Example Problem W-6

Uranium Sorption/Desorption Due to River Water/Groundwater Interaction

Abstract: *This problem addresses the significance of water chemistry on uranium mobility at the Hanford 300 Area. Laboratory-derived uranium sorption models were used in the simulation. To solve the chemical reactions in this problem, STOMP-W-R is used.*

Problem Description

This problem addresses water chemistry effects on uranium sorption during river water intrusion. Initially, uranium in the column is in equilibrium with the groundwater solution chemistry measured in a nearby well (Table 1). A steady flux rate of 1.44 m/d was specified for the reactive transport model. River water chemistry (Table 1) is specified at the boundary. A total of 54 reactions (Tables 2 and 3) were considered in the reaction network. The calcite dissolution/precipitation reaction in Table 3 is kinetic while the rest are equilibrium reactions.

Table 1. Solution Chemistry Composition for River Water and Groundwater in the Hanford 300 Area (from Yabusaki et al., 2008).

Components	River water	Ground water
pH	7.1	7.7
HCO_3^-	9.18e-4 M	2.66e-3 M
K^+	1.75e-5	1.50e-4
NO_3^-	8.55e-6	1.73e-4
Sr^{2+}	1.23e-6	0
Na^+	1.00e-4	9.87e-4
Ca^{2+}	3.74e-4	1.10e-3
Mg^{2+}	1.48e-4	4.10e-4
Cl^-	3.10e-5	2.75e-3
SO_4^{2-}	7.08e-5	3.25e-4

Table 2. Reaction Stoichiometry and Thermodynamics for Uranium (from Yabusaki et al., 2008).

Reaction	**log K (I = 0)**
$UO_2^{2+} + H_2O = UO_2OH^+ + H^+$	-5.25
$UO_2^{2+} + 2H_2O = UO_2(OH)_{2,aq} + 2H^+$	-12.15
$UO_2^{2+} + 3H_2O = UO_2(OH)_3^- + 3H^+$	-20.25
$UO_2^{2+} + 4H_2O = UO_2(OH)_4^{2-} + 4H^+$	-32.4
$2UO_2^{2+} + H_2O = (UO_2)_2OH^{3+} + H^+$	-2.70
$2UO_2^{2+} + 2H_2O = (UO_2)_2(OH)_2^{2+} + 2H^+$	-5.62
$3UO_2^{2+} + 4H_2O = (UO_2)_3(OH)_4^{2+} + 4H^+$	-11.90
$3UO_2^{2+} + 5H_2O = (UO_2)_3(OH)_5^+ + 5H^+$	-15.55
$3UO_2^{2+} + 7H_2O = (UO_2)_3(OH)_7^- + 7H^+$	-32.20
$4UO_2^{2+} + 7H_2O = (UO_2)_4(OH)_7^+ + 7H^+$	-21.9
$UO_2^{2+} + CO_3^{2-} = UO_2CO_3(aq)$	9.94
$UO_2^{2+} + 2CO_3^{2-} = UO_2(CO_3)_2^{2-}$	16.61
$UO_2^{2+} + 3CO_3^{2-} = UO_2(CO_3)_3^{4-}$	21.84
$2UO_2^{2+} + CO_3^{2-} + 3H_2O = (UO_2)_2CO_3(OH)_3^- + 3H^+$	-0.855
$Ca^{2+} + UO_2^{2+} + 3CO_3^{2-} = CaUO_2(CO_3)_3^{2-}$	25.64
$2Ca^{2+} + UO_2^{2+} + 3CO_3^{2-} = Ca_2UO_2(CO_3)_3$ (aq)	30.55
$UO_2^{2+} + NO_3^- = UO_2NO_3^+$	0.3
$UO_2^{2+} + Cl^- = UO_2Cl^+$	0.17
$UO_2^{2+} + 2Cl^- = UO_2Cl_2(aq)$	-1.1
$UO_2^{2+} + SO_4^{2-} = UO_2SO_4(aq)$	3.15
$UO_2^{2+} + 2SO_4^{2-} = UO_2(SO_4)_2^{2-}$	4.14
$SOH + UO_2^{2+} + H_2O = SOUO_2OH + 2H^+$	-5.235
$SOH + UO_2^{2+} + H_2CO_3 = SOHUO_2CO_3 + 2H^+$	-1.033

Table 3. Reaction Stoichiometry and Thermodynamics General Water Chemistry (from Yabusaki et al., 2008).

Reaction	**Log K**
$H^+ + HCO_3^- = H_2CO_3$	6.3414
$HCO_3^- = CO_3^{2-} + H^+$	-10.3249
$Ca^{2+} + HCO_3^- = CaCO_3(aq) + H^+$	-7.0088
$Ca^{2+} + Cl^- = CaCl^+$	-0.7004
$Ca^{2+} + 2Cl^- = CaCl_2(aq)$	-0.6535
$Ca^{2+} + HCO_3^- = CaHCO_3^+$	1.0420
$Ca^{2+} + NO_3^- = CaNO_3^+$	1.3
$Mg^{2+} + NO_3^- = MgNO_3^+$	1.3
$Ca^{2+} + H_2O = CaOH^+ + H^+$	-12.85
$Ca^{2+} + SO_4^{2-} = CaSO4(aq)$	2.1004
$H^+ + Cl^- = HCl(aq)$	0.6999
$H^+ + NO_3^- = HNO_3(aq)$	-1.3081
$K^+ + Cl^- = KCl(aq)$	-1.5004
$K^+ + SO_4^{2-} = KSO_4^-$	0.875
$Mg^{2+} + HCO_3^- = MgCO_3(aq) + H^+$	-7.3562
$Mg^{2+} + Cl^- = MgCl^+$	-0.1386
$Mg^{2+} + HCO_3^- = MgHCO_3^+$	1.0329
$Mg^{2+} + SO_4^{2-} = MgSO_4(aq)$	2.4125
$Na^+ + HCO_3^- = NaCO_3^- + H^+$	-9.8156
$Na^+ + Cl^- = NaCl$	-0.7821
$Na^+ + HCO_3^- = NaHCO_3$ (aq)	0.1557
$Na^+ + H_2O = NaOH(aq) + H^+$	-14.7986
$Na^+ + SO_4^{2-} = NaSO_4^-$	0.82
$H^+ + OH^- = H_2O$	13.9911
$Sr^{2+} + HCO_3^- = SrCO_3(aq) + H^+$	-7.4703
$Sr^{2+} + Cl^- = SrCl^+$	-0.2533
$Sr^{2+} + NO_3^- = SrNO_3^+$	0.8
$Sr^{2+} + H_2O = SrOH^+ + H^+$	-13.29
$Sr^{2+} + SO_4^{2-} = SrSO_4(aq)$	2.3
$Na^+ + NO_3^- = NaNO_3(aq)$	-0.2564
$Ca^{2+} + HCO_3^- = Calcite(s) + H^+$	-1.8542

Currently there are four reaction rate models available with the STOMP simulator when compiled with Eckechem: 1) Steefel-Lasagna Dissolution-Precipitation (a.k.a Transition-State Theory or TST), 2) Smith-Atkins Forward-Backward, 3) Valocchi Monod, and 4) Valocchi Sorption. This example uses the TST rate equation (Lasaga 1984; Steefel and Lasaga 1994), which is expressed as

$$R_k = A_m k \left[1 - \frac{Q}{K_{eq}} \right] \tag{1}$$

where m is the mineral index, R_k is the dissolution/precipitation rate (positive values indicate dissolution, and negative values precipitation), A_m is the specific reactive surface area, k is the rate constant (moles per unit mineral surface area and unit time) which is temperature dependent, K_{eq} is the equilibrium constant for the mineral-water reaction written for the destruction of one mole of mineral m, and Q is the ion activity product. The temperature dependence of the reaction rate constant can be expressed reasonably well via an Arrhenius equation (Lasaga 1984; Steefel and Lasaga 1994). Since many rate constants are reported at 25°C, it is convenient to approximate rate constant dependency as a function of temperature,

$$k = k_{25} \exp\left[\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{298.15}\right)\right] \tag{2}$$

where E_a is the activation energy, k_{25} is the rate constant at 25°C, R is the gas constant, and T is absolute temperature.

Solid species data must be entered into specific cards in the STOMP input file to distinguish them from aqueous (mobile) species for transport purposes. The density and molecular weight of each mineral species are listed in the *Solid Species Card*. The species name must be unique and distinct from aqueous and gas species names.

```
~Solid Species Card
4,
SOH,,,0.0,kg/kmol,
SOHUO2CO3,,,0.0,kg/kmol,
SOUO2OH,,,0.0,kg/kmol,
Calcite,2709.893,kg/m^3,100.0872,kg/kmol,
```

The specific surface area and volume fraction of each mineral are listed in the *Lithology Card*:

```
~Lithology Card
Column,1,
Calcite,0.1,m^2/g,0.01,Overwrite,
```

The TST rate parameters and equilibrium coefficients for each mineral are listed in the *Kinetic Reactions Card*, along with all species involved in the dissolution/precipitation reaction. Equilibrium coefficients for minerals can be taken from the EQ3/6 v8.0 database (Wolery and Jarek 2003) with the exception of organic matter, which is assumed to degrade at the forward rate. For this example, the equilibrium and rate coefficients were taken from Yabusaki et al. (2008).

```
~Kinetic Reactions Card
1,
KnRc-31,TST,Calcite,2,Ca++,1.0,HCO3-,1.0,2,Calcite,1.0,H+,1.0,
6.456542e-9,mol/m^2 s,15.e+3,cal/mol,25.0,C,
,1.8487,,,,
```

Kinetic rates defined in the kinetic reactions card will be used by the kinetic equations card. Kinetic equations define kinetic components which are the stoichiometrically weighted sum of species concentrations that vary in time according to a weighted sum of kinetic rates:

$$\frac{d\sum(a_i C_i)}{dt} = \sum c_k R_k \tag{3}$$

where C_i is the concentration of species i (expressed as aqueous molar concentration), and a_i is the stoichiometric coefficient of species i, and C_i is the component species concentration (expressed as aqueous molar concentration), c_k is the stoichiometric coefficient of reaction k, and R_i is the rate of reaction k. Required inputs include the component species name, number of species in the conservation equation, species names, and species stoichiometric coefficients. The component species name must begin with "Kinetic_" followed by the species name of a reactive species in the conservation equation (e.g., Kinetic_Calcite). This name specification is critical in that it links the named species with the kinetic equation, making the concentration for that species the primary unknown for the kinetic equation.

```
~Kinetic Equations Card
1,
Kinetic_Calcite,1,Calcite,1.00000e+00,
1,KnRc-31,1.00000e+00,
```

The relevant aqueous species for this simulation can be determined using EQ3/6 v8.0 (Wolery and Jarek 2003) or defined by users, but they must be defined in the *Aqueous Species Card*. Required input includes the species name, aqueous molecular diffusion coefficient for all species, activity coefficient model option, species charge, species diameter, and species molecular weight. The species name must be unique and distinct from gas and solid species names. Currently, the activity coefficient models include Davies, B-Dot, Pitzer and a constant coefficient option. If the constant coefficient option is chosen then the species charge, diameter, and molecular weight inputs are not required. This example uses the B-dot (Helgeson 1969) activity coefficient model:

```
~Aqueous Species Card
62,,,bdot,,
(UO2)2(OH)2++,2.0,4.5,A,0.0,kg/kmol,
(UO2)2CO3(OH)3-,-1.0,4.0,A,0.0,kg/kmol,
(UO2)2OH+++,3.0,3.0,A,0.0,kg/kmol,
(UO2)3(OH)4++,2.0,4.5,A,0.0,kg/kmol,
(UO2)3(OH)5+,1.0,4.0,A,0.0,kg/kmol,
(UO2)3(OH)7-,-1.0,4.0,A,0.0,kg/kmol,
(UO2)4(OH)7+,1.0,4.0,A,0.0,kg/kmol,
CO3--,-2.0,4.5,A,0.0,kg/kmol,
Ca++,2.0,6.0,A,0.0,kg/kmol,
Ca2UO2(CO3)3(aq),0.0,0.0,A,0.0,kg/kmol,
CaCO3(aq),0.0,3.0,A,0.0,kg/kmol,
CaCl+,1.0,4.0,A,0.0,kg/kmol,
CaCl2(aq),0.0,3.0,A,0.0,kg/kmol,
CaHCO3+,1.0,3.0,A,0.0,kg/kmol,
CaNO3+,1.0,4.0,A,0.0,kg/kmol,
CaOH+,1.0,4.0,A,0.0,kg/kmol,
CaSO4(aq),0.0,3.0,A,0.0,kg/kmol,
CaUO2(CO3)3--,-2.0,0.0,A,0.0,kg/kmol,
Cl-,-1.0,3.0,A,0.0,kg/kmol,
H+,1.0,9.0,A,0.0,kg/kmol,
H2CO3,0.0,3.0,A,0.0,kg/kmol,
HCO3-,-1.0,4.0,A,0.0,kg/kmol,
HCl(aq),0.0,3.0,A,0.0,kg/kmol,
HNO3(aq),0.0,3.0,A,0.0,kg/kmol,
K+,1.0,3.0,A,0.0,kg/kmol,
KCl(aq),0.0,3.0,A,0.0,kg/kmol,
KSO4-,-1.0,4.0,A,0.0,kg/kmol,
Mg++,2.0,8.0,A,0.0,kg/kmol,
MgCO3(aq),0.0,3.0,A,0.0,kg/kmol,
MgCl+,1.0,4.0,A,0.0,kg/kmol,
MgHCO3+,1.0,4.0,A,0.0,kg/kmol,
MgNO3+,1.0,4.0,A,0.0,kg/kmol,
MgSO4(aq),0.0,3.0,A,0.0,kg/kmol,
NO3-,-1.0,3.0,A,0.0,kg/kmol,
Na+,1.0,4.0,A,0.0,kg/kmol,
NaCO3-,-1.0,4.0,A,0.0,kg/kmol,
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NaCl(aq),0.0,3.0,A,0.0,kg/kmol,
NaHCO3(aq),0.0,3.0,A,0.0,kg/kmol,
NaNO3(aq),0.0,3.0,A,0.0,kg/kmol,
NaOH(aq),0.0,3.0,A,0.0,kg/kmol,
NaSO4-,-1.0,4.0,A,0.0,kg/kmol,
OH-,-1.0,3.5,A,0.0,kg/kmol,
SO4--,-2.0,4.0,A,0.0,kg/kmol,
Sr++,2.0,5.0,A,0.0,kg/kmol,
SrCO3(aq),0.0,3.0,A,0.0,kg/kmol,
SrCl+,1.0,4.0,A,0.0,kg/kmol,
SrNO3+,1.0,4.0,A,0.0,kg/kmol,
SrOH+,1.0,4.0,A,0.0,kg/kmol,
SrSO4(aq),0.0,3.0,A,0.0,kg/kmol,
UO2(CO3)2--,-2.0,4.0,A,0.0,kg/kmol,
UO2(CO3)3----,-4.0,4.0,A,0.0,kg/kmol,
UO2(OH)2(aq),0.0,3.0,A,0.0,kg/kmol,
UO2(OH)3-,-1.0,4.0,A,0.0,kg/kmol,
UO2(OH)4--,-2.0,4.0,A,0.0,kg/kmol,
UO2(SO4)2--,-2.0,4.0,A,0.0,kg/kmol,
UO2++,2.0,4.5,A,0.0,kg/kmol,
UO2CO3(aq),0.0,3.0,A,0.0,kg/kmol,
UO2Cl+,1.0,4.0,A,0.0,kg/kmol,
UO2Cl2(aq),0.0,3.0,A,0.0,kg/kmol,
UO2NO3+,1.0,4.0,A,0.0,kg/kmol,
UO2OH+,1.0,4.0,A,0.0,kg/kmol,
UO2SO4(aq),0.0,3.0,A,0.0,kg/kmol,
```

Geochemical models usually assume some reactions to be fast/equilibrium relative to the time scale of flow. This assumption is often justified for some reactions, especially those involving only aqueous species. Equilibrium reactions are not zero-rate reactions but have high reaction rates and reach equilibrium quickly when transport, other reactions, or changes in physical chemical conditions disturb them. Specifically, if the rate of a reaction is much greater than the characteristic time of the problem being solved, it should be classified as an equilibrium reaction.

Species associated with the equilibrium reactions are defined via the *Equilibrium Equations Card*. Required inputs include the number of species in the equilibrium equation (including the equilibrium species), the species names, the equilibrium reaction name, and the species stoichiometric coefficients. The equilibrium species is distinguished from the other species in the equilibrium equation by being the first species listed for the equilibrium equation. For this example, except for the calcite dissolution/precipitation reaction, all the reactions listed in Tables 2 and 3 are equilibrium reactions:

~Equilibrium Equations Card
53,
3,H2CO3,H+,1.00000e+00,HCO3-,1.00000e+00,EqRc-1,1.0,
3,CO3--,H+,-1.00000e+00,HCO3-,1.00000e+00,EqRc-2,1.0,
4,CaCO3(aq),Ca++,1.00000e+00,H+,-1.00000e+00,HCO3-,1.00000e+00,EqRc-3,1.0,
3,CaCl+,Ca++,1.00000e+00,Cl-,1.00000e+00,EqRc-4,1.0,
3,CaCl2(aq),Ca++,1.00000e+00,Cl-,2.00000e+00,EqRc-5,1.0,
3,CaHCO3+,Ca++,1.00000e+00,HCO3-,1.00000e+00,EqRc-6,1.0,
3,CaNO3+,Ca++,1.00000e+00,NO3-,1.00000e+00,EqRc-7,1.0,
3,MgNO3+,Mg++,1.00000e+00,NO3-,1.00000e+00,EqRc-8,1.0,
3,CaOH+,Ca++,1.00000e+00,H+,-1.00000e+00,EqRc-9,1.0,
3,CaSO4(aq),Ca++,1.00000e+00,SO4--,1.00000e+00,EqRc-10,1.0,
3,HCl(aq),Cl-,1.00000e+00,H+,1.00000e+00,EqRc-11,1.0,
3,HNO3(aq),H+,1.00000e+00,NO3-,1.00000e+00,EqRc-12,1.0,
3,KCl(aq),Cl-,1.00000e+00,K+,1.00000e+00,EqRc-13,1.0,
3,KSO4-,K+,1.00000e+00,SO4--,1.00000e+00,EqRc-14,1.0,
4,MgCO3(aq),H+,-1.00000e+00,HCO3-,1.00000e+00,Mg++,1.00000e+00,EqRc-15,1.0,
3,MgCl+,Cl-,1.00000e+00,Mg++,1.00000e+00,EqRc-16,1.0,
3,MgHCO3+,HCO3-,1.00000e+00,Mg++,1.00000e+00,EqRc-17,1.0,
3,MgSO4(aq),Mg++,1.00000e+00,SO4--,1.00000e+00,EqRc-18,1.0,
4,NaCO3-,H+,-1.00000e+00,HCO3-,1.00000e+00,Na+,1.00000e+00,EqRc-19,1.0,
3,NaCl(aq),Cl-,1.00000e+00,Na+,1.00000e+00,EqRc-20,1.0,
3,NaHCO3(aq),HCO3-,1.00000e+00,Na+,1.00000e+00,EqRc-21,1.0,
3,NaOH(aq),H+,-1.00000e+00,Na+,1.00000e+00,EqRc-22,1.0,
3,NaSO4-,Na+,1.00000e+00,SO4--,1.00000e+00,EqRc-23,1.0,
2,OH-,H+,-1.00000e+00,EqRc-24,1.0,
4,SrCO3(aq),H+,-1.00000e+00,HCO3-,1.00000e+00,Sr++,1.00000e+00,EqRc-25,1.0,
3,SrCl+,Cl-,1.00000e+00,Sr++,1.00000e+00,EqRc-26,1.0,
3,SrNO3+,NO3-,1.00000e+00,Sr++,1.00000e+00,EqRc-27,1.0,
3,SrOH+,H+,-1.00000e+00,Sr++,1.00000e+00,EqRc-28,1.0,
3,SrSO4(aq),SO4--,1.00000e+00,Sr++,1.00000e+00,EqRc-29,1.0,
3,NaNO3(aq),NO3-,1.00000e+00,Na+,1.00000e+00,EqRc-30,1.0,
5,UO2++,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,EqRc-31,1.0,
5,UO2(OH)2(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,1.00000e+00,HCO3-,-
3.00000e+00,EqRc-32,1.0,
4,UO2(OH)3-,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,HCO3-,-3.00000e+00,EqRc-
33,1.0,
5,UO2(OH)4--,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,-1.00000e+00,HCO3-,-
3.00000e+00,EqRc-34,1.0,
5,(UO2)2OH+++,Ca++,-4.00000e+00,Ca2UO2(CO3)3(aq),2.00000e+00,H+,5.00000e+00,HCO3-,-
6.00000e+00,EqRc-35,1.0,
5,(UO2)2(OH)2++,Ca++,-4.00000e+00,Ca2UO2(CO3)3(aq),2.00000e+00,H+,4.00000e+00,HCO3-,-
6.00000e+00,EqRc-36,1.0,
5,(UO2)3(OH)4++,Ca++,-6.00000e+00,Ca2UO2(CO3)3(aq),3.00000e+00,H+,5.00000e+00,HCO3-,-
9.00000e+00,EqRc-37,1.0,
5,(UO2)3(OH)5+,Ca++,-6.00000e+00,Ca2UO2(CO3)3(aq),3.00000e+00,H+,4.00000e+00,HCO3-,-
9.00000e+00,EqRc-38,1.0,
5,(UO2)3(OH)7-,Ca++,-6.00000e+00,Ca2UO2(CO3)3(aq),3.00000e+00,H+,2.00000e+00,HCO3-,-
9.00000e+00,EqRc-39,1.0,
5,(UO2)4(OH)7+,Ca++,-8.00000e+00,Ca2UO2(CO3)3(aq),4.00000e+00,H+,5.00000e+00,HCO3-,-
1.20000e+01,EqRc-40,1.0,
5,UO2CO3(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,2.00000e+00,HCO3-,-
2.00000e+00,EqRc-41,1.0,
5,UO2(CO3)2--,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,1.00000e+00,HCO3-,-
1.00000e+00,EqRc-42,1.0,

```
3,UO2(CO3)3----,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,EqRc-43,1.0,
5,(UO2)2CO3(OH)3-,Ca++,-4.00000e+00,Ca2UO2(CO3)3(aq),2.00000e+00,H+,2.00000e+00,HCO3-
,-5.00000e+00,EqRc-44,1.0,
3,CaUO2(CO3)3--,Ca++,-1.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,EqRc-45,1.0,
5,UO2OH+,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,2.00000e+00,HCO3-,-
3.00000e+00,EqRc-46,1.0,
6,UO2NO3+,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,NO3-,1.00000e+00,EqRc-47,1.0,
6,UO2Cl+,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,Cl-
,1.00000e+00,H+,3.00000e+00,HCO3-,-3.00000e+00,EqRc-48,1.0,
6,UO2Cl2(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,Cl-
,2.00000e+00,H+,3.00000e+00,HCO3-,-3.00000e+00,EqRc-49,1.0,
6,UO2SO4(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,SO4--,1.00000e+00,EqRc-50,1.0,
6,UO2(SO4)2--,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,SO4--,2.00000e+00,EqRc-51,1.0,
6,SOUO2OH,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,1.00000e+00,HCO3-,-
3.00000e+00,SOH,1.00000e+00,EqRc-52,1.0,
6,SOHUO2CO3,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,2.00000e+00,HCO3-,-
2.00000e+00,SOH,1.00000e+00,EqRc-53,1.0,
```

The *Equilibrium Reactions Card* specifies the equilibrium reaction constants to be considered in the simulation. This card is only used to specify the parameters used in the temperature dependent equations for equilibrium constants. Required inputs include the equilibrium reaction name and equation coefficients for the temperature dependent equilibrium constant. The equilibrium reaction names must be unique and distinct from the kinetic reaction names (e.g., EqRc-1, E1, Equil-Reac-1, er-1). This example uses equilibrium coefficients from Yabusaki et al. (2008).

```
~Equilibrium Reactions Card
53,
EqRc-1,0.0,6.341,0.0,0.0,0.0,1/mol,
EqRc-2,0.0,-10.325,0.0,0.0,0.0,1/mol,
EqRc-3,0.0,-7.009,0.0,0.0,0.0,1/mol,
EqRc-4,0.0,-0.700,0.0,0.0,0.0,1/mol,
EqRc-5,0.0,-0.653,0.0,0.0,0.0,1/mol,
EqRc-6,0.0,1.043,0.0,0.0,0.0,1/mol,
EqRc-7,0.0,1.300,0.0,0.0,0.0,1/mol,
EqRc-8,0.0,1.300,0.0,0.0,0.0,1/mol,
EqRc-9,0.0,-12.850,0.0,0.0,0.0,1/mol,
EqRc-10,0.0,2.100,0.0,0.0,0.0,1/mol,
EqRc-11,0.0,0.700,0.0,0.0,0.0,1/mol,
EqRc-12,0.0,-1.308,0.0,0.0,0.0,1/mol,
EqRc-13,0.0,-1.500,0.0,0.0,0.0,1/mol,
EqRc-14,0.0,0.875,0.0,0.0,0.0,1/mol,
EqRc-15,0.0,-7.356,0.0,0.0,0.0,1/mol,
EqRc-16,0.0,-0.139,0.0,0.0,0.0,1/mol,
EqRc-17,0.0,1.033,0.0,0.0,0.0,1/mol,
EqRc-18,0.0,2.413,0.0,0.0,0.0,1/mol,
EqRc-19,0.0,-9.816,0.0,0.0,0.0,1/mol,
```

```
EqRc-20,0.0,-0.782,0.0,0.0,0.0,1/mol,
EqRc-21,0.0,0.156,0.0,0.0,0.0,1/mol,
EqRc-22,0.0,-14.799,0.0,0.0,0.0,1/mol,
EqRc-23,0.0,0.820,0.0,0.0,0.0,1/mol,
EqRc-24,0.0,-13.991,0.0,0.0,0.0,1/mol,
EqRc-25,0.0,-7.470,0.0,0.0,0.0,1/mol,
EqRc-26,0.0,-0.253,0.0,0.0,0.0,1/mol,
EqRc-27,0.0,0.800,0.0,0.0,0.0,1/mol,
EqRc-28,0.0,-13.290,0.0,0.0,0.0,1/mol,
EqRc-29,0.0,2.300,0.0,0.0,0.0,1/mol,
EqRc-30,0.0,-0.256,0.0,0.0,0.0,1/mol,
EqRc-31,0.0,0.425,0.0,0.0,0.0,1/mol,
EqRc-32,0.0,-11.725,0.0,0.0,0.0,1/mol,
EqRc-33,0.0,-19.825,0.0,0.0,0.0,1/mol,
EqRc-34,0.0,-31.975,0.0,0.0,0.0,1/mol,
EqRc-35,0.0,-1.851,0.0,0.0,0.0,1/mol,
EqRc-36,0.0,-4.771,0.0,0.0,0.0,1/mol,
EqRc-37,0.0,-10.626,0.0,0.0,0.0,1/mol,
EqRc-38,0.0,-14.276,0.0,0.0,0.0,1/mol,
EqRc-39,0.0,-30.926,0.0,0.0,0.0,1/mol,
EqRc-40,0.0,-20.201,0.0,0.0,0.0,1/mol,
EqRc-41,0.0,0.040,0.0,0.0,0.0,1/mol,
EqRc-42,0.0,-3.615,0.0,0.0,0.0,1/mol,
EqRc-43,0.0,-8.710,0.0,0.0,0.0,1/mol,
EqRc-44,0.0,-10.331,0.0,0.0,0.0,1/mol,
EqRc-45,0.0,-4.910,0.0,0.0,0.0,1/mol,
EqRc-46,0.0,-4.825,0.0,0.0,0.0,1/mol,
EqRc-47,0.0,0.725,0.0,0.0,0.0,1/mol,
EqRc-48,0.0,0.595,0.0,0.0,0.0,1/mol,
EqRc-49,0.0,-0.675,0.0,0.0,0.0,1/mol,
EqRc-50,0.0,3.575,0.0,0.0,0.0,1/mol,
EqRc-51,0.0,4.565,0.0,0.0,0.0,1/mol,
EqRc-52,0.0,-4.810,0.0,0.0,0.0,1/mol,
EqRc-53,0.0,5.733,0.0,0.0,0.0,1/mol,
```

Often pH, rather than the concentration of the H^+ component, is defined for a system. pH may be associated with the aqueous species H^+ via the *Species Link Card*. This card associates reactive species with components in the coupled flow and transport equations and defines which species name defines the system pH, etc. Currently, the following coupled flow and transport components can be associated: aqueous water, gas water, aqueous CO_2, gas CO_2, aqueous salt, and solid salt. Required inputs include the number of reactive species links, species names, and linked components (i.e., Aqueous pH, Aqueous Water, Gas Water, Aqueous CO_2, Gas CO_2).

```
~Species Link Card
1,
H+,pH,
```

The final input card needed to define the reaction network is the *Conservation Equations Card*. This card specifies the conservation equations to be considered in the simulation. Conservation equations have the following general form:

$$\frac{d\sum\left(a_i C_i\right)}{dt} = 0 \tag{4}$$

where C_i is the concentration of species i (expressed as aqueous molar concentration), and a_i is the stoichiometric coefficient of species i, and C_i is the component species concentration (expressed as aqueous molar concentration). Required inputs include the component species name, the number of species in the conservation equation, the species names, and the species stoichiometric coefficients. The component species name must begin with "Total_" followed with the species name of a reactive species in the conservation equation (e.g., Total_Ca++, Total_HCO3-, Total_H+). This name specification is critical in that it links the named species with the conservation equation, making the concentration for that species the primary unknown for the conservation equation.

```
~Conservation Equations Card
12,
Total_Ca++,32,Ca++,1.00000e+00,(UO2)2(OH)2++,-4.00000e+00,(UO2)2CO3(OH)3-,-
4.00000e+00,(UO2)2OH+++,-4.00000e+00,(UO2)3(OH)4++,
-6.00000e+00,(UO2)3(OH)5+,-6.00000e+00,(UO2)3(OH)7-,-6.00000e+00,(UO2)4(OH)7+,-
8.00000e+00,CaCO3(aq),1.00000e+00,CaCl+,1.00000e+00,
CaCl2(aq),1.00000e+00,CaHCO3+,1.00000e+00,CaNO3+,1.00000e+00,CaOH+,1.00000e+00,CaSO4(
aq),1.00000e+00,CaUO2(CO3)3--,-1.00000e+00,
Calcite,1.00000e+00,SOHUO2CO3,-2.00000e+00,SOUO2OH,-2.00000e+00,UO2(CO3)2--,-
2.00000e+00,UO2(CO3)3----,-2.00000e+00,UO2(OH)2(aq),
-2.00000e+00,UO2(OH)3-,-2.00000e+00,UO2(OH)4--,-2.00000e+00,UO2(SO4)2--,-
2.00000e+00,UO2++,-2.00000e+00,UO2CO3(aq),-2.00000e+00,
UO2Cl+,-2.00000e+00,UO2Cl2(aq),-2.00000e+00,UO2NO3+,-2.00000e+00,UO2OH+,-
2.00000e+00,UO2SO4(aq),-2.00000e+00,
Total_Ca2UO2(CO3)3(aq),24,Ca2UO2(CO3)3(aq),1.00000e+00,(UO2)2(OH)2++,2.00000e+00,(UO2
)2CO3(OH)3-,2.00000e+00,
(UO2)2OH+++,2.00000e+00,(UO2)3(OH)4++,3.00000e+00,(UO2)3(OH)5+,3.00000e+00,(UO2)3(OH
)7-,3.00000e+00,(UO2)4(OH)7+,4.00000e+00,
CaUO2(CO3)3--,1.00000e+00,SOHUO2CO3,1.00000e+00,SOUO2OH,1.00000e+00,UO2(CO3)2--
,1.00000e+00,UO2(CO3)3----,1.00000e+00,
UO2(OH)2(aq),1.00000e+00,UO2(OH)3-,1.00000e+00,UO2(OH)4--,1.00000e+00,UO2(SO4)2--
,1.00000e+00,UO2++,1.00000e+00,UO2CO3(aq),
1.00000e+00,UO2Cl+,1.00000e+00,UO2Cl2(aq),1.00000e+00,UO2NO3+,1.00000e+00,UO2OH+,1.00
000e+00,UO2SO4(aq),1.00000e+00,
```

Total_Cl-,10,Cl-
,1.00000e+00,CaCl+,1.00000e+00,CaCl2(aq),2.00000e+00,HCl(aq),1.00000e+00,KCl(aq),1.00000e+00
,MgCl+,1.00000e+00,
NaCl(aq),1.00000e+00,SrCl+,1.00000e+00,UO2Cl+,1.00000e+00,UO2Cl2(aq),2.00000e+00,
Total_H+,34,H+,1.00000e+00,(UO2)2(OH)2++,4.00000e+00,(UO2)2CO3(OH)3-
,2.00000e+00,(UO2)2OH+++,5.00000e+00,(UO2)3(OH)4++,5.00000e+00,
(UO2)3(OH)5+,4.00000e+00,(UO2)3(OH)7-,2.00000e+00,(UO2)4(OH)7+,5.00000e+00,CO3--,-
1.00000e+00,CaCO3(aq),-1.00000e+00,
CaOH+,-1.00000e+00,Calcite,-
1.00000e+00,H2CO3,1.00000e+00,HCl(aq),1.00000e+00,HNO3(aq),1.00000e+00,MgCO3(aq),-
1.00000e+00,
NaCO3-,-1.00000e+00,NaOH(aq),-1.00000e+00,OH-,-
1.00000e+00,SOHUO2CO3,2.00000e+00,SOUO2OH,1.00000e+00,SrCO3(aq),-1.00000e+00,
SrOH+,-1.00000e+00,UO2(CO3)2--,1.00000e+00,UO2(OH)2(aq),1.00000e+00,UO2(OH)4--,-
1.00000e+00,UO2(SO4)2--,3.00000e+00,
UO2++,3.00000e+00,UO2CO3(aq),2.00000e+00,UO2Cl+,3.00000e+00,UO2Cl2(aq),3.00000e+00,UO
2NO3+,3.00000e+00,UO2OH+,2.00000e+00,
UO2SO4(aq),3.00000e+00,
Total_HCO3-,32,HCO3-,1.00000e+00,(UO2)2(OH)2++,-6.00000e+00,(UO2)2CO3(OH)3-,-
5.00000e+00,(UO2)2OH+++,-6.00000e+00,(UO2)3(OH)4++,
-9.00000e+00,(UO2)3(OH)5+,-9.00000e+00,(UO2)3(OH)7-,-9.00000e+00,(UO2)4(OH)7+,-
1.20000e+01,CO3--,1.00000e+00,CaCO3(aq),
1.00000e+00,CaHCO3+,1.00000e+00,Calcite,1.00000e+00,H2CO3,1.00000e+00,MgCO3(aq),1.00000
e+00,MgHCO3+,1.00000e+00,NaCO3-,1.00000e+00,
NaHCO3(aq),1.00000e+00,SOHUO2CO3,-2.00000e+00,SOUO2OH,-
3.00000e+00,SrCO3(aq),1.00000e+00,UO2(CO3)2--,-1.00000e+00,UO2(OH)2(aq),
-3.00000e+00,UO2(OH)3-,-3.00000e+00,UO2(OH)4--,-3.00000e+00,UO2(SO4)2--,-
3.00000e+00,UO2++,-3.00000e+00,UO2CO3(aq),-2.00000e+00,
UO2Cl+,-3.00000e+00,UO2Cl2(aq),-3.00000e+00,UO2NO3+,-3.00000e+00,UO2OH+,-
3.00000e+00,UO2SO4(aq),-3.00000e+00,
Total_K+,3,K+,1.00000e+00,KCl(aq),1.00000e+00,KSO4-,1.00000e+00,
Total_Mg++,6,Mg++,1.00000e+00,MgCO3(aq),1.00000e+00,MgCl+,1.00000e+00,MgHCO3+,1.0000
0e+00,MgNO3+,1.00000e+00,MgSO4(aq),1.00000e+00,
Total_NO3-,7,NO3-
,1.00000e+00,CaNO3+,1.00000e+00,HNO3(aq),1.00000e+00,MgNO3+,1.00000e+00,NaNO3(aq),1.0
0000e+00,SrNO3+,1.00000e+00,UO2NO3+,1.00000e+00,
Total_Na+,7,Na+,1.00000e+00,NaCO3-
,1.00000e+00,NaCl(aq),1.00000e+00,NaHCO3(aq),1.00000e+00,NaNO3(aq),1.00000e+00,NaOH(aq)
,1.00000e+00,NaSO4-,1.00000e+00,
Total_SO4--,8,SO4--,1.00000e+00,CaSO4(aq),1.00000e+00,KSO4-
,1.00000e+00,MgSO4(aq),1.00000e+00,NaSO4-,1.00000e+00,SrSO4(aq),1.00000e+00,UO2(SO4)2--
,2.00000e+00,UO2SO4(aq),1.00000e+00,
Total_SOH,3,SOH,1.00000e+00,SOHUO2CO3,1.00000e+00,SOUO2OH,1.00000e+00,
Total_Sr++,6,Sr++,1.00000e+00,SrCO3(aq),1.00000e+00,SrCl+,1.00000e+00,SrNO3+,1.00000e+00,Sr
OH+,1.00000e+00,SrSO4(aq),1.00000e+00,

The initial water chemistry used in the simulation is the groundwater solution listed in Table 23.1 at a temperature of 25 °C and a pH of 7.7. Any species not specified in the *Initial Conditions Card* are assumed to be less than 10^{-30}.

~Initial Conditions Card
Aqueous Pressure,Gas Pressure,
14,
Aqueous Pressure,102064.81,Pa,,,,,,,1,10,1,1,1,1,
Gas Pressure,102064.81,Pa,,,,,,,1,10,1,1,1,1,
Temperature,25,C,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,pH,7.7,,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,HCO3-,2.66e-3,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Ca++,1.1e-3,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Cl-,2.75e-3,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,K+,1.5e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Mg++,4.1e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,NO3-,1.73e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Na+,9.87e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,SO4--,3.25e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,SOH,0.605088,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Ca2UO2(CO3)3(aq),1.30295e-5,mol/liter,,,,,,,1,10,1,1,1,1,

Results

River water intrusion results in calcite dissolution, a decrease in the calcite mineral volume fraction, an increase in pH, and the liberation of calcium and bicarbonate. The node closer to the river water boundary has stronger sorption because of direct mixing with the river water solution. Figures 1 and 2 show uranium sorption with and without calcite reaction.

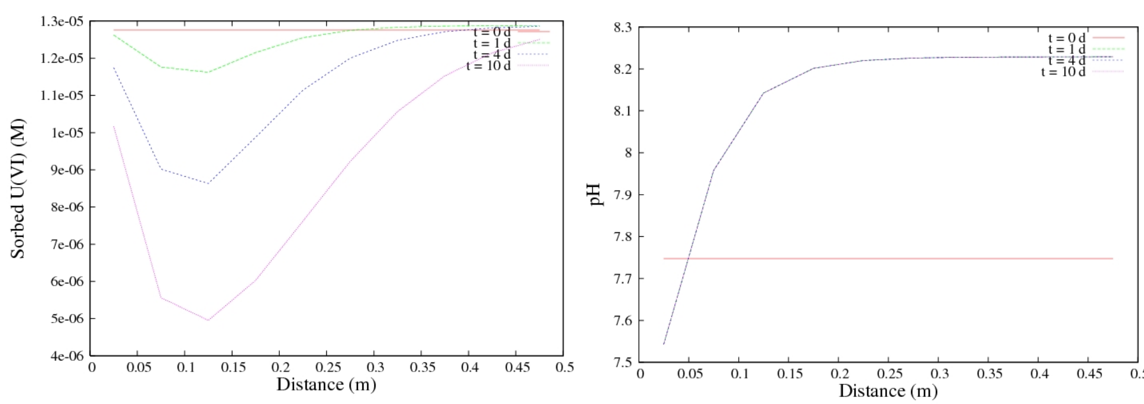

Figure 1. Change in pH and sorbed uranium vs. distance at different times, with calcite reaction

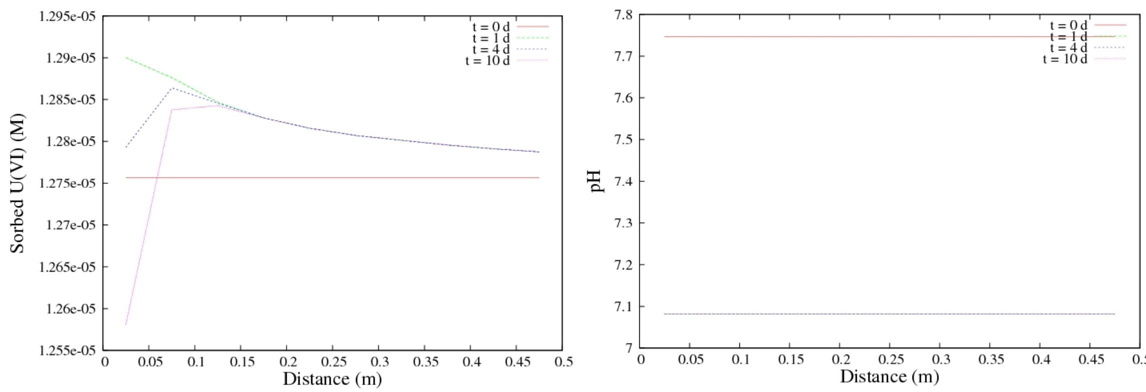

Figure 2. Change in pH and sorbed uranium vs. distance at different times, with no calcite reaction

References

Helgeson HC. 1969. "Thermodynamics of hydrothermal systems at elevated temperatures and pressures." *American Journal of Science*, 267(7):729-&.

Lasaga AC. 1984. "Chemical kinetics of water-rock interactions." *Journal of Geophysical Research*, 89(NB6):4009-4025.

Steefel CI and AC Lasaga. 1994. "A coupled model for transport of multiple chemical species and kinetic precipitation/dissolution reactions with applications to reactive flow in single phase hydrothermal system." *American Journal of Science*, 294(5):529-592.

Wolery TW and RL Jarek. 2003. Software User's Manual, EQ3/6, Version 8.0. Sandia National Laboratories, Albuquerque, New Mexico.

Yabusaki SB, Y Fang, and SR Waichler. 2008. "Building Conceptual Models of Field-Scale Uranium Reactive Transport in a Dynamic Vadose Zone-Aquifer-River System." *Water Resources Research* 44:W12403. doi:10.1029/2007WR006617

Exercises

Tip: save a backup copy of your original input file before making any of these modifications.

1. Change the initial total H+ concentration record in the *Initial Conditions Card* to:

   Overwrite Species Aqueous Volumetric,pH,7.7,,,,,,,,1,10,1,1,1,1,

   Compare your results with the original.

2. Change the initial condition from groundwater chemistry to river water chemistry and calculate the total H+ using pH.
3. Vary the calcite kinetic reaction rate by several orders or magnitude and observe the effects.

Input File

Input file for flow:

```
~Simulation Title Card
3.2,
STOMP Example Problem W-6: Flow,
Y Fang,
Pacific Northwest Laboratory,
Feb 2011,
10:15 AM PDT,
2,
300 Area Uranium
1D transport: equilibrium reactions, sorption sites, calcite precipitation

~Solution Control Card
Normal,
Water,
1,
0,day,1,yr,5,d,5,d,1.25,8,1.e-06,
10000,
0,

~Grid Card
Cartesian,
10,1,1,
0.0,m,10@0.05,m,
0,m,1.0,m,
0,m,1.0,m,

~Rock/Soil Zonation Card
1,
Column,1,10,1,1,1,1,

~Mechanical Properties Card
Column,2.75,g/cm^3,0.08,0.08,1.e-5,1/m,Millington and Quirk,

~Hydraulic Properties Card
Column,10.0,Darcy,10.0,Darcy,10.0,Darcy,

~Saturation Function Card
Column,van Genuchten,6.83,1/m,2.08,0.1213,,

~Aqueous Relative Permeability Card
Column,Mualem,,

~Solute/Porous Media Interaction Card
Column,,,,,

~Initial Conditions Card
Aqueous Pressure,Gas Pressure,
2,
Aqueous Pressure,102064.81,Pa,,,,,,,1,10,1,1,1,1,
Gas Pressure,102064.81,Pa,,,,,,,1,10,1,1,1,1,
```

```
~Boundary Conditions Card
2,
West,Aqueous Neumann,,
1,1,1,1,1,1,1,
0,hr,1.44,m/d,
East,Aqueous Dirichlet,
10,10,1,1,1,1,1,
0,day,102064.81,Pa,

~Output Options Card
3,
1,1,1,
50,1,1,
10,1,1,
1,1,yr,m,6,6,6,
1,
XNC aqueous volumetric flux,m/d,
0,
0,day,
```

Input file for reactive transport:

```
~Simulation Title Card
3.2,
STOMP Example Problem W-6: Reactive Transport,
Y Fang,
Pacific Northwest Laboratory,
Feb 2011,
10:15 AM PDT,
2,
300 Area Uranium
2D transport condition: equilibrium reactions, sorption sites, calcite precipitation

~Solution Control Card
Restart,
Water w/ ECKEChem Reduced Courant,0.25,
1,
0,day,10,d,0.005,day,5,d,1.25,8,1.e-06,
10000,
0,

~Grid Card
Cartesian,
10,1,1,
0,m,10@0.05,m,
0,m,1.0,m,
0,m,1.0,m,

~Rock/Soil Zonation Card
1,
Column,1,10,1,1,1,1,

~Mechanical Properties Card
Column,220,kg/m^3,0.25,0.25,1.e-5,1/m,Millington and Quirk,

~Hydraulic Properties Card
Column,10.0,Darcy,10.0,Darcy,10.0,Darcy,

~Saturation Function Card
Column,van Genuchten,6.83,1/m,2.08,0.1213,,

~Aqueous Relative Permeability Card
Column,Mualem,,
```

```
~Solute/Porous Media Interaction Card
Column,,,,,

~Aqueous Species Card
# totoal number of aqueous spec, species diffusion coeff, unit, activity model, activity
#62,,,davies,,
62,,,bdot,,
(UO2)2(OH)2++,2.0,4.5,A,0.0,kg/kmol,
(UO2)2CO3(OH)3-,-1.0,4.0,A,0.0,kg/kmol,
(UO2)2OH+++,3.0,3.0,A,0.0,kg/kmol,
(UO2)3(OH)4++,2.0,4.5,A,0.0,kg/kmol,
(UO2)3(OH)5+,1.0,4.0,A,0.0,kg/kmol,
(UO2)3(OH)7-,-1.0,4.0,A,0.0,kg/kmol,
(UO2)4(OH)7+,1.0,4.0,A,0.0,kg/kmol,
CO3--,-2.0,4.5,A,0.0,kg/kmol,
Ca++,2.0,6.0,A,0.0,kg/kmol,
Ca2UO2(CO3)3(aq),0.0,0.0,A,0.0,kg/kmol,
CaCO3(aq),0.0,3.0,A,0.0,kg/kmol,
CaCl+,1.0,4.0,A,0.0,kg/kmol,
CaCl2(aq),0.0,3.0,A,0.0,kg/kmol,
CaHCO3+,1.0,3.0,A,0.0,kg/kmol,
CaNO3+,1.0,4.0,A,0.0,kg/kmol,
CaOH+,1.0,4.0,A,0.0,kg/kmol,
CaSO4(aq),0.0,3.0,A,0.0,kg/kmol,
CaUO2(CO3)3--,-2.0,0.0,A,0.0,kg/kmol,
Cl-,-1.0,3.0,A,0.0,kg/kmol,
H+,1.0,9.0,A,0.0,kg/kmol,
H2CO3,0.0,3.0,A,0.0,kg/kmol,
HCO3-,-1.0,4.0,A,0.0,kg/kmol,
HCl(aq),0.0,3.0,A,0.0,kg/kmol,
HNO3(aq),0.0,3.0,A,0.0,kg/kmol,
K+,1.0,3.0,A,0.0,kg/kmol,
KCl(aq),0.0,3.0,A,0.0,kg/kmol,
KSO4-,-1.0,4.0,A,0.0,kg/kmol,
Mg++,2.0,8.0,A,0.0,kg/kmol,
MgCO3(aq),0.0,3.0,A,0.0,kg/kmol,
MgCl+,1.0,4.0,A,0.0,kg/kmol,
MgHCO3+,1.0,4.0,A,0.0,kg/kmol,
MgNO3+,1.0,4.0,A,0.0,kg/kmol,
MgSO4(aq),0.0,3.0,A,0.0,kg/kmol,
NO3-,-1.0,3.0,A,0.0,kg/kmol,
Na+,1.0,4.0,A,0.0,kg/kmol,
NaCO3-,-1.0,4.0,A,0.0,kg/kmol,
NaCl(aq),0.0,3.0,A,0.0,kg/kmol,
NaHCO3(aq),0.0,3.0,A,0.0,kg/kmol,
NaNO3(aq),0.0,3.0,A,0.0,kg/kmol,
NaOH(aq),0.0,3.0,A,0.0,kg/kmol,
NaSO4-,-1.0,4.0,A,0.0,kg/kmol,
OH-,-1.0,3.5,A,0.0,kg/kmol,
SO4--,-2.0,4.0,A,0.0,kg/kmol,
Sr++,2.0,5.0,A,0.0,kg/kmol,
SrCO3(aq),0.0,3.0,A,0.0,kg/kmol,
SrCl+,1.0,4.0,A,0.0,kg/kmol,
SrNO3+,1.0,4.0,A,0.0,kg/kmol,
SrOH+,1.0,4.0,A,0.0,kg/kmol,
SrSO4(aq),0.0,3.0,A,0.0,kg/kmol,
UO2(CO3)2--,-2.0,4.0,A,0.0,kg/kmol,
UO2(CO3)3----,-4.0,4.0,A,0.0,kg/kmol,
UO2(OH)2(aq),0.0,3.0,A,0.0,kg/kmol,
UO2(OH)3-,-1.0,4.0,A,0.0,kg/kmol,
UO2(OH)4--,-2.0,4.0,A,0.0,kg/kmol,
UO2(SO4)2--,-2.0,4.0,A,0.0,kg/kmol,
UO2++,2.0,4.5,A,0.0,kg/kmol,
UO2CO3(aq),0.0,3.0,A,0.0,kg/kmol,
UO2Cl+,1.0,4.0,A,0.0,kg/kmol,
```

UO2Cl2(aq),0.0,3.0,A,0.0,kg/kmol,
UO2NO3+,1.0,4.0,A,0.0,kg/kmol,
UO2OH+,1.0,4.0,A,0.0,kg/kmol,
UO2SO4(aq),0.0,3.0,A,0.0,kg/kmol,

~Solid Species Card
total number of solid species
4,
species name, mass density (calculated with molar volume), unit, molecular weight, unit
SOH,,,0.0,kg/kmol,
SOHUO2CO3,,,0.0,kg/kmol,
SOUO2OH,,,0.0,kg/kmol,
Calcite,2709.893,kg/m^3,100.0872,kg/kmol,

~Lithology Card
rock name, number of minerals
Column,1,
mineral name, surface area, unit, volume fraction
Calcite,0.1,m^2/g,0.01,Overwrite,

~Species Link Card
1,
H+,pH,

~Conservation Equations Card
12,
Total_Ca++,32,Ca++,1.00000e+00,(UO2)2(OH)2++,-4.00000e+00,(UO2)2CO3(OH)3-,-
4.00000e+00,(UO2)2OH+++,-4.00000e+00,(UO2)3(OH)4++,
-6.00000e+00,(UO2)3(OH)5+,-6.00000e+00,(UO2)3(OH)7-,-6.00000e+00,(UO2)4(OH)7+,-
8.00000e+00,CaCO3(aq),1.00000e+00,CaCl+,1.00000e+00,
CaCl2(aq),1.00000e+00,CaHCO3+,1.00000e+00,CaNO3+,1.00000e+00,CaOH+,1.00000e+00,CaSO4(aq),1.0000
0e+00,CaUO2(CO3)3--,-1.00000e+00,
Calcite,1.00000e+00,SOHUO2CO3,-2.00000e+00,SOUO2OH,-2.00000e+00,UO2(CO3)2--,-
2.00000e+00,UO2(CO3)3----,-2.00000e+00,UO2(OH)2(aq),
-2.00000e+00,UO2(OH)3-,-2.00000e+00,UO2(OH)4--,-2.00000e+00,UO2(SO4)2--,-2.00000e+00,UO2++,-
2.00000e+00,UO2CO3(aq),-2.00000e+00,
UO2Cl+,-2.00000e+00,UO2Cl2(aq),-2.00000e+00,UO2NO3+,-2.00000e+00,UO2OH+,-
2.00000e+00,UO2SO4(aq),-2.00000e+00,
Total_Ca2UO2(CO3)3(aq),24,Ca2UO2(CO3)3(aq),1.00000e+00,(UO2)2(OH)2++,2.00000e+00,(UO2)2CO3(OH
)3-,2.00000e+00,
(UO2)2OH+++,2.00000e+00,(UO2)3(OH)4++,3.00000e+00,(UO2)3(OH)5+,3.00000e+00,(UO2)3(OH)7-
,3.00000e+00,(UO2)4(OH)7+,4.00000e+00,
CaUO2(CO3)3--,1.00000e+00,SOHUO2CO3,1.00000e+00,SOUO2OH,1.00000e+00,UO2(CO3)2--
,1.00000e+00,UO2(CO3)3----,1.00000e+00,
UO2(OH)2(aq),1.00000e+00,UO2(OH)3-,1.00000e+00,UO2(OH)4--,1.00000e+00,UO2(SO4)2--
,1.00000e+00,UO2++,1.00000e+00,UO2CO3(aq),
1.00000e+00,UO2Cl+,1.00000e+00,UO2Cl2(aq),1.00000e+00,UO2NO3+,1.00000e+00,UO2OH+,1.00000e+00,U
O2SO4(aq),1.00000e+00,
Total_Cl-,10,Cl-
,1.00000e+00,CaCl+,1.00000e+00,CaCl2(aq),2.00000e+00,HCl(aq),1.00000e+00,KCl(aq),1.00000e+00,MgCl+,1.
00000e+00,
NaCl(aq),1.00000e+00,SrCl+,1.00000e+00,UO2Cl+,1.00000e+00,UO2Cl2(aq),2.00000e+00,
Total_H+,34,H+,1.00000e+00,(UO2)2(OH)2++,4.00000e+00,(UO2)2CO3(OH)3-
,2.00000e+00,(UO2)2OH+++,5.00000e+00,(UO2)3(OH)4++,5.00000e+00,
(UO2)3(OH)5+,4.00000e+00,(UO2)3(OH)7-,2.00000e+00,(UO2)4(OH)7+,5.00000e+00,CO3--,-
1.00000e+00,CaCO3(aq),-1.00000e+00,
CaOH+,-1.00000e+00,Calcite,-
1.00000e+00,H2CO3,1.00000e+00,HCl(aq),1.00000e+00,HNO3(aq),1.00000e+00,MgCO3(aq),-1.00000e+00,
NaCO3-,-1.00000e+00,NaOH(aq),-1.00000e+00,OH-,-
1.00000e+00,SOHUO2CO3,2.00000e+00,SOUO2OH,1.00000e+00,SrCO3(aq),-1.00000e+00,
SrOH+,-1.00000e+00,UO2(CO3)2--,1.00000e+00,UO2(OH)2(aq),1.00000e+00,UO2(OH)4--,-
1.00000e+00,UO2(SO4)2--,3.00000e+00,
UO2++,3.00000e+00,UO2CO3(aq),2.00000e+00,UO2Cl+,3.00000e+00,UO2Cl2(aq),3.00000e+00,UO2NO3+,3.0
0000e+00,UO2OH+,2.00000e+00,
UO2SO4(aq),3.00000e+00,

Total_HCO3-,32,HCO3-,1.00000e+00,(UO2)2(OH)2++,-6.00000e+00,(UO2)2CO3(OH)3-,-5.00000e+00,(UO2)2OH+++,-6.00000e+00,(UO2)3(OH)4++,
-9.00000e+00,(UO2)3(OH)5+,-9.00000e+00,(UO2)3(OH)7-,-9.00000e+00,(UO2)4(OH)7+,-1.20000e+01,CO3--,1.00000e+00,CaCO3(aq),
1.00000e+00,CaHCO3+,1.00000e+00,Calcite,1.00000e+00,H2CO3,1.00000e+00,MgCO3(aq),1.00000e+00,MgHCO3+,1.00000e+00,NaCO3-,1.00000e+00,
NaHCO3(aq),1.00000e+00,SOHUO2CO3,-2.00000e+00,SOUO2OH,-3.00000e+00,SrCO3(aq),1.00000e+00,UO2(CO3)2--,-1.00000e+00,UO2(OH)2(aq),
-3.00000e+00,UO2(OH)3-,-3.00000e+00,UO2(OH)4--,-3.00000e+00,UO2(SO4)2--,-3.00000e+00,UO2++,-3.00000e+00,UO2CO3(aq),-2.00000e+00,
UO2Cl+,-3.00000e+00,UO2Cl2(aq),-3.00000e+00,UO2NO3+,-3.00000e+00,UO2OH+,-3.00000e+00,UO2SO4(aq),-3.00000e+00,
Total_K+,3,K+,1.00000e+00,KCl(aq),1.00000e+00,KSO4-,1.00000e+00,
Total_Mg++,6,Mg++,1.00000e+00,MgCO3(aq),1.00000e+00,MgCl+,1.00000e+00,MgHCO3+,1.00000e+00,MgNO3+,1.00000e+00,MgSO4(aq),1.00000e+00,
Total_NO3-,7,NO3-,1.00000e+00,CaNO3+,1.00000e+00,HNO3(aq),1.00000e+00,MgNO3+,1.00000e+00,NaNO3(aq),1.00000e+00,SrNO3+,1.00000e+00,UO2NO3+,1.00000e+00,
Total_Na+,7,Na+,1.00000e+00,NaCO3-,1.00000e+00,NaCl(aq),1.00000e+00,NaHCO3(aq),1.00000e+00,NaNO3(aq),1.00000e+00,NaOH(aq),1.00000e+00,NaSO4-,1.00000e+00,
Total_SO4--,8,SO4--,1.00000e+00,CaSO4(aq),1.00000e+00,KSO4-,1.00000e+00,MgSO4(aq),1.00000e+00,NaSO4-,1.00000e+00,SrSO4(aq),1.00000e+00,UO2(SO4)2--,2.00000e+00,UO2SO4(aq),1.00000e+00,
Total_SOH,3,SOH,1.00000e+00,SOHUO2CO3,1.00000e+00,SOUO2OH,1.00000e+00,
Total_Sr++,6,Sr++,1.00000e+00,SrCO3(aq),1.00000e+00,SrCl+,1.00000e+00,SrNO3+,1.00000e+00,SrOH+,1.00000e+00,SrSO4(aq),1.00000e+00,

~Equilibrium Reactions Card
number of equilibirum reactions
53,
EqRc-1,0.0,6.341,0.0,0.0,0.0,1/mol,
EqRc-2,0.0,-10.325,0.0,0.0,0.0,1/mol,
EqRc-3,0.0,-7.009,0.0,0.0,0.0,1/mol,
EqRc-4,0.0,-0.700,0.0,0.0,0.0,1/mol,
EqRc-5,0.0,-0.653,0.0,0.0,0.0,1/mol,
EqRc-6,0.0,1.043,0.0,0.0,0.0,1/mol,
EqRc-7,0.0,1.300,0.0,0.0,0.0,1/mol,
EqRc-8,0.0,1.300,0.0,0.0,0.0,1/mol,
EqRc-9,0.0,-12.850,0.0,0.0,0.0,1/mol,
EqRc-10,0.0,2.100,0.0,0.0,0.0,1/mol,
EqRc-11,0.0,0.700,0.0,0.0,0.0,1/mol,
EqRc-12,0.0,-1.308,0.0,0.0,0.0,1/mol,
EqRc-13,0.0,-1.500,0.0,0.0,0.0,1/mol,
EqRc-14,0.0,0.875,0.0,0.0,0.0,1/mol,
EqRc-15,0.0,-7.356,0.0,0.0,0.0,1/mol,
EqRc-16,0.0,-0.139,0.0,0.0,0.0,1/mol,
EqRc-17,0.0,1.033,0.0,0.0,0.0,1/mol,
EqRc-18,0.0,2.413,0.0,0.0,0.0,1/mol,
EqRc-19,0.0,-9.816,0.0,0.0,0.0,1/mol,
EqRc-20,0.0,-0.782,0.0,0.0,0.0,1/mol,
EqRc-21,0.0,0.156,0.0,0.0,0.0,1/mol,
EqRc-22,0.0,-14.799,0.0,0.0,0.0,1/mol,
EqRc-23,0.0,0.820,0.0,0.0,0.0,1/mol,
EqRc-24,0.0,-13.991,0.0,0.0,0.0,1/mol,
EqRc-25,0.0,-7.470,0.0,0.0,0.0,1/mol,
EqRc-26,0.0,-0.253,0.0,0.0,0.0,1/mol,
EqRc-27,0.0,0.800,0.0,0.0,0.0,1/mol,
EqRc-28,0.0,-13.290,0.0,0.0,0.0,1/mol,
EqRc-29,0.0,2.300,0.0,0.0,0.0,1/mol,
EqRc-30,0.0,-0.256,0.0,0.0,0.0,1/mol,
EqRc-31,0.0,0.425,0.0,0.0,0.0,1/mol,
EqRc-32,0.0,-11.725,0.0,0.0,0.0,1/mol,
EqRc-33,0.0,-19.825,0.0,0.0,0.0,1/mol,
EqRc-34,0.0,-31.975,0.0,0.0,0.0,1/mol,

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EqRc-35,0.0,-1.851,0.0,0.0,0.0,1/mol,
EqRc-36,0.0,-4.771,0.0,0.0,0.0,1/mol,
EqRc-37,0.0,-10.626,0.0,0.0,0.0,1/mol,
EqRc-38,0.0,-14.276,0.0,0.0,0.0,1/mol,
EqRc-39,0.0,-30.926,0.0,0.0,0.0,1/mol,
EqRc-40,0.0,-20.201,0.0,0.0,0.0,1/mol,
EqRc-41,0.0,0.040,0.0,0.0,0.0,1/mol,
EqRc-42,0.0,-3.615,0.0,0.0,0.0,1/mol,
EqRc-43,0.0,-8.710,0.0,0.0,0.0,1/mol,
EqRc-44,0.0,-10.331,0.0,0.0,0.0,1/mol,
EqRc-45,0.0,-4.910,0.0,0.0,0.0,1/mol,
EqRc-46,0.0,-4.825,0.0,0.0,0.0,1/mol,
EqRc-47,0.0,0.725,0.0,0.0,0.0,1/mol,
EqRc-48,0.0,0.595,0.0,0.0,0.0,1/mol,
EqRc-49,0.0,-0.675,0.0,0.0,0.0,1/mol,
EqRc-50,0.0,3.575,0.0,0.0,0.0,1/mol,
EqRc-51,0.0,4.565,0.0,0.0,0.0,1/mol,
EqRc-52,0.0,-4.810,0.0,0.0,0.0,1/mol,
EqRc-53,0.0,5.733,0.0,0.0,0.0,1/mol,

~Equilibrium Equations Card
# number of equilibrium reactions
53,
3,H2CO3,H+,1.00000e+00,HCO3-,1.00000e+00,EqRc-1,1.0,
3,CO3--,H+,-1.00000e+00,HCO3-,1.00000e+00,EqRc-2,1.0,
4,CaCO3(aq),Ca++,1.00000e+00,H+,-1.00000e+00,HCO3-,1.00000e+00,EqRc-3,1.0,
3,CaCl+,Ca++,1.00000e+00,Cl-,1.00000e+00,EqRc-4,1.0,
3,CaCl2(aq),Ca++,1.00000e+00,Cl-,2.00000e+00,EqRc-5,1.0,
3,CaHCO3+,Ca++,1.00000e+00,HCO3-,1.00000e+00,EqRc-6,1.0,
3,CaNO3+,Ca++,1.00000e+00,NO3-,1.00000e+00,EqRc-7,1.0,
3,MgNO3+,Mg++,1.00000e+00,NO3-,1.00000e+00,EqRc-8,1.0,
3,CaOH+,Ca++,1.00000e+00,H+,-1.00000e+00,EqRc-9,1.0,
3,CaSO4(aq),Ca++,1.00000e+00,SO4--,1.00000e+00,EqRc-10,1.0,
3,HCl(aq),Cl-,1.00000e+00,H+,1.00000e+00,EqRc-11,1.0,
3,HNO3(aq),H+,1.00000e+00,NO3-,1.00000e+00,EqRc-12,1.0,
3,KCl(aq),Cl-,1.00000e+00,K+,1.00000e+00,EqRc-13,1.0,
3,KSO4-,K+,1.00000e+00,SO4--,1.00000e+00,EqRc-14,1.0,
4,MgCO3(aq),H+,-1.00000e+00,HCO3-,1.00000e+00,Mg++,1.00000e+00,EqRc-15,1.0,
3,MgCl+,Cl-,1.00000e+00,Mg++,1.00000e+00,EqRc-16,1.0,
3,MgHCO3+,HCO3-,1.00000e+00,Mg++,1.00000e+00,EqRc-17,1.0,
3,MgSO4(aq),Mg++,1.00000e+00,SO4--,1.00000e+00,EqRc-18,1.0,
4,NaCO3-,H+,-1.00000e+00,HCO3-,1.00000e+00,Na+,1.00000e+00,EqRc-19,1.0,
3,NaCl(aq),Cl-,1.00000e+00,Na+,1.00000e+00,EqRc-20,1.0,
3,NaHCO3(aq),HCO3-,1.00000e+00,Na+,1.00000e+00,EqRc-21,1.0,
3,NaOH(aq),H+,-1.00000e+00,Na+,1.00000e+00,EqRc-22,1.0,
3,NaSO4-,Na+,1.00000e+00,SO4--,1.00000e+00,EqRc-23,1.0,
2,OH-,H+,-1.00000e+00,EqRc-24,1.0,
4,SrCO3(aq),H+,-1.00000e+00,HCO3-,1.00000e+00,Sr++,1.00000e+00,EqRc-25,1.0,
3,SrCl+,Cl-,1.00000e+00,Sr++,1.00000e+00,EqRc-26,1.0,
3,SrNO3+,NO3-,1.00000e+00,Sr++,1.00000e+00,EqRc-27,1.0,
3,SrOH+,H+,-1.00000e+00,Sr++,1.00000e+00,EqRc-28,1.0,
3,SrSO4(aq),SO4--,1.00000e+00,Sr++,1.00000e+00,EqRc-29,1.0,
3,NaNO3(aq),NO3-,1.00000e+00,Na+,1.00000e+00,EqRc-30,1.0,
5,UO2++,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-3.00000e+00,EqRc-
31,1.0,
5,UO2(OH)2(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,1.00000e+00,HCO3-,-
3.00000e+00,EqRc-32,1.0,
4,UO2(OH)3-,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,HCO3-,-3.00000e+00,EqRc-33,1.0,
5,UO2(OH)4--,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,-1.00000e+00,HCO3-,-
3.00000e+00,EqRc-34,1.0,
5,(UO2)2OH+++,Ca++,-4.00000e+00,Ca2UO2(CO3)3(aq),2.00000e+00,H+,5.00000e+00,HCO3-,-
6.00000e+00,EqRc-35,1.0,
5,(UO2)2(OH)2++,Ca++,-4.00000e+00,Ca2UO2(CO3)3(aq),2.00000e+00,H+,4.00000e+00,HCO3-,-
6.00000e+00,EqRc-36,1.0,
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5,(UO2)3(OH)4++,Ca++,-6.00000e+00,Ca2UO2(CO3)3(aq),3.00000e+00,H+,5.00000e+00,HCO3-,-
9.00000e+00,EqRc-37,1.0,
5,(UO2)3(OH)5+,Ca++,-6.00000e+00,Ca2UO2(CO3)3(aq),3.00000e+00,H+,4.00000e+00,HCO3-,-
9.00000e+00,EqRc-38,1.0,
5,(UO2)3(OH)7-,Ca++,-6.00000e+00,Ca2UO2(CO3)3(aq),3.00000e+00,H+,2.00000e+00,HCO3-,-
9.00000e+00,EqRc-39,1.0,
5,(UO2)4(OH)7+,Ca++,-8.00000e+00,Ca2UO2(CO3)3(aq),4.00000e+00,H+,5.00000e+00,HCO3-,-
1.20000e+01,EqRc-40,1.0,
5,UO2CO3(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,2.00000e+00,HCO3-,-
2.00000e+00,EqRc-41,1.0,
5,UO2(CO3)2--,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,1.00000e+00,HCO3-,-
1.00000e+00,EqRc-42,1.0,
3,UO2(CO3)3----,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,EqRc-43,1.0,
5,(UO2)2CO3(OH)3-,Ca++,-4.00000e+00,Ca2UO2(CO3)3(aq),2.00000e+00,H+,2.00000e+00,HCO3-,-
5.00000e+00,EqRc-44,1.0,
3,CaUO2(CO3)3--,Ca++,-1.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,EqRc-45,1.0,
5,UO2OH+,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,2.00000e+00,HCO3-,-3.00000e+00,EqRc-
46,1.0,
6,UO2NO3+,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-3.00000e+00,NO3-
,1.00000e+00,EqRc-47,1.0,
6,UO2Cl+,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,Cl-,1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,EqRc-48,1.0,
6,UO2Cl2(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,Cl-,2.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,EqRc-49,1.0,
6,UO2SO4(aq),Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,SO4--,1.00000e+00,EqRc-50,1.0,
6,UO2(SO4)2--,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,3.00000e+00,HCO3-,-
3.00000e+00,SO4--,2.00000e+00,EqRc-51,1.0,
6,SOUO2OH,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,1.00000e+00,HCO3-,-
3.00000e+00,SOH,1.00000e+00,EqRc-52,1.0,
6,SOHUO2CO3,Ca++,-2.00000e+00,Ca2UO2(CO3)3(aq),1.00000e+00,H+,2.00000e+00,HCO3-,-
2.00000e+00,SOH,1.00000e+00,EqRc-53,1.0,

~Kinetic Reactions Card
1,
KnRc-31,TST,Calcite,2,Ca++,1.0,HCO3-,1.0,2,Calcite,1.0,H+,1.0,
6.456542e-39,mol/m^2 s,15.e+3,cal/mol,25.0,C,
,1.8487,,,,

~Kinetic Equations Card
1,
Kinetic_Calcite,1,Calcite,1.00000e+00,
1,KnRc-31,1.00000e+00,

~Initial Conditions Card
Aqueous Pressure,Gas Pressure,
#Well w/o Uranium
14,
Aqueous Pressure,102064.81,Pa,,,,,,,1,10,1,1,1,1,
Gas Pressure,102064.81,Pa,,,,,,,1,10,1,1,1,1,
Temperature,25,C,,,,,,,1,10,1,1,1,1,
#Overwrite Species Aqueous Volumetric,pH,7.7,,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,H+,8.24818e-5,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,HCO3-,2.66e-3,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Ca++,1.1e-3,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Cl-,2.75e-3,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,K+,1.5e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Mg++,4.1e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,NO3-,1.73e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Na+,9.87e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,SO4--,3.25e-4,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,SOH,0.605088,mol/liter,,,,,,,1,10,1,1,1,1,
Overwrite Species Aqueous Volumetric,Ca2UO2(CO3)3(aq),1.30295e-5,mol/liter,,,,,,,1,10,1,1,1,1,
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~Boundary Conditions Card
2,
West,Aqueous Neumann,Species Aqueous Conc.,
10,H+,HCO3-,K+,NO3-,Na+,Ca++,Mg++,Cl-,SO4--,Ca2UO2(CO3)3(aq),
1,1,1,1,1,1,1,
0,hr,1.44,m/d,
#Well w/ Uranium
1.29599e-4,mol/liter,9.18e-4,mol/liter,1.75e-5,mol/liter,
8.55e-6,mol/liter,1e-4,mol/liter,3.74e-4,mol/liter,
1.48e-4,mol/liter,3.1e-5,mol/liter,7.08e-5,mol/liter,0.e-6,mol/liter,
East,Aqueous Dirichlet,Species Outflow,
0,
10,10,1,1,1,1,1,
0,day,102064.81,Pa,

~Output Options Card
3,
1,1,1,
5,1,1,
10,1,1,
1,1,d,m,6,6,6,
9,
Species Aqueous Concentration,Total_H+,mol/L,
Species Aqueous Concentration,H+,mol/L,
Species Aqueous Concentration,Total_Ca2UO2(CO3)3(aq),mol/L,
Species Aqueous Concentration,Ca2UO2(CO3)3(aq),mol/L,
Species Aqueous Concentration,CaUO2(CO3)3--,mol/L,
Species Aqueous Concentration,UO2(CO3)3----,mol/L,
Species Aqueous Concentration,SOUO2OH,mol/L,
Species Aqueous Concentration,SOHUO2CO3,mol/L,
Species Aqueous Concentration,calcite,mol/L,
4,
0,day,
1,d,
4,d,
10,d,
4,
Species Aqueous Concentration,H+,mol/L,
Species Aqueous Concentration,Total_Ca2UO2(CO3)3(aq),mol/L,
Species Aqueous Concentration,SOUO2OH,mol/L,
Species Aqueous Concentration,SOHUO2CO3,mol/L,
```