**Example for PhreeqC script for groundwater from Tel shoket6 borehole, carbonate aquifer at temperature of 20⁰C**

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.7.0-15749\database\llnl.dat

SOLUTION\_MASTER\_SPECIES

Al Al+3 0 Al 26.9815

Si SiO2 0 SiO2 28.0855

SOLUTION\_SPECIES

Al+3 = Al+3

-llnl\_gamma 9.0000

log\_k 0

-delta\_H 0 kJ/mol # Calculated enthalpy of reaction Al+3

SiO2 = SiO2

-llnl\_gamma 3.0000

log\_k 0

-delta\_H 0 kJ/mol # Calculated enthalpy of reaction SiO2

# Enthalpy of formation: -209.775 kcal/mol

4H2O + Al+3 = Al(OH)4- + 4 H+

-llnl\_gamma 4.0

log\_k -22.851

-analytic 6.761926e+02 2.074159e-01 -3.498514e+04 -2.620590e+02 9.728766e+05 -6.794820e-05

-Vm 8.4938 12.9576 0.6570 -3.3147 1.0403 #TS01

H2O + Al+3 = Al(OH)+2 + H+

-llnl\_gamma 4.5

log\_k -4.964

-analytic 4.876919e+02 1.174365e-01 -2.522243e+04 -1.831424e+02 1.126238e+06 -2.890362e-05

-Vm -0.4532 -8.8878 9.2434 -2.4116 1.5897 #TS01

3H2O + Al+3 = Al(OH)3 + 3 H+

-llnl\_gamma 3.0

log\_k -17.044

-analytic 1.698129e+03 4.425076e-01 -8.348751e+04 -6.455354e+02 3.670657e+06 -1.242598e-04

-Vm 5.4624 5.5560 3.5662 -3.0087 0 #TS01

2H2O + Al+3 = Al(OH)2+ + 2 H+

-llnl\_gamma 4.0

log\_k -10.921

-analytic 1.378643e+03 3.661170e-01 -6.661347e+04 -5.249904e+02 2.937298e+06 -1.044802e-04 # TS01

-Vm 2.4944 -1.6909 6.4146 -2.7091 0.5324 # TS01

Al+3 + SiO2 + 2 H2O = AlH3SiO4+2 + H+

-llnl\_gamma 4.5

log\_k -2.613

-analytic 2.028449e+03 5.556364e-01 -9.187336e+04 -7.763264e+02 4.216938e+06 -1.677843e-04

-Vm 0.16 -7.23 8.61 -2.4800 0.88000 # TS01

4H2O + Na+ + Al+3 = NaAl(OH)4 + 4 H+

-llnl\_gamma 3.0

log\_k -22.9

-analytic -1.711218e+02 -9.243056e-02 -3.384201e+03 7.554937e+01 -3.703544e+05 4.899537e-05

-Vm 9.1267 14.3411 0.1121 -3.3719 0 # TS01

SiO2 + H2O = HSiO3- + H+

-llnl\_gamma 4.0

log\_k -9.842

-analytic 5.434886e+03 1.537747e+00 -2.417723e+05 -2.094080e+03 1.190645e+07 -4.999253e-04

-Vm 2.9735 -0.5158 5.9467 -2.7575 1.5511

SiO2 + Na+ + H2O = NaHSiO3 + H+

-llnl\_gamma 3.0

log\_k -8.011

-analytic 6.170122e+03 1.686468e+00 -2.788451e+05 -2.367426e+03 1.412272e+07 -5.219411e-04

-Vm 3.4928 0.75 5.4483 -2.8100 -0.038

SiO2 + Mg+2 + H2O = Mg(HSiO3)+ + H+

-llnl\_gamma 4.0

log\_k -8.582

-analytic 6.991775e+03 1.925345e+00 -3.158859e+05 -2.683919e+03 1.595435e+07 -5.970318e-04

-Vm 0.6289 -6.2428 8.1967 -2.5209 0.9177

SiO2 + Ca+2 + H2O = Ca(HSiO3)+ + H+

-llnl\_gamma 4.0

log\_k -8.832

-analytic -8.283895E+02 -3.440430E-01 2.115267E+04 3.404640E+02 -2.962864E+05 1.357884E-04

-Vm 1.0647 -5.1787 7.7785 -2.5649 0.5831

PHASES

Illite

K.85Fe.25Al2.35Si3.4O10(OH)2 + 8.4000 H+ = 0.8500 K+ + 2.3500 Al+3 + 5.2000 H2O + 3.4000 SiO2 + 0.2500 Fe+2

log\_k 9.68

-analytic 5.1079e2 1.2823e-1 -8.3236e3 -2.0525e2 0.0000E+00 -3.9850e-5

-Vm 140.67

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Step 1: Get initial solution composition by Tel shoket6 borehole with carbonate aquifer and gas at 20C##########

SOLUTION 0

temp 20

pH 7.22

units mmol/l

Br 0.0025

C 4.062

Ca 1.2975

Cl 1.8052 charge

K 0.0588

Mg 1.0286

Na 1.9575

S 0.3227

-water 1 # kg

GAS\_PHASE 0

-fixed\_pressure ###Consider a gas phase of CH4, H2O and CO2 (fixed\_pressure) as main gas components in the subsurface###

-pressure 1

-temperature 20

CO2(g) 0

CH4(g) 0

H2O(g) 0

Reaction 1

CO2(g) 1

CH4(g) 0

H2O(g) 0

0.002 moles

EQUILIBRIUM\_PHASES 0

Calcite 0 80.58

Dolomite 0 5.64

Quartz 0 3.86

K-Feldspar 0 0.32

Illite 0 0.12

Kaolinite 0 0.18

Save Solution 1

SELECTED\_OUTPUT 1

-file Base\_Mk Tel Shoket 6\_0.002mol\_Carbonate aquifer\_200c.out

-temperature true

-pH true

-totals Ca Mg C Si Al Fe Na

-saturation\_indices CO2(g)

-equilibrium\_phases Quartz K-feldspar Albite Calcite Kaolinite Pyrite Dolomite Siderite Illite1

-gases CO2(g) CH4(g) H2O(g)

End

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Step 2: Recalculate the changes of gas phase and minerals at 20 C ##

Use Solution 1

GAS\_PHASE 1

-fixed\_pressure

-pressure 1

-temperature 20

CO2(g) 0

CH4(g) 0

H2O(g) 0

Reaction 1

CO2(g) 1

CH4(g) 0

H2O(g) 0

0.002 moles

REACTION\_TEMPERATURE 1

20

REACTION\_PRESSURE 1

1

EQUILIBRIUM\_PHASES 1

Calcite 0 80.58

Dolomite 0 5.64

Quartz 0 3.86

K-Feldspar 0 0.32

Illite 0 0.12

Kaolinite 0 0.18

Save Solution 2

Save GAS\_PHASE 2

Save EQUILIBRIUM\_PHASES 2

END

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Step 3: Increase Step-wisely the temperature and pressure of the system to mimic burial. ##########

Use Solution 2

Use GAS\_PHASE 2

Use EQUILIBRIUM\_PHASES 2

REACTION\_TEMPERATURE 1

30

REACTION\_PRESSURE 1

50.35

Save Solution 3

Save GAS\_PHASE 3

Save EQUILIBRIUM\_PHASES 3

END

Use Solution 3

Use GAS\_PHASE 3

USE EQUILIBRIUM\_PHASES 3

REACTION\_TEMPERATURE 2

40

REACTION\_PRESSURE 2

99.69

Save Solution 4

Save GAS\_PHASE 4

Save EQUILIBRIUM\_PHASES 4

END

Use Solution 4

Use GAS\_PHASE 4

USE EQUILIBRIUM\_PHASES 4

REACTION\_TEMPERATURE 3

50

REACTION\_PRESSURE 3

140.04

Save Solution 5

Save GAS\_PHASE 5

Save EQUILIBRIUM\_PHASES 5

END

Use Solution 5

Use GAS\_PHASE 5

USE EQUILIBRIUM\_PHASES 5

REACTION\_TEMPERATURE 4

60

REACTION\_PRESSURE 4

198.38

Save Solution 6

Save GAS\_PHASE 6

Save EQUILIBRIUM\_PHASES 6

END

Use Solution 6

Use GAS\_PHASE 6

USE EQUILIBRIUM\_PHASES 6

REACTION\_TEMPERATURE 5

70

REACTION\_PRESSURE 5

247.73

Save Solution 7

Save GAS\_PHASE 7

Save EQUILIBRIUM\_PHASES 7

END

Use Solution 7

Use GAS\_PHASE 7

USE EQUILIBRIUM\_PHASES 7

REACTION\_TEMPERATURE 6

80

REACTION\_PRESSURE 6

297.08

Save Solution 8

Save GAS\_PHASE 8

Save EQUILIBRIUM\_PHASES 8

END

Use Solution 8

Use GAS\_PHASE 8

USE EQUILIBRIUM\_PHASES 8

REACTION\_TEMPERATURE 7

90

REACTION\_PRESSURE 7

364.42

Save Solution 9

Save GAS\_PHASE 9

Save EQUILIBRIUM\_PHASES 9

END

Use Solution 9

Use GAS\_PHASE 9

USE EQUILIBRIUM\_PHASES 9

REACTION\_TEMPERATURE 8

100

REACTION\_PRESSURE 8

395.77

Save Solution 10

Save GAS\_PHASE 10

Save EQUILIBRIUM\_PHASES 10

END

Use Solution 10

Use GAS\_PHASE 10

USE EQUILIBRIUM\_PHASES 10

REACTION\_TEMPERATURE 9

110

REACTION\_PRESSURE 9

445.12

Save Solution 11

Save GAS\_PHASE 11

Save EQUILIBRIUM\_PHASES 11

END

Use Solution 11

Use GAS\_PHASE 11

USE EQUILIBRIUM\_PHASES 11

REACTION\_TEMPERATURE 10

120

REACTION\_PRESSURE 10

494.46

Save Solution 12

Save GAS\_PHASE 12

Save EQUILIBRIUM\_PHASES 12

END

Use Solution 12

Use GAS\_PHASE 12

USE EQUILIBRIUM\_PHASES 12

REACTION\_TEMPERATURE 11

130

REACTION\_PRESSURE 11

543.81

Save Solution 13

Save GAS\_PHASE 13

Save EQUILIBRIUM\_PHASES 13

END

Use Solution 13

Use GAS\_PHASE 13

USE EQUILIBRIUM\_PHASES 13

REACTION\_TEMPERATURE 12

140

REACTION\_PRESSURE 12

593.15

Save Solution 14

Save GAS\_PHASE 14

Save EQUILIBRIUM\_PHASES 14

END

Use Solution 14

Use GAS\_PHASE 14

USE EQUILIBRIUM\_PHASES 14

REACTION\_TEMPERATURE 13

150

REACTION\_PRESSURE 13

642.50

Save Solution 15

Save GAS\_PHASE 15

Save EQUILIBRIUM\_PHASES 15

END

Use Solution 15

Use GAS\_PHASE 15

USE EQUILIBRIUM\_PHASES 15

REACTION\_TEMPERATURE 14

160

REACTION\_PRESSURE 14

691.85

Save Solution 16

Save GAS\_PHASE 16

Save EQUILIBRIUM\_PHASES 16

END

Use Solution 16

Use GAS\_PHASE 16

USE EQUILIBRIUM\_PHASES 16

REACTION\_TEMPERATURE 15

170

REACTION\_PRESSURE 15

741.19

Save Solution 17

Save GAS\_PHASE 17

Save EQUILIBRIUM\_PHASES 17

END

Use Solution 17

Use GAS\_PHASE 17

USE EQUILIBRIUM\_PHASES 17

REACTION\_TEMPERATURE 16

180

REACTION\_PRESSURE 16

790.54

Save Solution 18

Save GAS\_PHASE 18

Save EQUILIBRIUM\_PHASES 18

END

Use Solution 18

Use GAS\_PHASE 18

USE EQUILIBRIUM\_PHASES 18

REACTION\_TEMPERATURE 17

190

REACTION\_PRESSURE 17

839.88

Save Solution 19

Save GAS\_PHASE 19

Save EQUILIBRIUM\_PHASES 19

END

Use Solution 19

Use GAS\_PHASE 19

USE EQUILIBRIUM\_PHASES 19

REACTION\_TEMPERATURE 18

200

REACTION\_PRESSURE 18

889.23

Save Solution 20

Save GAS\_PHASE 20

Save EQUILIBRIUM\_PHASES 20

END