

From: "Dave Levy" <DLey@telesto-inc.com>
To: "Michalak, Paul" <pxm2@nrc.gov>
Date: 1/6/06 5:19PM
Subject: Gas Hills Model - 40-0299

Paul:

Attached is a PDF with 2 versions of the SWFR Gas Hills model-re-run. I'll give a call Monday morning to discuss.

Thanks.

Dave

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Subject: Gas Hills Model
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Created By: DLevy@telesto-inc.com

Recipients

nrc.gov

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TITLE A-9 area (SW flow regime). FILE: SWFR1td_nrc2.in
#Concentration vs Time (0 to 1000 years) at the POE
#Using flow rate of 0.167 ft/d - DECREASING SOURCE TERM TO 90% REDUCTION
#DISPERSIVITY = 50
#SOLID PHASES ALLOWED
#Revised in 2005 for Pb-210
#Revised in 2006 for Solutions in Cells 6-54 and Source sulfate

PRINT

-reset false

KNOBS

-iterations 100
-tolerance 1.00E-13
-step_size 100
-pe_step_size 10
-diagonal_scale TRUE
-debug_prep FALSE
-debug_set FALSE
-debug_model FALSE
-debug_inverse FALSE
-logfile FALSE

SELECTED_OUTPUT

-file C:\SWFR1td_nrc2.dat

USER_PUNCH

-headings As Be Cl Pb U Ni Se SO4 Th Ra sOPb+
-headings wOPb+ PbX2 Anglesite sOHUO2+2
-headings wOUO2+ USiO4(C) Uraninite sONi+ wONi+
-headings NiSe sOHRa+2 wORa+ RaX2 RaSO4 wSeO4-
-headings wOHSeO4-2 wSeO3- wOHSeO3-2 Se(A)
-headings FeSe2 sSO4- wSO4- sOHSO4-2 wOHSO4-2
-headings gypsum wOTh+3 wOTh(OH)+2 wOTh(OH)2+
-headings wOTh(OH)3 wOTh(OH)4- sH2AsO3 wH2AsO3
-headings sH2AsO4 wH2AsO4 sHAsO4- wHAsO4- sAsO4-2
-headings wAsO4-2 sOHAsO4-3 wOHAsO4-3 sOBe+ wOBe+
-headings Calcite Ca Mg Na K HCO3 SO4 Cl TDS
-start
10 REM Convert to ppm and show molalities
20 PUNCH TOT("As")*74.9216*1000
30 PUNCH TOT("Be")*9.0122*1000
40 PUNCH TOT("Cl")*35.453*1000
50 PUNCH TOT("Pb")*207.19*1000/1.29e-11
60 PUNCH TOT("U")*238.029*1000
70 PUNCH TOT("Ni")*58.71*1000
80 PUNCH TOT("Se")*78.96*1000
90 PUNCH TOT("S(6)")*96.0616*1000
100 PUNCH TOT("Th")*232.038*1000/4.96e-8
110 PUNCH TOT("Ra")*226*1000/1.01e-9
120 PUNCH MOL("Hfo_sOPb+")
130 PUNCH MOL("Hfo_wOPb+")
140 PUNCH MOL("PbX2")
150 PUNCH EQUI("Anglesite")
160 PUNCH MOL("Hfo_sOHUO2+2")
170 PUNCH MOL("Hfo_wOUO2+")
180 PUNCH EQUI("USiO4(C)")
190 PUNCH EQUI("Uraninite")
200 PUNCH MOL("Hfo_sONi+")
210 PUNCH MOL("Hfo_wONi+")
220 PUNCH EQUI("NiSe")
230 PUNCH MOL("Hfo_sOHRa+2")
240 PUNCH MOL("Hfo_wORa+")
250 PUNCH MOL("RaX2")
260 PUNCH EQUI("RaSO4")
270 PUNCH MOL("Hfo_wSeO4-")

```

280 PUNCH MOL("Hfo_wOHSeO4-2")
290 PUNCH MOL("Hfo_wSeO3-")
300 PUNCH MOL("Hfo_wOHSeO3-2")
310 PUNCH EQUI("Se(A)")
320 PUNCH EQUI("Ferroselite")
330 PUNCH MOL("Hfo_sSO4-")
340 PUNCH MOL("Hfo_wSO4-")
350 PUNCH MOL("Hfo_sOHSO4-2")
360 PUNCH MOL("Hfo_wOHSO4-2")
370 PUNCH EQUI("gypsum")
380 PUNCH MOL("Hfo_wOTh+3")
390 PUNCH MOL("Hfo_wOTh(OH)+2")
400 PUNCH MOL("Hfo_wOTh(OH)2+")
410 PUNCH MOL("Hfo_wOTh(OH)3")
420 PUNCH MOL("Hfo_wOTh(OH)4-")
430 PUNCH MOL("Hfo_sh2AsO3")
440 PUNCH MOL("Hfo_wh2AsO3")
450 PUNCH MOL("Hfo_sh2AsO4")
460 PUNCH MOL("Hfo_wh2AsO4")
470 PUNCH MOL("Hfo_sHAsO4-")
480 PUNCH MOL("Hfo_wHAsO4-")
490 PUNCH MOL("Hfo_sAsO4-2")
500 PUNCH MOL("Hfo_wAsO4-2")
510 PUNCH MOL("Hfo_sOHasO4-3")
520 PUNCH MOL("Hfo_wOHasO4-3")
530 PUNCH MOL("Hfo_sOBe+")
540 PUNCH MOL("Hfo_wOBe+")
550 PUNCH EQUI("Calcite")
560 PUNCH TOT("Ca")*40.08*1000
570 PUNCH TOT("Mg")*24.312*1000
580 PUNCH TOT("Na")*22.9898*1000
590 PUNCH TOT("K")*39.102*1000
600 PUNCH MOL("HCO3-")*61.018*1000
610 PUNCH TOT("S(6)")*96.0616*1000
620 PUNCH TOT("Cl")*35.453*1000
630 A = (TOT("Ca")*40.08*1000)+(TOT("Mg")*24.312*1000)
640 B = (TOT("Na")*22.9898*1000)+(TOT("K")*39.102*1000)
650 C = MOL("HCO3-")*61.018*1000
660 D = TOT("S(6)")*96.0616*1000
670 E = TOT("Cl")*35.453*1000
680 PUNCH A+B+C+D+E
-end

```

PRINT

-selected_output false

SOLUTION 0 # Initial Source Term

units	ppm	
pe	8	
pH	4.33	
Th	2.22e-6	
Pb	2.44e-9	#Revised ACL 2005 (189 pCi/L)
Be	1.7	
Ca	710	#increased to obtain CB for SO4 <15%
Mg	174	#increased to obtain CB for SO4 <15%
Na	117	#increased to obtain CB for SO4 <15%
K	15	
Fe(2)	160	#increased to obtain CB for SO4 <15%
Cl	161	
As	1.36	
Ni	9.34	
Se	0.53	
Si	56.4	
U	34.1	
Alkalinity	2.44	as HCO3

S(6) 3500 #previously 2650
Ra 3.57e-7

SOLUTION 1-5 GW8 January 2001

units	ppm
pe	7
pH	4.73
S(6)	1540
Cl	97
Alkalinity	2.0 as HCO3
Ca	418
Na	30.6
Mg	70.8
K	17.6
Fe(2)	127
As	0.007
Be	0.076
Th	7.97e-8
Pb	2.58e-10
Ra	6.25e-8
Ni	1.31
Se	0.001
U	10.3

SOLUTION 6-54 GW-4 # Most recent data from GW-4 replaces MW-74 January 2001

units	ppm
pe	6
pH	4.3 #May-05
S(6)	1950 #Aug-01
Cl	110 #Aug-01
#Alkalinity	35 as HCO3
Ca	271 #May-01
Na	43.4 #Mar-01
Mg	88.1 #Mar-01
K	18.1 #Mar-01
Fe(2)	174 #Aug-01
As	0.0015 #1/2DL Aug-01
Be	0.001 # 1/2 DL Aug-01
#Th	negative value reported
Pb	3.93e-11 #Aug-01
Ra	4.59e-8 #Aug-01
Ni	0.65 #Aug-01
Se	0.011 #Aug-01
U	0.0547 #Aug-01
#S(-2)	not measured

EQUILIBRIUM_PHASES 1-54

Calcite	0.0	0.0
Gypsum	0.0	0.0
USiO4(c)	0.0	0.0
Ferroselite	0.0	0.0
Se(A)	0.0	0.0
RaSO4	0.0	0.0
NiSe	0.0	0.0
Anglesite	0.0	0.0

SURFACE 1-5

-equilibrate 1		
Hfo_wOH	0.086	600
Hfo_sOH	0.0021	45.9

SURFACE 6-54

-equilibrate 6		
Hfo_wOH	0.086	600
Hfo_sOH	0.0021	45.9

EXCHANGE 1-5
-equilibrate 1
X 1.2

EXCHANGE 6-54
-equilibrate 6
X 1.2

TRANSPORT
-lengths 54*30.5
-dispersivities 54*50
-cells 54
-shifts 4
-punch_cells 54

PRINT
-selected_output true

END

PRINT
-selected_output false

SOLUTION 0 #33% REDUCTION

units	ppm	
pe	5.6	
pH	4.47	
Th	1.47e-6	
Pb	1.63e-9	#Revised ACL 2005
Ra	2.41E-07	
U	22.62	
Be	1.13	
Ca	570	
Mg	137	
Na	94	
K	16.2	
Fe(2)	109	
Cl	114.6	
As	0.90	
Ni	6.20	
Se	0.35	
Si	37.4	
Alkalinity	4.0 as HCO3	
S(6)	2546	#previously 1980.5

TRANSPORT
-lengths 54*30.5
-dispersivities 54*50
-cells 54
-shifts 2
-punch_cells 54

PRINT
-selected_output true

END

PRINT
-selected_output false

SOLUTION 0 #50% Reduction

units	ppm
pe	5.5
pH	4.57
Th	1.12e-6

```
Pb      1.22e-9   #Revised ACL 2005
Ra      1.86E-07
U       17.16
Be      0.85
Ca      503
Mg      119
Na      83
K       16.8
Fe(2)   85
Cl      92.5
As      0.68
Ni      4.7
Se      0.27
Si      28.31
Alkalinity 4.73 as HCO3
S(6)    2089 #previously 1661
```

TRANSPORT

```
-lengths      54*30.5
-dispersivities 54*50
-cells        54
-shifts       4
-punch_cells  54
```

PRINT

```
-selected_output true
```

END

PRINT

```
selected_output false
```

SOLUTION 0 #75% Reduction

```
units      ppm
pe         5.1
pH         4.85
Th         5.65E-07
Pb         6.1e-10   #Revised ACL 2005
Ra         1.0E-07
U          8.62
Be         0.43
Ca         398
Mg         91
Na         66
K          17.7
Fe(2)      47
Cl         58
As         0.34
Ni         2.36
Se         0.13
Si         14.2
Alkalinity 5.88 as HCO3
S(6)      1375 #previously 1161
```

TRANSPORT

```
-lengths      54*30.5
-dispersivities 54*50
-cells        54
-shifts       12
-punch_cells  54
```

PRINT

```
selected_output true
```

END

PRINT .
selected_output false

SOLUTION 0 #90% Reduction

units	ppm	
pe	4.4	
pH	5.27	
Th	2.33E-07	
Pb	2.45e-10	#Revised ACL 2005
Ra	4.84e-8	
U	3.5	
Be	0.17	
Ca	334	
Mg	74	
Na	56	
K	18.2	
Fe(2)	24	
Cl	37.3	
As	0.14	
Ni	0.96	
Se	0.05	
Si	5.66	
Alkalinity	6.56	as HCO3
S(6)	946	#previously 860.7

TRANSPORT

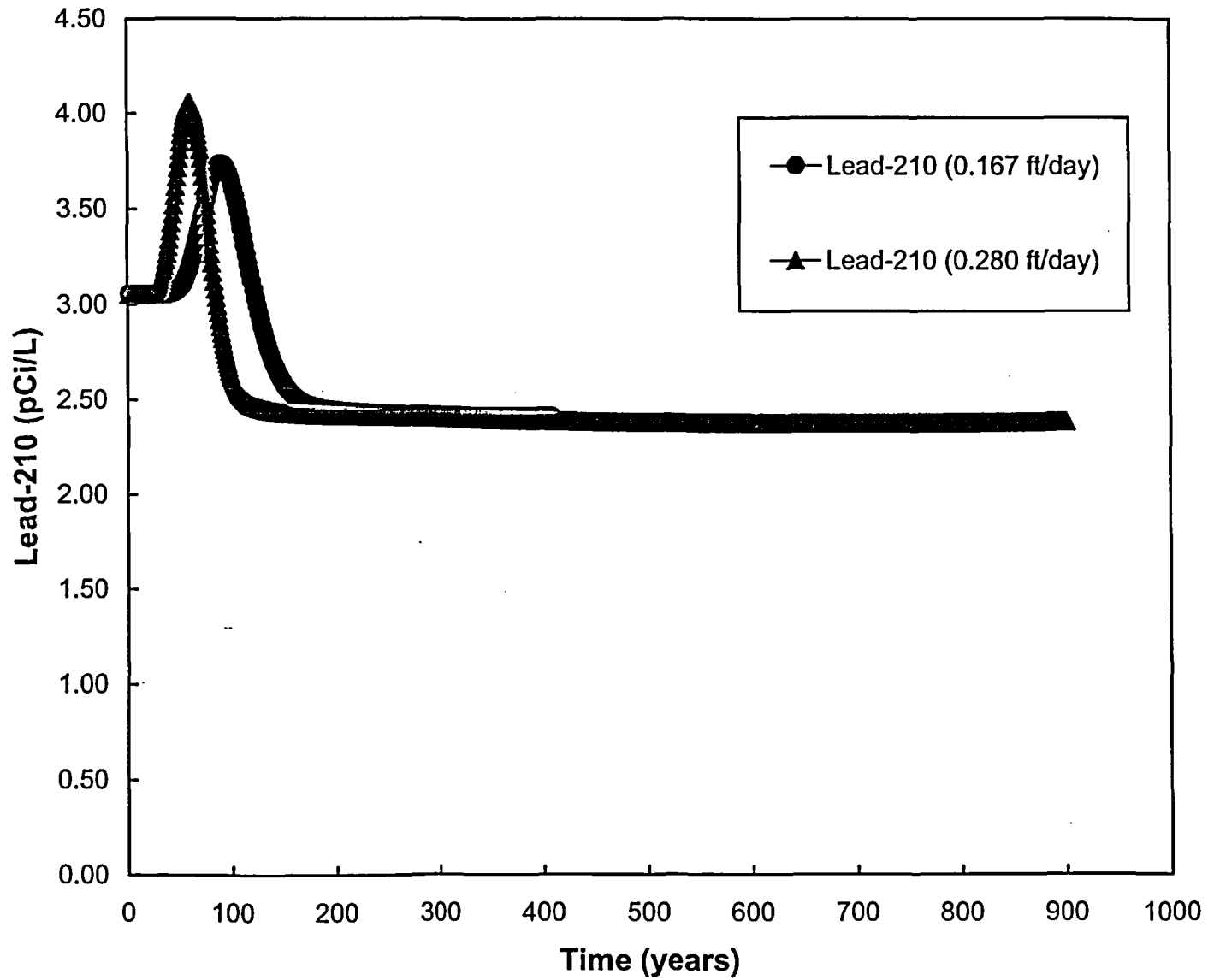
-lengths	54*30.5
-dispersivities	54*50
-cells	54
-shifts	588
-punch_cells	54

PRINT
-selected_output true

END

PRINT
selected_output false

Figure 2: Predicted Lead-210 Concentrations at the POE for the Southwestern Flow Regime for a 1000-Year Time Frame Using the Proposed Revised ACL of 189 pCi/L.



TITLE · A-9 area (SW flow regime). FILE: SWFR1td_nrc3.in
#Concentration vs Time (0 to 1000 years) at the POE
#Using flow rate of 0.167 ft/d - DECREASING SOURCE TERM TO 90% REDUCTION
#DISPERSIVITY = 50
#SOLID PHASES ALLOWED
#Revised in 2005 for Pb-210
#Revised in 2006 for Solutions in Cells 6-54 and Source sulfate

PRINT

-reset false

KNOBS

-iterations 100
-tolerance 1.00E-13
-step_size 100
-pe_step_size 10
-diagonal_scale TRUE
-debug_prep FALSE
-debug_set FALSE
-debug_model FALSE
-debug_inverse FALSE
-logfile FALSE

SELECTED OUTPUT

-file C:\SWFR1td_nrc3.dat

USER_PUNCH

-headings As Be Cl Pb U Ni Se SO4 Th Ra sOPb+
-headings wOPb+ PbX2 Anglesite sOHUO2+2
-headings wOUO2+ USiO4(C) Uraninite sONi+ wONi+
-headings NiSe sOHRA+2 wORA+ RaX2 RaSO4 wSeO4-
-headings wOHSeO4-2 wSeO3- wOHSeO3-2 Se(A)
-headings FeSe2 sSO4- wSO4- sOHSO4-2 wOHSO4-2
-headings gypsum wOTH+3 wOTH(OH)+2 wOTH(OH)2+
-headings wOTH(OH)3 wOTH(OH)4- sH2AsO3 wH2AsO3
-headings sH2AsO4 wH2AsO4 sHASO4- wHASO4- sAsO4-2
-headings wAsO4-2 sOHAsO4-3 wOHAsO4-3 sOBe+ wOBe+
-headings Calcite Ca Mg Na K HCO3 SO4 Cl TDS
-start
10 REM Convert to ppm and show molalities
20 PUNCH TOT("As")*74.9216*1000
30 PUNCH TOT("Be")*9.0122*1000
40 PUNCH TOT("Cl")*35.453*1000
50 PUNCH TOT("Pb")*207.19*1000/1.29e-11
60 PUNCH TOT("U")*238.029*1000
70 PUNCH TOT("Ni")*58.71*1000
80 PUNCH TOT("Se")*78.96*1000
90 PUNCH TOT("S(6)")*96.0616*1000
100 PUNCH TOT("Th")*232.038*1000/4.96e-8
110 PUNCH TOT("Ra")*226*1000/1.01e-9
120 PUNCH MOL("Hfo_sOPb+")
130 PUNCH MOL("Hfo_wOPb+")
140 PUNCH MOL("PbX2")
150 PUNCH EQUI("Anglesite")
160 PUNCH MOL("Hfo_sOHUO2+2")
170 PUNCH MOL("Hfo_wOUO2+")
180 PUNCH EQUI("USiO4(C)")
190 PUNCH EQUI("Uraninite")
200 PUNCH MOL("Hfo_sONi+")
210 PUNCH MOL("Hfo_wONi+")
220 PUNCH EQUI("NiSe")
230 PUNCH MOL("Hfo_sOHRA+2")
240 PUNCH MOL("Hfo_wORA+")
250 PUNCH MOL("RaX2")
260 PUNCH EQUI("RaSO4")
270 PUNCH MOL("Hfo_wSeO4-")

```

280 PUNCH MOL("Hfo_wOHSeO4-2")
290 PUNCH MOL("Hfo_wSeO3-")
300 PUNCH MOL("Hfo_wOHSeO3-2")
310 PUNCH EQUI("Se(A) ")
320 PUNCH EQUI("Ferroselite")
330 PUNCH MOL("Hfo_sSO4-")
340 PUNCH MOL("Hfo_wSO4-")
350 PUNCH MOL("Hfo_sOHSO4-2")
360 PUNCH MOL("Hfo_wOHSO4-2")
370 PUNCH EQUI("gypsum")
380 PUNCH MOL("Hfo_wOTh+3")
390 PUNCH MOL("Hfo_wOTh(OH)+2")
400 PUNCH MOL("Hfo_wOTh(OH)2+")
410 PUNCH MOL("Hfo_wOTh(OH)3")
420 PUNCH MOL("Hfo_wOTh(OH)4-")
430 PUNCH MOL("Hfo_sH2AsO3")
440 PUNCH MOL("Hfo_wH2AsO3")
450 PUNCH MOL("Hfo_sH2AsO4")
460 PUNCH MOL("Hfo_wH2AsO4")
470 PUNCH MOL("Hfo_sHAsO4-")
480 PUNCH MOL("Hfo_wHAsO4-")
490 PUNCH MOL("Hfo_sAsO4-2")
500 PUNCH MOL("Hfo_wAsO4-2")
510 PUNCH MOL("Hfo_sOHasO4-3")
520 PUNCH MOL("Hfo_wOHasO4-3")
530 PUNCH MOL("Hfo_sOBe+")
540 PUNCH MOL("Hfo_wOBe+")
550 PUNCH EQUI("Calcite")
560 PUNCH TOT("Ca")*40.08*1000
570 PUNCH TOT("Mg")*24.312*1000
580 PUNCH TOT("Na")*22.9898*1000
590 PUNCH TOT("K")*39.102*1000
600 PUNCH MOL("HCO3-")*61.018*1000
610 PUNCH TOT("S(6)")*96.0616*1000
620 PUNCH TOT("Cl")*35.453*1000
630 A = (TOT("Ca")*40.08*1000)+(TOT("Mg")*24.312*1000)
640 B = (TOT("Na")*22.9898*1000)+(TOT("K")*39.102*1000)
650 C = MOL("HCO3-")*61.018*1000
660 D = TOT("S(6)")*96.0616*1000
670 E = TOT("Cl")*35.453*1000
680 PUNCH A+B+C+D+E
-end

```

PRINT

-selected_output false

SOLUTION 0 # Initial Source Term

units	ppm	
pe	8	
pH	4.33	
Th	2.22e-6	
Pb	2.44e-9	#Revised ACL 2005 (189 pCi/L)
Be	1.7	
Ca	710	#increased to obtain CB for SO4 <15%
Mg	174	#increased to obtain CB for SO4 <15%
Na	117	#increased to obtain CB for SO4 <15%
K	15	
Fe(2)	160	#increased to obtain CB for SO4 <15%
Cl	161	
As	1.36	
Ni	9.34	
Se	0.53	
Si	56.4	
U	34.1	
Alkalinity	2.44	as HCO3

S(6) 3500 #previously 2650
Ra 3.57e-7

SOLUTION 1-5 GW8 January 2001

units	ppm
pe	7
pH	4.73
S(6)	1540
Cl	97
Alkalinity	2.0 as HCO3
Ca	418
Na	30.6
Mg	70.8
K	17.6
Fe(2)	127
As	0.007
Be	0.076
Th	7.97e-8
Pb	2.58e-10
Ra	6.25e-8
Ni	1.31
Se	0.001
U	10.3

SOLUTION 6-54 MW-72 # Data from MW-72 replaces MW-74 January 2001

units	ppm
pe	6
pH	6.48 #Jun-04
S(6)	1190 #Jun-04
Cl	115 #Jun-04
Alkalinity	400 as HCO3 #Jan-01
Ca	580 #Jan-01
Na	25 #Jan-01
Mg	63 #Jan-01
K	17 #Jan-01
Fe(2)	4 #Jan-01
As	0.0081 #Jun-05
Be	0.0001 #Jun-05
#Th	negative value reported
Pb	2.97e-11 #Jan-01
Ra	2.42e-8 #Jan-01
Ni	0.0179 #Jun-05
Se	0.017 #Jun-05
U	0.609 #Jun-05
#S(-2)	not measured

EQUILIBRIUM_PHASES 1-54

Calcite	0.0	0.0
Gypsum	0.0	0.0
USiO4(c)	0.0	0.0
Ferroselite	0.0	0.0
Se(A)	0.0	0.0
RaSO4	0.0	0.0
NiSe	0.0	0.0
Anglesite	0.0	0.0

SURFACE 1-5

-equilibrate 1			
Hfo_wOH	0.086	600	45.9
Hfo_sOH	0.0021		

SURFACE 6-54

-equilibrate 6			
Hfo_wOH	0.086	600	45.9
Hfo_sOH	0.0021		

EXCHANGE 1-5
-equilibrate 1
X 1.2

EXCHANGE 6-54
-equilibrate 6
X 1.2

TRANSPORT
-lengths 54*30.5
-dispersivities 54*50
-cells 54
-shifts 4
-punch_cells 54

PRINT
-selected_output true

END

PRINT
-selected_output false

SOLUTION 0 #33% REDUCTION

units	ppm	
pe	5.6	
pH	4.47	
Th	1.47e-6	
Pb	1.63e-9	#Revised ACL 2005
Ra	2.41E-07	
U	22.62	
Be	1.13	
Ca	570	
Mg	137	
Na	94	
K	16.2	
Fe(2)	109	
Cl	114.6	
As	0.90	
Ni	6.20	
Se	0.35	
Si	37.4	
Alkalinity	4.0 as HCO3	
S(6)	2546	#previously 1980.5

TRANSPORT
-lengths 54*30.5
-dispersivities 54*50
-cells 54
-shifts 2
-punch_cells 54

PRINT
-selected_output true

END

PRINT
-selected_output false

SOLUTION 0 #50% Reduction

units	ppm
pe	5.5
pH	4.57
Th	1.12e-6

Pb 1.22e-9 #Revised ACL 2005
Ra 1.86E-07
U 17.16
Be 0.85
Ca 503
Mg 119
Na 83
K 16.8
Fe(2) 85
Cl 92.5
As 0.68
Ni 4.7
Se 0.27
Si 28.31
Alkalinity 4.73 as HCO3
S(6) 2089 #previously 1661

TRANSPORT

-lengths 54*30.5
-dispersivities 54*50
-cells 54
-shifts 4
-punch_cells 54

PRINT

-selected_output true

END

PRINT

selected_output false

SOLUTION 0 #75% Reduction

units	ppm	
pe	5.1	
pH	4.85	
Th	5.65E-07	
Pb	6.1e-10	#Revised ACL 2005
Ra	1.0E-07	
U	8.62	
Be	0.43	
Ca	398	
Mg	91	
Na	66	
K	17.7	
Fe(2)	47	
Cl	58	
As	0.34	
Ni	2.36	
Se	0.13	
Si	14.2	
Alkalinity	5.88	as HCO3
S(6)	1375	#previously 1161

TRANSPORT

-lengths 54*30.5
-dispersivities 54*50
-cells 54
-shifts 12
-punch_cells 54

PRINT

selected_output true

END

PRINT.
selected_output false

SOLUTION 0 #90% Reduction

units	ppm	
pe	4.4	
pH	5.27	
Th	2.33E-07	
Pb	2.45e-10	#Revised ACL 2005
Ra	4.84e-8	
U	3.5	
Be	0.17	
Ca	334	
Mg	74	
Na	56	
K	18.2	
Fe(2)	24	
Cl	37.3	
As	0.14	
Ni	0.96	
Se	0.05	
Si	5.66	
Alkalinity	6.56	as HCO3
S(6)	946	#previously 860.7

TRANSPORT

-lengths	54*30.5
-dispersivities	54*50
-cells	54
-shifts	588
-punch_cells	54

PRINT
-selected_output true

END

PRINT
selected_output false

Figure 2: Predicted Lead-210 Concentrations at the POE for the Southwestern Flow Regime for a 1000-Year Time Frame Using the Proposed Revised ACL of 189 pCi/L.

