

Uranium chemistry in groundwater

PhreeqC Code

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TITLE Seawater

SOLUTION_MASTER_SPECIES
  U      U+4      0.0      238.0290      238.0290
  U(4)   U+4      0.0      238.0290
  U(5)   UO2+     0.0      238.0290
  U(6)   UO2+2    0.0      238.0290

SOLUTION_SPECIES
  #primary master species for U
  #is also secondary master species for U(4)
  U+4 = U+4
      log_k      0.0
  U+4 + 4 H2O = U(OH)4 + 4 H+
      log_k      -8.538
      delta_h     24.760 kcal
  U+4 + 5 H2O = U(OH)5- + 5 H+
      log_k      -13.147
      delta_h     27.580 kcal
  #secondary master species for U(5)
  U+4 + 2 H2O = UO2+ + 4 H+ + e-
      log_k      -6.432
      delta_h     31.130 kcal
  #secondary master species for U(6)
  U+4 + 2 H2O = UO2+2 + 4 H+ + 2 e-
      log_k      -9.217
      delta_h     34.430 kcal
  UO2+2 + H2O = UO2OH+ + H+
      log_k      -5.782
      delta_h     11.015 kcal
  2UO2+2 + 2H2O = (UO2)2(OH)2+2 + 2H+
      log_k      -5.626
      delta_h     -36.04 kcal
  3UO2+2 + 5H2O = (UO2)3(OH)5+ + 5H+
      log_k      -15.641
      delta_h     -44.27 kcal
  UO2+2 + CO3-2 = UO2CO3
      log_k      10.064
      delta_h     0.84 kcal
  UO2+2 + 2CO3-2 = UO2(CO3)2-2
      log_k      16.977
      delta_h     3.48 kcal
  UO2+2 + 3CO3-2 = UO2(CO3)3-4
      log_k      21.397
      delta_h     -8.78 kcal

PHASES
  Uraninite

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    UO2 + 4 H+ = U+4 + 2 H2O
    log_k          -3.490
    delta_h        -18.630 kcal
    Carnotite
K2(UO2)2(VO4)2 = 2K+ + 2UO2+2 + 2VO4-3
    log_k          -56.730
    delta_h        55 kcal

    Autunite
Ca(UO2)2(PO4)2 = Ca+2 + 2UO2+2 + 2PO4-3
    log_k          -48.360
    delta_h        0.0

SOLUTION 1
    units      ppm
    pH         8.22
    pe         8.451
    temp       25.0
    redox      N(5)/N(-3)
    pH         6.5
    S(6) 3.3 as S04
    N(5) 0.58 as N03
    P(5) 0.1
    U          0.01
    V          0.01
    Cl         0.22
    Na         0.38
    K          0.36
    Ca         0.20
    Mg         0.30
    Alkalinity 0.68 as HCO3
    N(-3) 0.81 as NH4
SAVE solution 1
SELECTED_OUTPUT
    -file ex21.txt
    -step true
    -pH true
    -pe true
    -reaction true
    -temperature true
    -alkalinity true
    -si CO2(g) CH4(g) N2(g) NH3(g)
    -gases CO2(g) N2(g) NH3(g)
    -totals Ca Na Cl S(6) N(5) Na K
    -molalities Ca+2 Na+ Cl-

END
TITLE Soil Processes
USE solution 1
EQUILIBRIUM_PHASES 1
    Autunite 0.0
    Carnotite 0.0

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Hydroxylapatite 0.0
Fluorite 0.0
SAVE solution 1
SELECTED_OUTPUT
  -file ex22.txt
  -step true
  -pH true
  -pe true
  -reaction true
  -temperature true
  -alkalinity true
  -si CO2(g) CH4(g) N2(g) NH3(g)
  -gases CO2(g) N2(g) NH3(g)
  -totals Ca Na Cl S(6) N(5) Na K
  -molalities Ca+2 Na+ Cl-
END
TITLE Evaporate water from soil
REACTION 1
  H2O      -1.0
  50.5 moles in 10 steps
REACTION_Temperature 1
  25
USE solution 1
SAVE solution 1
SELECTED_OUTPUT
  -file ex23.txt
  -step true
  -pH true
  -pe true
  -reaction true
  -temperature true
  -alkalinity true
  -si CO2(g) CH4(g) N2(g) NH3(g)
  -gases CO2(g) N2(g) NH3(g)
  -totals Ca Na Cl S(6) N(5) Na K
  -molalities Ca+2 Na+ Cl-
END
TITLE Vary temperature
REACTION_TEMPERATURE 2
  10.0 25.0 in 160 steps
USE solution 1
SAVE solution 1
SELECTED_OUTPUT
  -file ex24.txt
  -step true
  -pH true
  -pe true
  -reaction true
  -temperature true
  -alkalinity true
  -si CO2(g) CH4(g) N2(g) NH3(g)
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    -gases CO2(g) N2(g) NH3(g)
    -totals Ca Na Cl S(6) N(5) Na K
    -molalities Ca+2 Na+ Cl-
END
TITLE

SURFACE_SPECIES
  Hfo_sOH + H+ = Hfo_sOH2+
  log_k 7.18
  Hfo_sOH = Hfo_sO- + H+
  log_k -8.82
  Hfo_sOH + Zn+2 = Hfo_sOZn+ + H+
  log_k 0.66
  Hfo_wOH + H+ = Hfo_wOH2+
  log_k 7.18
  Hfo_wOH = Hfo_wO- + H+
  log_k -8.82
  Hfo_wOH + Zn+2 = Hfo_wOZn+ + H+
  log_k -2.32

USE solution 1

SURFACE 1
  Hfo_sOH      5e-6    600.    0.09
  Hfo_wOH      2e-4
SAVE solution 1
SELECTED_OUTPUT
  -file ex25.txt
  -step true
  -pH true
  -pe true
  -reaction true
  -temperature true
  -alkalinity true
  -si CO2(g) CH4(g) N2(g) NH3(g)
  -gases CO2(g) N2(g) NH3(g)
  -totals Ca Na Cl S(6) N(5) Na K
  -molalities Ca+2 Na+ Cl-
END
TITLE Redox Reaction
USE solution 1
REACTION 1
  CH2O 0.1 # add 0.1 mol CH2O;
  0.1 moles in 100 steps
SAVE solution 1
SELECTED_OUTPUT
  -file ex26.txt
  -step true
  -pH true
  -pe true
  -reaction true

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-temperature true
-alkalinity true
-si CO2(g) CH4(g) N2(g) NH3(g)
-gases CO2(g) N2(g) NH3(g)
-totals Ca Na Cl S(6) N(5) Na K
-molalities Ca+2 Na+ Cl-

END
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