Datashare 62:

From shale oil to biogenic shale gas: Retracing organic–inorganic interactions in the Alum Shale (Furongian–Lower Ordovician) in southern Sweden

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OIL DEGRADATION ALUM SHALE

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#**************************************************************************************
# USE PHREEQC INTERACTIVE3.0 COMPUTER CODE AND ITS PHREEQC.DAT DATABASE
#**************************************************************************************

SELECTED_OUTPUT
-FILE OIL DEGRADATION ALUM SHALE.XLS
-EQUILIBRIUM_PHASES CALCITE KAOLINITE PYRITE QUARTZ K-FELDSPAR CHLORITE(14A) ANORTHITE
-GASES CH4(G) CO2(G) H2(G)
-TOTALS ACETATE C(−4) C(4) S(−2) S(6) CA MG NA K SI AL CL
-ALKALINITY

#- - - - - - - - - - - - - - - - - - - ACETATE SPECIES DEFINITION (FROM MINTEQ.V4.DAT)
SOLUTION_MASTER_SPECIES
ACETATE                 ACETATE-        1.0         59.045         59.045

SOLUTION_SPECIES
ACETATE- = ACETATE-
        LOG_K 0

H++ ACETATE- = H(ACETATE)
        LOG_K   4.757
        DELTA_H         0.41            KJ
        -GAMMA 0        0
                #               ID:                     3309921
                #       LOG K SOURCE:                   NIST46.4
                #       DELTA H SOURCE:                 NIST46.4
                #     T AND IONIC STRENGTH:             0.00 25.0

CA+2 + ACETATE- = CA(ACETATE)+
        LOG_K   1.18
        DELTA_H             4           KJ
        -GAMMA 0            0
                #               ID:                     1509920
                #       LOG K SOURCE:                   NIST46.4
                #       DELTA H SOURCE:                 NIST46.4
                #     T AND IONIC STRENGTH:             0.00 25.0
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NA+ + ACETATE- = NA(ACETATE)
        LOG_K   −0.18
        DELTA_H         12              KJ
        -GAMMA 0        0
                #               ID:                     5009920
                #       LOG K SOURCE:                   NIST46.4
                #       DELTA H SOURCE:                 NIST46.4
                #     T AND IONIC STRENGTH:             0.00 25.0

K+ + ACETATE- = K(ACETATE)
        LOG_K           −0.1955
        DELTA_H             4.184           KJ
        -GAMMA 0            0
                #           ID:                     4109921
                #       LOG K SOURCE:                   NIST46.4
                #       DELTA H SOURCE:                 NIST46.2
                #    T AND IONIC STRENGTH:              0.10 25.0

FE+2 + ACETATE- = FE(ACETATE)+
        LOG_K               1.4
        DELTA_H             0               KJ
        -GAMMA 0            0
                #           ID:                     2809920
                #       LOG K SOURCE:                   NIST46.4
                #       DELTA H SOURCE:                 NIST46.2
                #    T AND IONIC STRENGTH:              0.00 25.0
FE+3 + ACETATE- = FE(ACETATE)+2
        LOG_K               4.0234
        DELTA_H             0               KJ
        -GAMMA 0            0
                #           ID:                     2819920
                #       LOG K SOURCE:                   NIST46.4
                #       DELTA H SOURCE:                 NIST46.2
                #    T AND IONIC STRENGTH:              0.10 20.0
FE+3 + 2ACETATE- = FE(ACETATE)2+
        LOG_K               7.5723
        DELTA_H             0               KJ
        -GAMMA 0            0
                #               ID:                     2819921
                #         LOG K SOURCE:                 NIST46.4
                #         DELTA H SOURCE:               NIST46.2
                #       T AND IONIC STRENGTH:           0.10 20.0
FE+3 + 3ACETATE- = FE(ACETATE)3
        LOG_K               9.5867
        DELTA_H             0               KJ
        -GAMMA 0            0
                #               ID:                     2819922
                #         LOG K SOURCE:                 NIST46.4
                #         DELTA H SOURCE:               NIST46.2
                #       T AND IONIC STRENGTH:           0.10 20.0


#- - - - - - - - - - - - - - - - - - - - GENERIC FRESHWATER (MELTING WATER)
SOLUTION 1
-TEMP                   4.0
-PH                     7.0
-UNITS                  MMOL/L
-DENSITY                1.000
#- - - - - - GENERIC FRESHWATER EQUILIBRATES WITH PRIMARY ROCK MINERAL ASSEMBLAGE
#- - - - - - - - - - - - - - - - - AT 20 BAR HYDROSTATIC PRESSURE (CA. 200 M DEPTH)
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#- - - - - - - - - - - - - - - - - - - - - - - - - - - - - CO2 PARTIAL PRESSURE IS 0.032 BAR
EQUILIBRIUM_PHASES 1
CALCITE             0.0     10.0
QUARTZ              0.0     10.0
KAOLINITE           0.0     10.0
PYRITE              0.0     10.0
K-MICA              0.0     10.0 DISSOLVE ONLY
K-FELDSPAR          0.0     10.0
CHLORITE(14A)       0.0     10.0
ANORTHITE           0.0     0.02
CO2(G)             −1.5     0.01
REACTION_PRESSURE 1
20.0
SAVE SOLUTION 2
END

#- - - - - - - - - - - - - - - - - - - - - - - - - - - - -  GENERIC NA+/CL- DOMINATED BRINE
SOLUTION 3
-TEMP      4.0
-PH      7.0
-UNITS      MMOL/L
-DENSITY      1.001
NA                  10.0
CL                  10.0 CHARGE
S(6)                0.1

#- - - - - -  GENERIC BRINE EQUILIBRATES WITH PRIMARY ROCK MINERAL ASSEMBLAGE
#- - - - - - - - - - - - - - - - -  AT 20 BAR HYDROSTATIC PRESSURE (CA. 200 M DEPTH)
#- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - CO2 PARTIAL PRESSURE IS 0.032 BAR
EQUILIBRIUM_PHASES 3
CALCITE             0.0     10.0
QUARTZ              0.0     10.0
KAOLINITE           0.0     10.0
PYRITE              0.0     10.0
K-MICA              0.0     10.0 DISSOLVE ONLY
K-FELDSPAR          0.0     10.0
CHLORITE(14A)       0.0             10.0
ANORTHITE           0.0     0.02
CO2(G)             −1.5             0.01
REACTION_PRESSURE 3
20.0
SAVE SOLUTION 4
END

#- - - - - - - - - - - - - - - - - - - - - - - -  COMPOSITIONAL MIXING OF GENERIC BRINE AND FRESHWATER
#- - - - - - - - - - - - - - - - AND CONCURRENT EQUILIBRATION WITH PRIMARY ROCK MINERAL ASSEMBLAGE
#- - - - - - - - - - - - - - – - - - - - - - - - - - - - - - - - - AT A DEPTH OF 200 M (DUE TO DIFFUSION)
#- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - 95% OF FRESHWATER PLUS 5% OF BRINE
MIX 5
2 0.95
4 0.05
EQUILIBRIUM_PHASES 5
CALCITE             0.0     10.0
QUARTZ              0.0     10.0
KAOLINITE           0.0     10.0
PYRITE              0.0     10.0
K-MICA              0.0     10.0 DISSOLVE ONLY
K-FELDSPAR          0.0     10.0
CHLORITE(14A)       0.0             10.0
ANORTHITE           0.0     0.02
```

```
CO2(G)                  −1.5        0.01
REACTION_PRESSURE 5
20.0
SAVE SOLUTION 6
END

#- - - - - - - - - - - - - ORGANIC-INORGANIC INTERACTIONS DUE TO HYDROCARBON DEGRADATION
#- - - - - - - - - - - - - CONCURRENT EQUILIBRATION WITH PRIMARY ROCK MINERAL ASSEMBLAGE
##- - - - - FORMATION OF A (POTENTIAL) FIXED-PRESSURE GAS PHASE AT 20 BAR IS ALLOWED
USE SOLUTION 6
EQUILIBRIUM_PHASES 6
CALCITE             0.0     10.0
QUARTZ              0.0     10.0
KAOLINITE           0.0     10.0
PYRITE              0.0     10.0
K-MICA              0.0     10.0 DISSOLVE ONLY
K-FELDSPAR          0.0     10.0
CHLORITE(14A)       0.0          10.0
ANORTHITE           0.0     0.02
REACTION_PRESSURE 6
20.0
REACTION 6
# HDP FORMATION SUMMARIZED BY THE OVERALL REACTION:
# R-CH2-CH2-CH3 + 4H2O = R + 2CO2 + CH4 + 5H2 (HDP); ACCORDING TO SEEWALD (2003)
CO2     1.98
CH4     0.98
H2      5.0
H(ACETATE)  0.02
0.015  0.020  0.025  0.030  0.035  0.040  0.045  0.05  0.055  0.06  MOLES

GAS_PHASE 6 FIXED-PRESSURE GAS PHASE
-FIXED_PRESSURE
-PRESSURE  20
CO2(G)  0.0
CH4(G)  0.0
H2(G)  0.0
H2S(G)  0.0
SAVE SOLUTION 7
END
```