'temperature points' 8 0. 25. 60. 100. 150. 200. 250. 300.
'Debye-Huckel adh' 0.4939 0.5114 0.5465 0.5995 0.6855 0.7994 0.9593 1.2180
'Debye-Huckel bdh' 0.3253 0.3288 0.3346 0.3421 0.3525 0.3639 0.3766 0.3925
'Debye-Huckel bdt' 0.0374 0.0410 0.0440 0.0460 0.0470 0.0470 0.0340 0.0000

'HCO3-' 4.0 -1.0 61.0171
'H13CO3-' 4.0 -1.0 62.0171
'CH4(aq)' 3.0 0.0 16.00
'13CH4(aq)' 3.0 0.0 17.00
'H2O' 3.0 0.0 18.0153
'Ca++' 6.0 2.0 40.0780

'Cl-' 3.0 -1.0 35.4527
'Fe++' 6.0 2.0 55.8470
'Fe+++' 9.0 3.0 55.8470
'H+' 9.0 1.0 1.0079
'H2(aq)' 9.0 0.0 1.0079
'HPO4--' 4.0 -2.0 95.9793
'HS-' 3.0 -1.0 33.08
'K+' 3.0 1.0 39.0983
'Mg++' 8.0 2.0 24.3050
'NH4+' 3.0 1.0 18.0306
'Na+' 4.0 1.0 22.9898
'SO4--' 4.0 -2.0 96.0636
'H2(aq)' 3.0 0.0 2.0159
'End of primary' 0.0 0.0 0.0

'CO2(aq)' 3 -1.0000 'H2O' 1.0000 'H+' 1.0000 'HCO3-' -6.5804
-6.3447 -6.2684 -6.3882 -6.7235 -7.1969 -7.7868 -8.5280
3.0 0.0 44.0098
'CO3--' 2 -1.0000 'H+' 1.0000 'HCO3-' 10.6241 10.3288 10.1304
10.0836 10.2003 10.4648 10.8707 11.4638 4.5 -2.0 60.0092
'13CO2(aq)' 3 -1.0000 'H2O' 1.0000 'H+' 1.0000 'H13CO3-'
-6.575157231 -6.340786483 -6.266007282 -6.387191367 -6.723849202
-7.198317074 -7.789078905 -8.530989082 3.0 0.0 44.0098
'13CO3--' 2 -1.0000 'H+' 1.0000 'H13CO3-' 10.62438416 10.32896851
10.1304358 10.08351465 10.20009546 10.46450148 10.87032548 11.46336275 4.5
-2.0 60.0092

'NH3(aq)' 2 -1.0000 'H+' 1.0000 'NH4+' 10.0691 9.2410 8.2847
7.4010 6.5156 5.7992 5.1995 4.6767 2.5 0.0 18.0385
'H2PO4-' 2 1.0000 'H+' 1.0000 'HPO4--' -7.3231 -7.2054 -7.1888
-7.2876 -7.5259 -7.8671 -8.3189 -8.9357 4.0 -1.0 96.9872
'H3PO4(aq)' 2 1.0000 'HPO4--' 2.0000 'H+' -9.3933 -9.3751
-9.5434 -9.8805 -10.4425 -11.1429 -12.0169 -13.1928 3.0 0.0
97.9952
'PO4---' 2 -1.0000 'H+' 1.0000 'HPO4--' 12.6048 12.3218 12.1275
12.0760 12.1809 12.4313 12.8214 13.3896 4.0 -3.0 94.9714
'H2S(aq)' 2 1.0000 'H+' 1.0000 'HS-' -7.4159 -6.9877 -6.6467
-6.4827 -6.4960 -6.6831 -7.0225 -7.5536 3.0 0.0 34.0819
'S--' 2 -1.0000 'H+' 1.0000 'HS-' 13.7100 12.9351 12.0082
11.1018 10.1202 9.2545 8.4250 7.5568 5.0 -2.0 32.0660
'FeS(aq)' 3 -1.00 'H+' 1.00 'Fe++' 1.00 'HS-' -4.6480 -4.6480 -4.6480 -4.6480 -4.6480
-4.6480 -4.6480 -4.6480 3.0 0.0 87.9110
'End of secondary' 1 0. '0' 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.

'CO2(g)' 0.0000 1 1.0000 'CO2(aq)' -0.4 -0.4 -0.4 -0.4 -0.4 -0.4 -0.4 -0.4
44.0098
'13CO2(g)' 0.0000 1 1.0000 '13CO2(aq)' -0.400510835 -0.400461052
-0.400403915 -0.400351746 -0.400300412 -0.400259931 -0.40022719 -0.400200164
44.0098
'CH4(g)' 0.0000 1 1.0000 'CH4(aq)' -2.5846 -2.8502 -3.0228
-3.0582 -2.9646 -2.7795 -2.5344 -2.2310 16.0428
'13CH4(g)' 0.0000 1 1.0000 '13CH4(aq)' -2.584947575 -2.850547575
-3.023147575 -3.058547575 -2.964947575 -2.779847575 -2.534747575
-2.231347575 16.0428

'H2S(g)' 0.0000 2 1.0000 'H+' 1.0000 'HS-' -8.0781 -7.9759
-7.9295 -7.9572 -8.0759 -8.2750 -8.5671 -9.0074 34.0819
'End of gases' 0. 1 1. '0' 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.

'Calcite-Ca' 36.9340 4 -1.0000 'H+' 1.0000 'Ca++' 0.989305424
'HCO3-' 0.010694576 'H13CO3-' 2.2257 1.8487 1.3330 0.7743
0.0999 -0.5838 -1.3262 -2.2154 100.0872
'Calcite-Mg' 36.9340 4 -1.0000 'H+' 1.0000 'Mg++' 0.989305424
'HCO3-' 0.010694576 'H13CO3-' 2.2257 1.8487 1.3330 0.7743

0.0999 -0.5838 -1.3262 -2.2154 84.21413
'Pyrite_FeS' 23.94 3 -1.00 'H2(aq)' 1.00 'H2S(aq)' 1.00 'Mackinawite' -6.5285
-5.9811 -5.3527 -4.7789 -4.2142 -3.7689 -3.4087 -3.1113 119.9790
'CH2O_SO4' 28.81 7 -1 'SO4--' -0.264 'H+' 1.0 'H2S(aq)' 1.978281341 'HCO3-'
0.021718659 'H13CO3-' 0.302 'NH4+' 0.019 'HPO4--' 4 4 4 4 4 4 4 4 67.037
'CH2O_ME' 28.81 9 -0.264 'H2O' 0.989712522 'CH4(aq)' 0.010287478 '13CH4(aq)'
0.727578763 'CO2(aq)' 0.008421237 '13CO2(aq)' 0.260979678 'HCO3-' 0.003020322
'H13CO3-' 0.302 'NH4+' 0.019 'HPO4--' 4 4 4 4 4 4 4 4 67.037
'Mackinawite' 23.94 3 -1.0 'H+' 1.0 'Fe++' 1.0 'HS-' -4.648 -4.648 -4.648 -4.648
-4.648 -4.648 -4.648 -4.648 87.911
'End of minerals' 0. 1 0. '0' 0. 0. 0. 0. 0. 0. 0. 0. 0.

Begin aqueous kinetics
AOM 1 'monod' 5 -1.0 'SO4--' -1 'CH4(aq)' 1 'HCO3-' 1.0 'HS-' 1.0 'H2O' 5.8
0.5e-4 2 'SO4--' 5e-4 'CH4(aq)' 5e-3
'Inhibition' 0
13AOM 1 'monod' 5 -1.0 'SO4--' -1.0 '13CH4(aq)' 1.0 'H13CO3-' 1.0 'HS-' 1.0
'H2O' 5.8
0.3960396e-6 2 'SO4--' 5e-4 '13CH4(aq)' 4e-5
'Inhibition' 0
CO2_reduction 1 'monod' 5 -4.0 'H2(aq)' -1.0 'HCO3-' -1.0 'H+' 1.0 'CH4(aq)' 3.0
'H2O' 40.25
2.35e-5 2 'H2(aq)' 1e-6 'HCO3-' 1e-2
'Inhibition' 1 'SO4--' 1e-4

13CO2_reduction 1 'monod' 5 -4.0 'H2(aq)' -1.0 'H13CO3-' -1.0 'H+' 1.0
'13CH4(aq)' 3.0 'H2O' 40.25
1.9E-07 2 'H2(aq)' 1e-6 'H13CO3-' 8.8730E-05
'Inhibition' 1 'SO4--' 1e-4

End of aqueous kinetic

Begin mineral kinetics
+--
CH2O_SO4
label = default
type = monod
rate(25C) = -12.40

```
   activation = 0.0    (kcal/mole)
   monod_terms :    SO4--    100e-06
   inhibition :
   1 ch2o_so4 + 14 h+ + 53 so4-2 --> 53 h2s(aq) +    1 hpo4-2 + 16 nh4+ + 106 hco3-
+---------------------------------------------------
CH2O_ME
   label = default
   type    = monod
   rate(25C) = -12.40
   activation = 0.0    (kcal/mole)
   monod_terms :
   inhibition : SO4--    1600.0e-06 HCO3- 15e-3 CH4(aq) 15e-3
   1 ch2o_so4 + 14 h+ + 53 so4-2 --> 53 h2s(aq) +    1 hpo4-2 + 16 nh4+ + 106 hco3-
+---------------------------------------------------
Calcite-Ca
   label = default
   type    = tst
   rate(25C) = -6.19
   activation = 15.0    (kcal/mole)
   dependence : HCO3- 1.0
   1.0 Calcite + 1.0 H+ =    1.0 Ca+2 + 1.0 HCO3-
+---------------------------------------------------
Calcite-Mg
   label = default
   type    = tst
   rate(25C) = -6.19
   activation = 15.0    (kcal/mole)
   dependence : HCO3- 1.0
   1.0 Calcite + 1.0 H+ =    1.0 Ca+2 + 1.0 HCO3-
+---------------------------------------------------
Pyrite_FeS
   label = default
   type    = tst
   rate(25C) = -8
   activation = 15.0    (kcal/mole)
   dependence :
+---------------------------------------------------
Mackinawite
```

label = default
type = tst
rate(25C) = -8.90
activation = 0.0 (kcal/mole)
dependence :
1.0 FeS(am) + 1.0 H+ = 1.0 Fe+2 + 1.0 HS-
+----------

End of mineral kinetics
Begin exchange
'NaX' 2 1.0 'Na+' 1.0 'X-' 0.00 0.000
'KX' 2 1.0 'K+' 1.0 'X-' -0.48 0.000
'CaX2' 2 1.0 'Ca++' 2.0 'X-' -0.99 0.000
'MgX2' 2 1.0 'Mg++' 2.0 'X-' -0.86 0.000
'NH4X' 2 1.0 'NH4+' 1.0 'X-' -0.48 0.000
'NaXhan_zach1' 2 1.0 'Na+' 1.0 'Xhan_zach1-' 6.76 0.000
'NaXhan_zach2' 2 1.0 'Na+' 1.0 'Xhan_zach2-' 2.20 0.000
'CsXhan_zach1' 2 1.0 'Cs+' 1.0 'Xhan_zach1-' 0.00 0.000
'CsXhan_zach2' 2 1.0 'Cs+' 1.0 'Xhan_zach2-' 0.00 0.000
'NaXhan1' 2 1.0 'Na+' 1.0 'Xhan_col1-' 6.99 0.000
'NaXhan2' 2 1.0 'Na+' 1.0 'Xhan_col2-' 2.52 0.000
'CsXhan1' 2 1.0 'Cs+' 1.0 'Xhan_col1-' 0.00 0.000
'CsXhan2' 2 1.0 'Cs+' 1.0 'Xhan_col2-' 0.00 0.000
'NaXhan1' 2 1.0 'Na+' 1.0 'Xhan1-' 7.388 0.000
'NaXhan2' 2 1.0 'Na+' 1.0 'Xhan2-' 4.301 0.000
'NaXhan3' 2 1.0 'Na+' 1.0 'Xhan3-' 1.906 0.000
'KXhan1' 2 1.0 'K+' 1.0 'Xhan1-' 5.034 0.000
'KXhan2' 2 1.0 'K+' 1.0 'Xhan2-' 2.287 0.000
'KXhan3' 2 1.0 'K+' 1.0 'Xhan3-' 1.050 0.000
'Ca0.5Xhan1' 2 0.5 'Ca++' 1.0 'Xhan1-' 7.906 0.000
'Ca0.5Xhan2' 2 0.5 'Ca++' 1.0 'Xhan2-' 5.202 0.000
'Ca0.5Xhan3' 2 0.5 'Ca++' 1.0 'Xhan3-' 1.764 0.000
'CsXhan1' 2 1.0 'Cs+' 1.0 'Xhan1-' 0.00 0.000
'CsXhan2' 2 1.0 'Cs+' 1.0 'Xhan2-' 0.00 0.000
'CsXhan3' 2 1.0 'Cs+' 1.0 'Xhan3-' 0.00 0.000
'NaXhan1' 2 1.0 'Na+' 1.0 'Xhan1a-' 6.99 0.000
'NaXhan2' 2 1.0 'Na+' 1.0 'Xhan2a-' 2.34 0.000
'CsXhan1' 2 1.0 'Cs+' 1.0 'Xhan1a-' 0.00 0.000
'CsXhan2' 2 1.0 'Cs+' 1.0 'Xhan2a-' 0.00 0.000

End of exchange