604	-0.746	-0.142
NaSO4-	2.369e-03	1.742e-03	-2.625	-2.759	-0.133
NaHCO3	2.047e-04	2.235e-04	-3.689	-3.651	0.038
NaCO3-	1.429e-04	1.051e-04	-3.845	-3.978	-0.133
NaOH	8.809e-07	9.615e-07	-6.055	-6.017	0.038
O (0)	0.000e+00				
O2	0.000e+00	0.000e+00	-77.091	-77.053	0.038
S (-2)	1.564e-03				
HS-	1.547e-03	1.021e-03	-2.810	-2.991	-0.181
H2S	1.693e-05	1.848e-05	-4.771	-4.733	0.038
S-2	1.635e-07	3.981e-08	-6.786	-7.400	-0.614
S (6)	1.478e-02				
SO4-2	8.977e-03	2.110e-03	-2.047	-2.676	-0.629
MgSO4	2.810e-03	3.067e-03	-2.551	-2.513	0.038
NaSO4-	2.369e-03	1.742e-03	-2.625	-2.759	-0.133
CaSO4	5.593e-04	6.105e-04	-3.252	-3.214	0.038
KSO4-	6.602e-05	4.856e-05	-4.180	-4.314	-0.133
HSO4-	2.605e-10	1.916e-10	-9.584	-9.718	-0.133
Si	1.056e-04				
H4SiO4	9.517e-05	1.039e-04	-4.022	-3.983	0.038
H3SiO4-	1.042e-05	7.664e-06	-4.982	-5.116	-0.133
H2SiO4-2	5.844e-10	1.710e-10	-9.233	-9.767	-0.534

```

-----Saturation indices-----
Phase          SI log IAP  log KT

```

Anhydrite	-1.12	-5.46	-4.33	CaSO4
Aragonite	1.28	-6.99	-8.26	CaCO3
Calcite	1.43	-6.99	-8.42	CaCO3
CH4 (g)	-3.26	-49.10	-45.84	CH4
Chalcedony	-0.26	-3.97	-3.71	SiO2
Chrysotile	5.46	39.34	33.88	Mg3Si2O5(OH)4
CO2 (g)	-3.82	-22.03	-18.21	CO2
Dolomite	3.53	-13.25	-16.77	CaMg(CO3)2
Gypsum	-0.88	-5.47	-4.59	CaSO4:2H2O
H2 (g)	-6.71	-6.77	-0.06	H2
H2O (g)	-1.87	-0.00	1.86	H2O
H2S (g)	-3.88	-47.56	-43.69	H2S
O2 (g)	-74.27	13.53	87.80	O2
Quartz	0.19	-3.97	-4.17	SiO2
Sepiolite	3.48	19.59	16.12	Mg2Si3O7.5OH:3H2O
Sepiolite (d)	0.93	19.59	18.66	Mg2Si3O7.5OH:3H2O
SiO2 (a)	-1.15	-3.97	-2.82	SiO2
Sulfur	-3.16	-40.79	-37.63	S
Talc	8.45	31.40	22.95	Mg3Si4O10(OH)2

-----  
End of simulation.

-----  
Reading input data for simulation 8.  
-----

Mix 6  
1 0.6  
2 0.4  
Save Solution 3  
End

-----  
Beginning of batch-reaction calculations.  
-----

Reaction step 1.  
Using mix 6.  
Mixture 6.

6.000e-01 Solution 1lakustrine water  
4.000e-01 Solution 2seawater

-----Solution composition-----

Elements	Molality	Moles
C	5.174e-03	5.174e-03
Ca	5.524e-03	5.524e-03
Cl	2.603e-01	2.603e-01
K	4.729e-03	4.729e-03
Mg	2.557e-02	2.558e-02
Na	2.017e-01	2.018e-01
S	1.312e-02	1.312e-02
Si	1.178e-04	1.178e-04

-----Description of solution-----

pH	=	8.992	Charge balance
pe	=	-5.620	Adjusted to redox equilibrium
Activity of water	=	0.991	
Ionic strength	=	3.064e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	8.120e-03	
Total CO2 (mol/kg)	=	5.172e-03	
Temperature (deg C)	=	11.200	
Electrical balance (eq)	=	-2.224e-02	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-4.10	
Iterations	=	11	
Total H	=	1.110316e+02	
Total O	=	5.557352e+01	

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	4.667e-06	3.162e-06	-5.331	-5.500	-0.169
H+	1.299e-09	1.020e-09	-8.887	-8.992	-0.105
H2O	5.551e+01	9.913e-01	1.744	-0.004	0.000
C(-4)	1.576e-06				
CH4	1.576e-06	1.692e-06	-5.802	-5.772	0.031
C(4)	5.172e-03				
HCO3-	3.562e-03	2.583e-03	-2.448	-2.588	-0.140
MgCO3	4.503e-04	4.832e-04	-3.347	-3.316	0.031

	CO3-2	3.086e-04	8.524e-05	-3.511	-4.069	-0.559
	MgHCO3+	2.886e-04	2.131e-04	-3.540	-3.671	-0.132
	NaHCO3	1.971e-04	2.115e-04	-3.705	-3.675	0.031
	CaCO3	1.582e-04	1.697e-04	-3.801	-3.770	0.031
	NaCO3-	1.509e-04	1.114e-04	-3.821	-3.953	-0.132
	CaHCO3+	4.942e-05	3.583e-05	-4.306	-4.446	-0.140
	CO2	7.006e-06	7.519e-06	-5.155	-5.124	0.031
Ca		5.524e-03				
	Ca+2	4.889e-03	1.445e-03	-2.311	-2.840	-0.529
	CaSO4	4.271e-04	4.583e-04	-3.369	-3.339	0.031
	CaCO3	1.582e-04	1.697e-04	-3.801	-3.770	0.031
	CaHCO3+	4.942e-05	3.583e-05	-4.306	-4.446	-0.140
	CaOH+	3.158e-07	2.332e-07	-6.501	-6.632	-0.132
Cl		2.603e-01				
	Cl-	2.603e-01	1.782e-01	-0.585	-0.749	-0.164
H (0)		2.467e-10				
	H2	1.233e-10	1.324e-10	-9.909	-9.878	0.031
K		4.729e-03				
	K+	4.682e-03	3.206e-03	-2.330	-2.494	-0.164
	KSO4-	4.653e-05	3.435e-05	-4.332	-4.464	-0.132
	KOH	1.007e-08	1.081e-08	-7.997	-7.966	0.031
Mg		2.557e-02				
	Mg+2	2.281e-02	7.342e-03	-1.642	-2.134	-0.492
	MgSO4	2.011e-03	2.158e-03	-2.697	-2.666	0.031
	MgCO3	4.503e-04	4.832e-04	-3.347	-3.316	0.031
	MgHCO3+	2.886e-04	2.131e-04	-3.540	-3.671	-0.132
	MgOH+	9.505e-06	7.018e-06	-5.022	-5.154	-0.132
Na		2.017e-01				
	Na+	1.997e-01	1.456e-01	-0.700	-0.837	-0.137
	NaSO4-	1.641e-03	1.212e-03	-2.785	-2.917	-0.132
	NaHCO3	1.971e-04	2.115e-04	-3.705	-3.675	0.031
	NaCO3-	1.509e-04	1.114e-04	-3.821	-3.953	-0.132
	NaOH	8.719e-07	9.356e-07	-6.060	-6.029	0.031
O (0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-77.427	-77.396	0.031
S (-2)		1.877e-03				
	HS-	1.858e-03	1.259e-03	-2.731	-2.900	-0.169
	H2S	1.821e-05	1.954e-05	-4.740	-4.709	0.031
	S-2	2.105e-07	5.537e-08	-6.677	-7.257	-0.580
S (6)		1.124e-02				
	SO4-2	7.115e-03	1.820e-03	-2.148	-2.740	-0.592
	MgSO4	2.011e-03	2.158e-03	-2.697	-2.666	0.031
	NaSO4-	1.641e-03	1.212e-03	-2.785	-2.917	-0.132
	CaSO4	4.271e-04	4.583e-04	-3.369	-3.339	0.031
	KSO4-	4.653e-05	3.435e-05	-4.332	-4.464	-0.132
	HSO4-	1.841e-10	1.359e-10	-9.735	-9.867	-0.132
Si		1.178e-04				
	H4SiO4	1.048e-04	1.124e-04	-3.980	-3.949	0.031
	H3SiO4-	1.301e-05	9.606e-06	-4.886	-5.017	-0.132
	H2SiO4-2	8.128e-10	2.415e-10	-9.090	-9.617	-0.527

-----Saturation indices-----						
Phase	SI	log IAP	log KT			
Anhydrite	-1.25	-5.58	-4.33	CaSO4		
Aragonite	1.35	-6.91	-8.26	CaCO3		
Calcite	1.51	-6.91	-8.41	CaCO3		
CH4 (g)	-3.05	-49.01	-45.96	CH4		
Chalcedony	-0.22	-3.94	-3.72	SiO2		
Chrysotile	5.65	39.65	33.99	Mg3Si2O5 (OH) 4		
CO2 (g)	-3.84	-22.05	-18.21	CO2		
Dolomite	3.64	-13.11	-16.75	CaMg (CO3) 2		
Gypsum	-1.00	-5.59	-4.59	CaSO4:2H2O		
H2 (g)	-6.68	-6.74	-0.06	H2		
H2O (g)	-1.89	-0.00	1.88	H2O		
H2S (g)	-3.86	-47.68	-43.82	H2S		
O2 (g)	-74.62	13.48	88.10	O2		
Quartz	0.24	-3.94	-4.18	SiO2		
Sepiolite	3.71	19.85	16.14	Mg2Si3O7.5OH:3H2O		
Sepiolite (d)	1.19	19.85	18.66	Mg2Si3O7.5OH:3H2O		
SiO2 (a)	-1.11	-3.94	-2.83	SiO2		
Sulfur	-3.19	-40.94	-37.75	S		
Talc	8.72	31.77	23.05	Mg3Si4O10 (OH) 2		

-----  
End of simulation.

-----  
Reading input data for simulation 9.

-----  
Mix 7

1 0.7  
 2 0.3  
 Save Solution 3  
 End

-----  
 Beginning of batch-reaction calculations.  
 -----

Reaction step 1.  
 Using mix 7.  
 Mixture 7.

7.000e-01 Solution 1lakustrine water  
 3.000e-01 Solution 2Seawater

-----Solution composition-----

Elements	Molality	Moles
C	5.771e-03	5.771e-03
Ca	4.455e-03	4.455e-03
Cl	1.956e-01	1.956e-01
K	3.610e-03	3.611e-03
Mg	1.928e-02	1.929e-02
Na	1.517e-01	1.518e-01
S	9.890e-03	9.891e-03
Si	1.300e-04	1.300e-04

-----Description of solution-----

pH = 9.075 Charge balance  
 pe = -5.721 Adjusted to redox equilibrium  
 Activity of water = 0.993  
 Ionic strength = 2.320e-01  
 Mass of water (kg) = 1.000e+00  
 Total alkalinity (eq/kg) = 9.188e-03  
 Total CO2 (mol/kg) = 5.768e-03  
 Temperature (deg C) = 10.400  
 Electrical balance (eq) = -1.734e-02  
 Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -4.22  
 Iterations = 12  
 Total H = 1.110345e+02  
 Total O = 5.556225e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.115e-06	3.582e-06	-5.291	-5.446	-0.155
H+	1.057e-09	8.406e-10	-8.976	-9.075	-0.099
H2O	5.551e+01	9.934e-01	1.744	-0.003	0.000
C (-4)	2.770e-06				
CH4	2.770e-06	2.922e-06	-5.558	-5.534	0.023
C (4)	5.768e-03				
HCO3-	4.045e-03	3.000e-03	-2.393	-2.523	-0.130
MgCO3	4.978e-04	5.251e-04	-3.303	-3.280	0.023
CO3-2	3.878e-04	1.174e-04	-3.411	-3.930	-0.519
MgHCO3+	2.647e-04	1.975e-04	-3.577	-3.704	-0.127
CaCO3	1.896e-04	2.000e-04	-3.722	-3.699	0.023
NaHCO3	1.784e-04	1.882e-04	-3.749	-3.725	0.023
NaCO3-	1.507e-04	1.124e-04	-3.822	-3.949	-0.127
CaHCO3+	4.724e-05	3.504e-05	-4.326	-4.455	-0.130
CO2	6.932e-06	7.312e-06	-5.159	-5.136	0.023
Ca	4.455e-03				
Ca+2	3.922e-03	1.243e-03	-2.407	-2.905	-0.499
CaSO4	2.960e-04	3.123e-04	-3.529	-3.505	0.023
CaCO3	1.896e-04	2.000e-04	-3.722	-3.699	0.023
CaHCO3+	4.724e-05	3.504e-05	-4.326	-4.455	-0.130
CaOH+	3.268e-07	2.438e-07	-6.486	-6.613	-0.127
Cl	1.956e-01				
Cl-	1.956e-01	1.381e-01	-0.709	-0.860	-0.151
H (0)	2.720e-10				
H2	1.360e-10	1.435e-10	-9.866	-9.843	0.023
K	3.610e-03				
K+	3.582e-03	2.528e-03	-2.446	-2.597	-0.151
KSO4-	2.867e-05	2.139e-05	-4.543	-4.670	-0.127
KOH	9.823e-09	1.036e-08	-8.008	-7.985	0.023
Mg	1.928e-02				
Mg+2	1.724e-02	5.865e-03	-1.764	-2.232	-0.468
MgSO4	1.275e-03	1.345e-03	-2.894	-2.871	0.023
MgCO3	4.978e-04	5.251e-04	-3.303	-3.280	0.023
MgHCO3+	2.647e-04	1.975e-04	-3.577	-3.704	-0.127
MgOH+	8.433e-06	6.292e-06	-5.074	-5.201	-0.127
Na	1.517e-01				

	Na+	1.504e-01	1.115e-01	-0.823	-0.953	-0.130
	NaSO4-	9.877e-04	7.370e-04	-3.005	-3.133	-0.127
	NaHCO3	1.784e-04	1.882e-04	-3.749	-3.725	0.023
	NaCO3-	1.507e-04	1.124e-04	-3.822	-3.949	-0.127
	NaOH	8.257e-07	8.710e-07	-6.083	-6.060	0.023
O (0)		0.000e+00				
	O2	0.000e+00	0.000e+00	-77.778	-77.755	0.023
S (-2)		2.189e-03				
	HS-	2.169e-03	1.519e-03	-2.664	-2.818	-0.155
	H2S	1.892e-05	1.996e-05	-4.723	-4.700	0.023
	S-2	2.628e-07	7.627e-08	-6.580	-7.118	-0.537
S (6)		7.702e-03				
	SO4-2	5.114e-03	1.453e-03	-2.291	-2.838	-0.546
	MgSO4	1.275e-03	1.345e-03	-2.894	-2.871	0.023
	NaSO4-	9.877e-04	7.370e-04	-3.005	-3.133	-0.127
	CaSO4	2.960e-04	3.123e-04	-3.529	-3.505	0.023
	KSO4-	2.867e-05	2.139e-05	-4.543	-4.670	-0.127
	HSO4-	1.181e-10	8.812e-11	-9.928	-10.055	-0.127
Si		1.300e-04				
	H4SiO4	1.138e-04	1.201e-04	-3.944	-3.921	0.023
	H3SiO4-	1.613e-05	1.203e-05	-4.792	-4.920	-0.127
	H2SiO4-2	1.113e-09	3.450e-10	-8.953	-9.462	-0.509

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.41	-5.74	-4.34	CaSO4
Aragonite	1.42	-6.84	-8.26	CaCO3
Calcite	1.58	-6.84	-8.41	CaCO3
CH4 (g)	-2.82	-48.91	-46.08	CH4
Chalcedony	-0.19	-3.91	-3.73	SiO2
Chrysotile	5.81	39.91	34.10	Mg3Si2O5(OH)4
CO2 (g)	-3.86	-22.08	-18.22	CO2
Dolomite	3.74	-13.00	-16.73	CaMg(CO3)2
Gypsum	-1.16	-5.75	-4.59	CaSO4:2H2O
H2 (g)	-6.64	-6.71	-0.07	H2
H2O (g)	-1.91	-0.00	1.91	H2O
H2S (g)	-3.86	-47.81	-43.95	H2S
O2 (g)	-74.98	13.41	88.40	O2
Quartz	0.28	-3.91	-4.20	SiO2
Sepiolite	3.91	20.08	16.16	Mg2Si3O7.5OH:3H2O
Sepiolite (d)	1.42	20.08	18.66	Mg2Si3O7.5OH:3H2O
SiO2 (a)	-1.08	-3.91	-2.84	SiO2
Sulfur	-3.23	-41.10	-37.87	S
Talc	8.94	32.09	23.15	Mg3Si4O10(OH)2

-----  
End of simulation.

-----  
Reading input data for simulation 10.

-----  
Mix 8  
1 0.8  
2 0.2  
Save Solution 3  
End

-----  
Beginning of batch-reaction calculations.

-----  
Reaction step 1.

Using mix 8.

Mixture 8.

8.000e-01 Solution 1lakustrine water

2.000e-01 Solution 2Seawater

-----Solution composition-----		
Elements	Molality	Moles
C	6.367e-03	6.368e-03
Ca	3.386e-03	3.386e-03
Cl	1.308e-01	1.309e-01
K	2.492e-03	2.493e-03
Mg	1.299e-02	1.299e-02
Na	1.017e-01	1.018e-01
S	6.663e-03	6.664e-03
Si	1.421e-04	1.422e-04

-----Description of solution-----  
 pH = 9.174 Charge balance  
 pe = -5.848 Adjusted to redox equilibrium  
 Activity of water = 0.996  
 Ionic strength = 1.571e-01



Mass of water (kg) = 1.000e+00  
 Total alkalinity (eq/kg) = 1.025e-02  
 Total CO2 (mol/kg) = 6.362e-03  
 Temperature (deg C) = 9.600  
 Electrical balance (eq) = -1.245e-02  
 Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -4.47  
 Iterations = 14  
 Total H = 1.110374e+02  
 Total O = 5.555098e+01

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.736e-06	4.196e-06	-5.241	-5.377	-0.136
H+	8.261e-10	6.697e-10	-9.083	-9.174	-0.091
H2O	5.551e+01	9.955e-01	1.744	-0.002	0.000
C (-4)	5.835e-06				
CH4	5.835e-06	6.050e-06	-5.234	-5.218	0.016
C (4)	6.362e-03				
HCO3-	4.562e-03	3.492e-03	-2.341	-2.457	-0.116
MgCO3	5.262e-04	5.456e-04	-3.279	-3.263	0.016
CO3-2	4.882e-04	1.676e-04	-3.311	-3.776	-0.464
CaCO3	2.289e-04	2.373e-04	-3.640	-3.625	0.016
MgHCO3+	2.220e-04	1.693e-04	-3.654	-3.771	-0.118
NaHCO3	1.457e-04	1.511e-04	-3.836	-3.821	0.016
NaCO3-	1.388e-04	1.059e-04	-3.858	-3.975	-0.118
CaHCO3+	4.353e-05	3.332e-05	-4.361	-4.477	-0.116
CO2	6.644e-06	6.888e-06	-5.178	-5.162	0.016
Ca	3.386e-03				
Ca+2	2.948e-03	1.039e-03	-2.530	-2.983	-0.453
CaCO3	2.289e-04	2.373e-04	-3.640	-3.625	0.016
CaSO4	1.648e-04	1.708e-04	-3.783	-3.767	0.016
CaHCO3+	4.353e-05	3.332e-05	-4.361	-4.477	-0.116
CaOH+	3.361e-07	2.563e-07	-6.474	-6.591	-0.118
Cl	1.308e-01				
Cl-	1.308e-01	9.625e-02	-0.883	-1.017	-0.133
H (0)	3.163e-10				
H2	1.582e-10	1.640e-10	-9.801	-9.785	0.016
K	2.492e-03				
K+	2.479e-03	1.824e-03	-2.606	-2.739	-0.133
KSO4-	1.320e-05	1.007e-05	-4.879	-4.997	-0.118
KOH	9.065e-09	9.399e-09	-8.043	-8.027	0.016
Mg	1.299e-02				
Mg+2	1.162e-02	4.323e-03	-1.935	-2.364	-0.429
MgSO4	6.170e-04	6.397e-04	-3.210	-3.194	0.016
MgCO3	5.262e-04	5.456e-04	-3.279	-3.263	0.016
MgHCO3+	2.220e-04	1.693e-04	-3.654	-3.771	-0.118
MgOH+	7.060e-06	5.384e-06	-5.151	-5.269	-0.118
Na	1.017e-01				
Na+	1.010e-01	7.695e-02	-0.996	-1.114	-0.118
NaSO4-	4.376e-04	3.337e-04	-3.359	-3.477	-0.118
NaHCO3	1.457e-04	1.511e-04	-3.836	-3.821	0.016
NaCO3-	1.388e-04	1.059e-04	-3.858	-3.975	-0.118
NaOH	7.289e-07	7.558e-07	-6.137	-6.122	0.016
O (0)	0.000e+00				
O2	0.000e+00	0.000e+00	-78.177	-78.161	0.016
S (-2)	2.498e-03				
HS-	2.479e-03	1.814e-03	-2.606	-2.741	-0.136
H2S	1.881e-05	1.950e-05	-4.726	-4.710	0.016
S-2	3.241e-07	1.076e-07	-6.489	-6.968	-0.479
S (6)	4.164e-03				
SO4-2	2.932e-03	9.591e-04	-2.533	-3.018	-0.485
MgSO4	6.170e-04	6.397e-04	-3.210	-3.194	0.016
NaSO4-	4.376e-04	3.337e-04	-3.359	-3.477	-0.118
CaSO4	1.648e-04	1.708e-04	-3.783	-3.767	0.016
KSO4-	1.320e-05	1.007e-05	-4.879	-4.997	-0.118
HSO4-	5.986e-11	4.565e-11	-10.223	-10.341	-0.118
Si	1.421e-04				
H4SiO4	1.220e-04	1.265e-04	-3.914	-3.898	0.016
H3SiO4-	2.016e-05	1.538e-05	-4.695	-4.813	-0.118
H2SiO4-2	1.537e-09	5.200e-10	-8.813	-9.284	-0.471

-----Saturation indices-----

Phase	SI	log IAP	log KT	
Anhydrite	-1.67	-6.00	-4.34	CaSO4
Aragonite	1.49	-6.76	-8.25	CaCO3
Calcite	1.65	-6.76	-8.41	CaCO3
CH4 (g)	-2.52	-48.73	-46.21	CH4

Chalcedony	-0.15	-3.89	-3.74	SiO2
Chrysotile	5.94	40.15	34.21	Mg3Si2O5(OH)4
CO2(g)	-3.90	-22.12	-18.22	CO2
Dolomite	3.81	-12.90	-16.71	CaMg(CO3)2
Gypsum	-1.41	-6.01	-4.59	CaSO4:2H2O
H2(g)	-6.58	-6.65	-0.07	H2
H2O(g)	-1.93	-0.00	1.93	H2O
H2S(g)	-3.88	-47.97	-44.09	H2S
O2(g)	-75.40	13.30	88.70	O2
Quartz	0.32	-3.89	-4.21	SiO2
Sepiolite	4.09	20.27	16.19	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	1.61	20.27	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-1.05	-3.89	-2.85	SiO2
Sulfur	-3.32	-41.31	-38.00	S
Talc	9.12	32.37	23.25	Mg3Si4O10(OH)2

-----  
End of simulation.

-----  
Reading input data for simulation 11.

-----  
Mix 9  
1 0.9  
2 0.1  
Save Solution 3  
End  
-----

-----  
Beginning of batch-reaction calculations.

-----  
Reaction step 1.

Using mix 9.

Mixture 9.

9.000e-01 Solution 1lakustrine water

1.000e-01 Solution 2Seawater

-----Solution composition-----

Elements	Molality	Moles
C	6.964e-03	6.965e-03
Ca	2.317e-03	2.317e-03
Cl	6.613e-02	6.614e-02
K	1.374e-03	1.374e-03
Mg	6.702e-03	6.703e-03
Na	5.174e-02	5.175e-02
S	3.435e-03	3.436e-03
Si	1.543e-04	1.543e-04

-----Description of solution-----

pH	=	9.312	Charge balance
pe	=	-6.081	Adjusted to redox equilibrium
Activity of water	=	0.998	
Ionic strength	=	8.173e-02	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	1.126e-02	
Total CO2 (mol/kg)	=	6.926e-03	
Temperature (deg C)	=	8.800	
Electrical balance (eq)	=	-7.550e-03	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-5.19	
Iterations	=	13	
Total H	=	1.110403e+02	
Total O	=	5.553972e+01	

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.883e-06	5.379e-06	-5.162	-5.269	-0.107
H+	5.822e-10	4.873e-10	-9.235	-9.312	-0.077
H2O	5.551e+01	9.977e-01	1.744	-0.001	0.000
C(-4)	3.845e-05				
CH4	3.845e-05	3.918e-05	-4.415	-4.407	0.008
C(4)	6.926e-03				
HCO3-	5.104e-03	4.106e-03	-2.292	-2.387	-0.094
CO3-2	6.315e-04	2.645e-04	-3.200	-3.578	-0.378
MgCO3	5.037e-04	5.133e-04	-3.298	-3.290	0.008
CaCO3	2.917e-04	2.972e-04	-3.535	-3.527	0.008
MgHCO3+	1.505e-04	1.200e-04	-3.822	-3.921	-0.098
NaCO3-	1.071e-04	8.543e-05	-3.970	-4.068	-0.098
NaHCO3	9.326e-05	9.503e-05	-4.030	-4.022	0.008

	CaHCO3+	3.793e-05	3.051e-05	-4.421	-4.515	-0.094
	CO2	5.880e-06	5.992e-06	-5.231	-5.222	0.008
Ca	2.317e-03					
	Ca+2	1.959e-03	8.279e-04	-2.708	-3.082	-0.374
	CaCO3	2.917e-04	2.972e-04	-3.535	-3.527	0.008
	CaHCO3+	3.793e-05	3.051e-05	-4.421	-4.515	-0.094
	CaSO4	2.814e-05	2.868e-05	-4.551	-4.542	0.008
	CaOH+	3.527e-07	2.813e-07	-6.453	-6.551	-0.098
Cl	6.613e-02					
	Cl-	6.613e-02	5.182e-02	-1.180	-1.285	-0.106
H(0)	4.990e-10					
	H2	2.495e-10	2.543e-10	-9.603	-9.595	0.008
K	1.374e-03					
	K+	1.372e-03	1.076e-03	-2.863	-2.968	-0.106
	KSO4-	1.564e-06	1.247e-06	-5.806	-5.904	-0.098
	KOH	7.492e-09	7.635e-09	-8.125	-8.117	0.008
Mg	6.702e-03					
	Mg+2	5.964e-03	2.608e-03	-2.224	-2.584	-0.359
	MgCO3	5.037e-04	5.133e-04	-3.298	-3.290	0.008
	MgHCO3+	1.505e-04	1.200e-04	-3.822	-3.921	-0.098
	MgSO4	7.863e-05	8.012e-05	-4.104	-4.096	0.008
	MgOH+	5.175e-06	4.127e-06	-5.286	-5.384	-0.098
Na	5.174e-02					
	Na+	5.149e-02	4.115e-02	-1.288	-1.386	-0.097
	NaCO3-	1.071e-04	8.543e-05	-3.970	-4.068	-0.098
	NaHCO3	9.326e-05	9.503e-05	-4.030	-4.022	0.008
	NaSO4-	4.727e-05	3.770e-05	-4.325	-4.424	-0.098
	NaOH	5.462e-07	5.566e-07	-6.263	-6.254	0.008
O(0)	0.000e+00					
	O2	0.000e+00	0.000e+00	-78.842	-78.834	0.008
S(-2)	2.779e-03					
	HS-	2.761e-03	2.158e-03	-2.559	-2.666	-0.107
	H2S	1.702e-05	1.734e-05	-4.769	-4.761	0.008
	S-2	4.038e-07	1.654e-07	-6.394	-6.781	-0.387
S(6)	6.566e-04					
	SO4-2	5.010e-04	2.037e-04	-3.300	-3.691	-0.391
	MgSO4	7.863e-05	8.012e-05	-4.104	-4.096	0.008
	NaSO4-	4.727e-05	3.770e-05	-4.325	-4.424	-0.098
	CaSO4	2.814e-05	2.868e-05	-4.551	-4.542	0.008
	KSO4-	1.564e-06	1.247e-06	-5.806	-5.904	-0.098
	HSO4-	8.717e-12	6.952e-12	-11.060	-11.158	-0.098
Si	1.543e-04					
	H4SiO4	1.279e-04	1.304e-04	-3.893	-3.885	0.008
	H3SiO4-	2.639e-05	2.104e-05	-4.579	-4.677	-0.098
	H2SiO4-2	2.270e-09	9.186e-10	-8.644	-9.037	-0.393

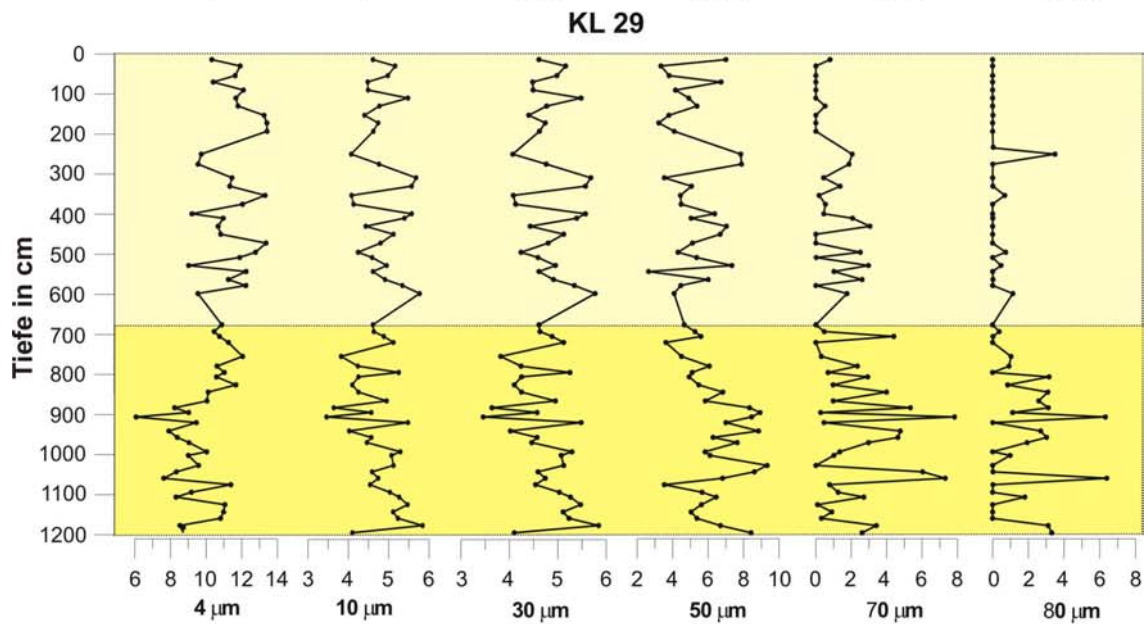
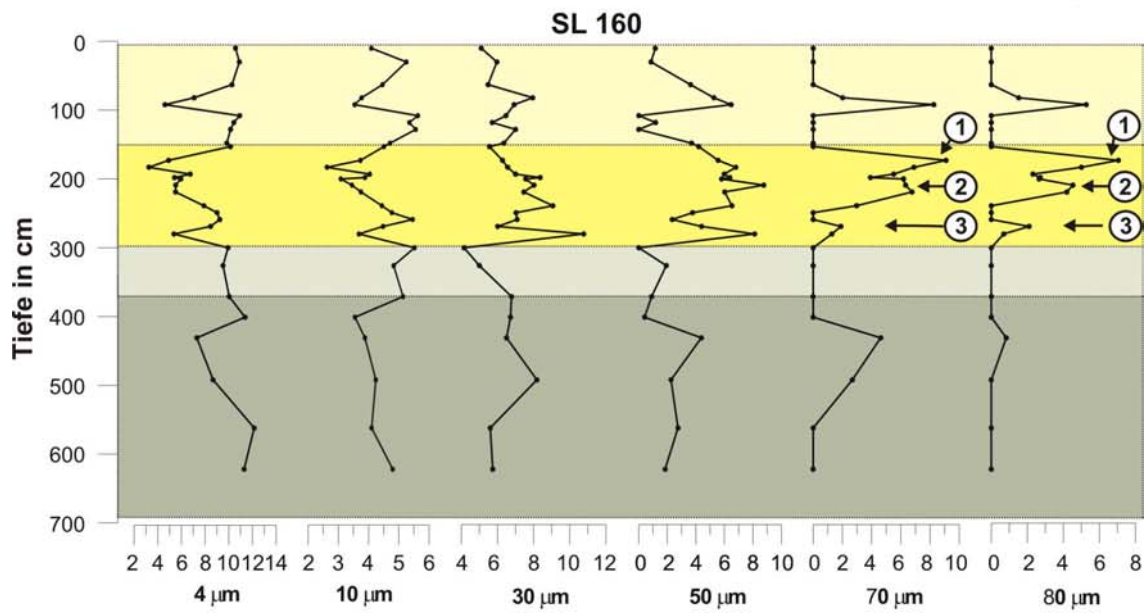
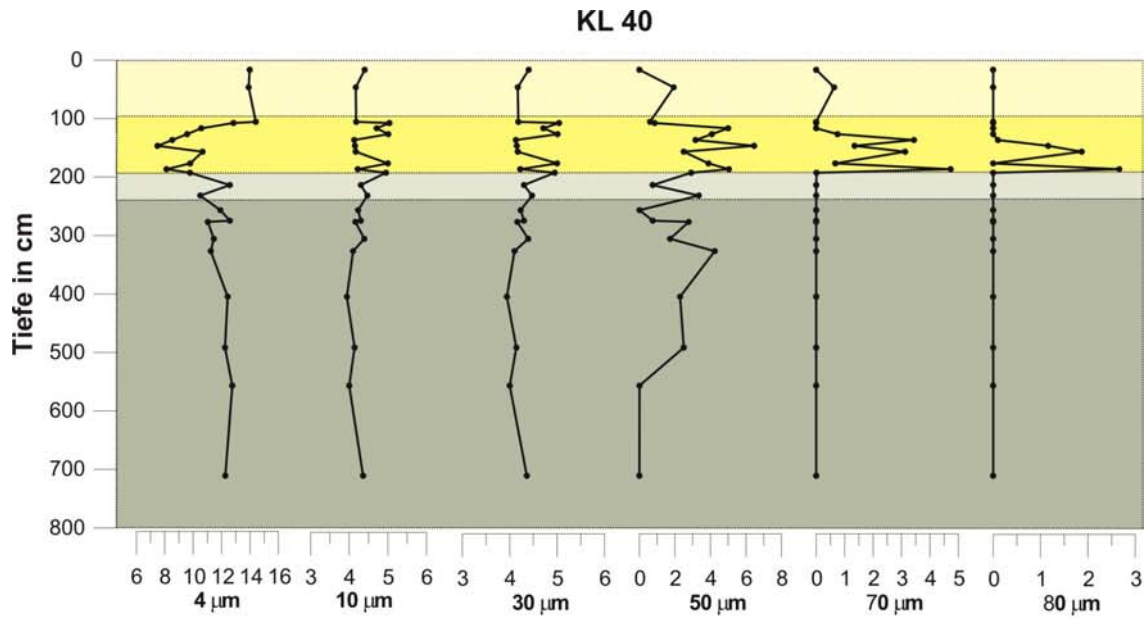
-----Saturation indices-----						
Phase	SI	log IAP	log KT			
Anhydrite	-2.44	29.41	31.85	CaSO4		
Aragonite	1.59	36.98	35.39	CaCO3		
Calcite	1.75	36.98	35.24	CaCO3		
CH4(g)	-1.71	-4.41	-2.69	CH4		
Chalcedony	-0.13	-3.88	-3.75	SiO2		
Chrysotile	6.03	40.35	34.32	Mg3Si2O5(OH)4		
CO2(g)	-3.97	21.44	25.41	CO2		
Dolomite	3.87	74.46	70.59	CaMg(CO3)2		
Gypsum	-2.18	29.41	31.59	CaSO4:2H2O		
H2(g)	-6.39	-6.46	-0.07	H2		
H2O(g)	-1.95	-0.00	1.95	H2O		
H2S(g)	-3.94	-11.98	-8.04	H2S		
O2(g)	-76.08	12.92	89.00	O2		
Quartz	0.34	-3.88	-4.22	SiO2		
Sepiolite	4.22	20.43	16.21	Mg2Si3O7.5OH:3H2O		
Sepiolite(d)	1.77	20.43	18.66	Mg2Si3O7.5OH:3H2O		
SiO2(a)	-1.03	-3.88	-2.85	SiO2		
Sulfur	-3.58	-5.52	-1.94	S		
Talc	9.24	32.59	23.35	Mg3Si4O10(OH)2		

-----  
End of simulation.  
-----

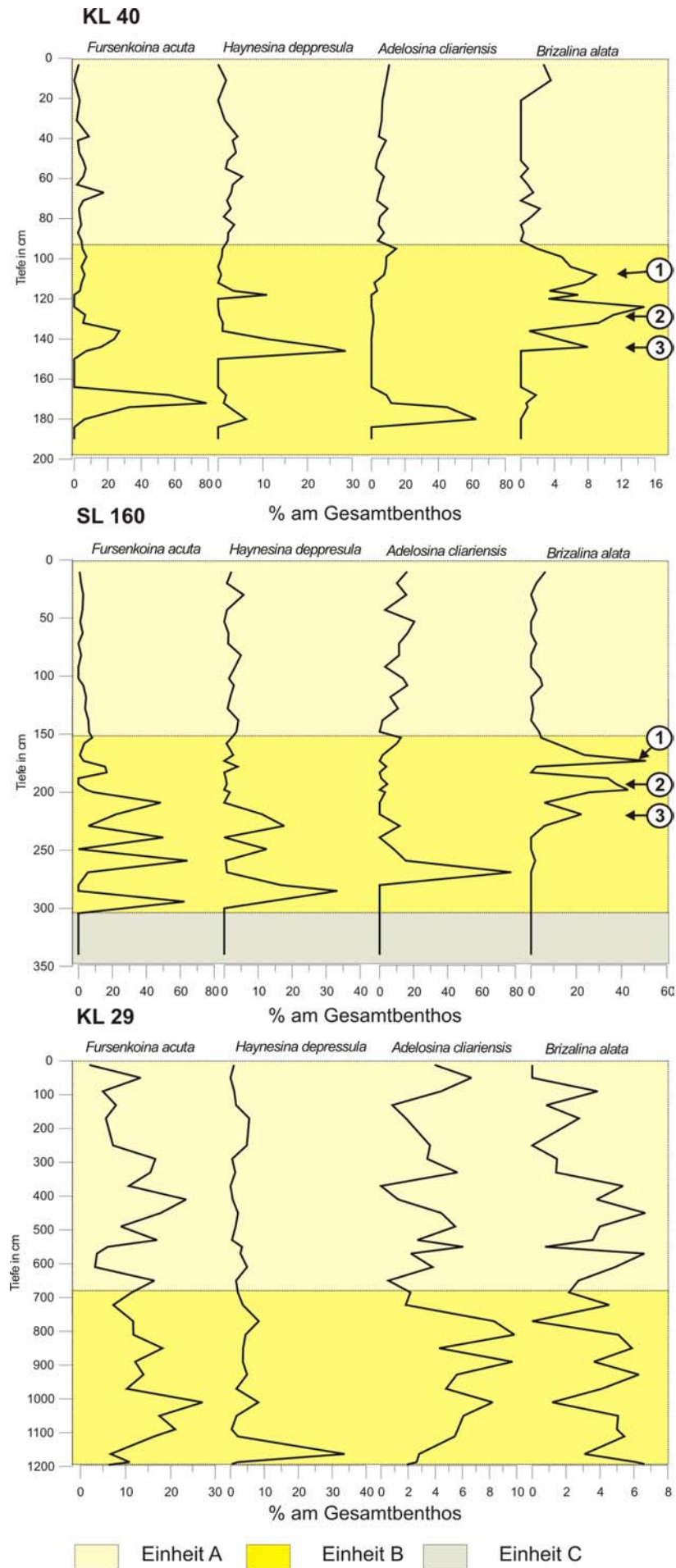
-----  
Reading input data for simulation 12.  
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-----  
End of run.  
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-----  
No memory leaks  
-----



Einheit A
  Einheit B
  Einheit C
  Einheit D



paläozeanographische/ paläoklimatologische Veränderung	Stanley & Blanpied (1980;) Aksu et al. (1999a)	Chagatay et al. (2000)	Ryan et al.(1997) Ballard et al. (2000)	Sperling et al. (2003)	Entwickeltes Modell dieser Arbeit
Lakustrine Phase des Marmarameeres (seit 40000a BP)	Keine Aussagen	Keine Aussagen	Keine Aussagen	Keine Aussagen	von 17000a bis 13000a Veränderung des Klimas zu warm-humiden Bedingungen; Zunahme des fluviatilen Eintrags von Sediment mit erhöhten Anteilen von mafischen Bestandteilen (Ni-Cr-Anomalie). Anoxische Bedingungen; Bildung von Sulfiden
Meeresspiegel überschreitet Dardanellen-Schwelle (-65m NN)	12000a-11000a	12000a-11000a	12000a-11000a	12000a-11000a	13000a, synsedimentäre Ausfällung eines Kalzit- Horizonts
Meeresspiegel überschreitet Bosporus-Schwelle (-35 NN)	9500a, Ausfluss aus dem Schwarzen Meer	10600a, Ausfluss aus dem Schwarzen Meer	7150a, Ausfluss aus dem Marmarameer ins Schwarze Meer	8700a, Ausfluss aus dem Marmarameer ins Schwarze Meer	8700a, Ausfluss aus dem Marmarameer in das Schwarze Meer
Zweischicht- Wasserkörper im Marmarameer	ab 9500a	ab 10600a	ab 7000a	ab 7000a	ab 7000a
Gründe für Sapropel- Bildung	Zweigeschichteter Wasserkörper, hohe Bioproduktivität durch Nährstoff- eintrag aus dem Schwarzen Meer	Zweigeschichteter Wasserkörper, hohe Bioproduktivität durch Nährstoff- eintrag aus dem Schwarzen Meer	Zweigeschichteter Wasserkörper, hohe Bioproduktivität durch Nährstoff- eintrag aus dem Schwarzen Meer	Reorganisation der biochemischen Zyklen	Nährstoffanreicherung im Oberflächenwasser durch aufsteigendes Tiefenwasser bei gleichzeitig erhöhten erosiven Eintrag durch humides Klima
Ablagerungszeitraum des Sapropels	9500 -7150a	10600-6400a	Keine Aussage zu Marmarameer	9500- 6500a	11500- 7800a