308

Scientific Notebook # 258

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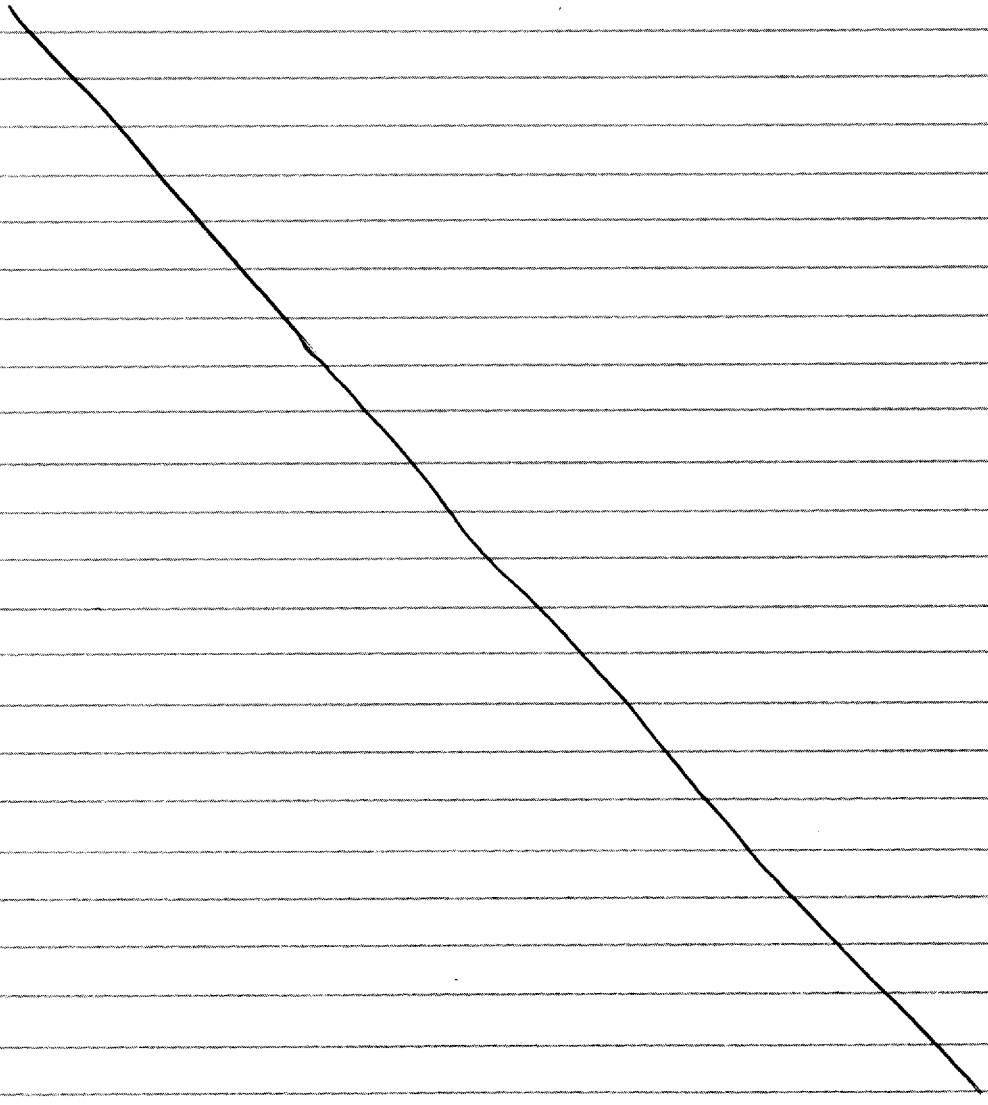
20-1402-871
KTI on Radionuclide Transport
02/04/98

Contents

Page

Objectives (20-1402-871) - KTI on Radionuclide Transport (02/04/98)

The purpose of the research discussed in this scientific notebook is to evaluate available geochemical, geological, and hydrologic data in the vicinity of Yucca Mountain to help constrain radionuclide transport from the proposed repository. Uses of these data may include delineation of regional flow patterns, placing constraints on the potential for dilution of radionuclide-bearing waters through mixing between different bodies of groundwater, geochemical information related to retardation (sorption, precipitation, dissolution. Computer codes that may be used include the EPA geochemistry code MINTEQA2, the USGS hydrochemistry code NETPATH, GIS software such as ArcView, and commercial software such as Microsoft Excel, SigmaPlot, and WordPerfect.



03-17-98

NETPATH Test Model Results (20-1402-871) - KTI on Radionuclide Transport (03/17/98)

Test model results from NETPATH 2.0, installed on CNWRA equipment, are identical to those achieved in *An interactive code (NETPATH) for modeling net geochemical reactions along a flow path (version 2.0)* by Plummer, et al. Model results for np-2.dat; np-5-5.dat; and np-6.dat are presented here.

np-2.out

Initial Well: GSL, Bear R. weighted 1961
Final Well : GSL, S. arm at RR Oct. 1960.

NETPATH 2.13
December 30, 1996

Constraints: 5	Phases: 5	Parameters
Carbon Calcium Chloride	Sulfur Sodium	CO2 GAS NaCl ARAGONIT MIRABILI GYPSUM	Mixing: No Evaporation: Yes Rayleigh Calcs: No

	Final	Initial
C	6.3060	6.0210
S	291.4270	0.6980
CA	11.2170	1.6980
NA	5428.6160	9.4490
CL	5834.6400	9.2340

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000
NaCl	NA	1.0000	CL	1.0000				
ARAGONIT	CA	1.0000	C	1.0000	RS	4.0000		
MIRABILI	NA	2.0000	S	1.0000	RS	6.0000		
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000

5 models checked
3 models found

MODEL 1

CO2 GAS	-4.32887	
NaCl	-2.26579	
ARAGONIT	-1.68460	
MIRABILI	-0.34995	
Evaporation factor:	837.323	1.194g H2O remain

MODEL 2

CO2 GAS	-4.13876	
ARAGONIT	-1.87226	
MIRABILI	-0.42879	
GYPSUM	0.19201	
Evaporation factor:	631.865	1.583g H2O remain

MODEL 3

NaCl	49.32956	
ARAGONIT	-5.95771	
MIRABILI	-2.14518	
GYPSUM	4.37229	
Evaporation factor:	99.629	10.037g H2O remain

np-5-5.out

Initial Well : Chapelle-Knobel (1985) Fd-12
Final Well : Chapelle-Knobel (1985) Ff-35

Constraints: 3	Phases: 3	Parameters
Carbon Calcium Sodium	CALCITE H-Exch CO2 GAS	Mixing: No Evaporation: No Rayleigh Calcs: Yes Init C-14 50.00 (TDC) (User-defined)

	Final	Initial
C	5.9742	3.0741
CA	0.0749	1.0232
NA	6.0930	0.1653

CALCITE	CA	1.0000 C	1.0000 RS	4.0000 I1	1.1000 I2	0.0000
H-Exch	NA	1.6000 CA	-1.0000			
CO2 GAS	C	1.0000 RS	4.0000 I1	-22.0000 I2	0.0000	

1 model checked
1 model found

MODEL 1

CALCITE	2.75643
H-Exch	3.70478
CO2 GAS	0.14373

	Computed	Observed
Carbon-13	-6.5051	-6.2000
C-14 (% mod)	25.7278*	3.1000
Sulfur-34	0.0000	Undefined
Strontium-87	Insufficient data	
Nitrogen-15	Insufficient data	

Adjusted C-14 age in years: 17494.* * = based on User-defined

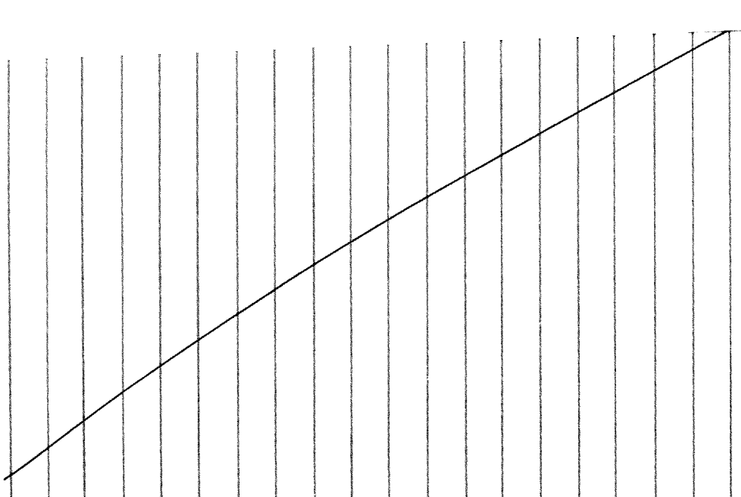
Model (for initial A0)	A0 (initial)	Computed (no decay)	Observed	age (final)
Original Data	33.90	17.44	3.10	14281.
Mass Balance	55.75	28.69	3.10	18394.
Vogel	85.00	43.74	3.10	21880.
Tamers	52.75	27.15	3.10	17937.
Ingerson and Pearson	50.40	25.93	3.10	17559.
Mook	34.25	17.62	3.10	14366.
Fontes and Garnier	50.35	25.91	3.10	17551.
Eichinger	47.91	24.65	3.10	17141.
User-defined	50.00	25.73	3.10	17494.

Data used for Carbon-13

Initial Value: -12.6000 Modeled Final Value: -6.5051

2 dissolving phases:

Phase	Delta C	Isotopic composition (o/oo)
CALCITE	2.75643	1.1000
CO2 GAS	0.14373	-22.0000



03/17/98

Data used for C-14 (% mod)

Initial Value: 50.0000 Modeled Final Value: 25.7278

2 dissolving phases:

Phase	Delta C	Isotopic composition (% modern)
CALCITE	2.75643	0.0000
CO2 GAS	0.14373	0.0000

Data used for Sulfur-34

Initial Value: 0.0000 Modeled Final Value: 0.0000

No incoming or outgoing phases

Data used for Strontium-87
Insufficient data

Data used for Nitrogen-15
Insufficient data

np-6.out

Initial Well : Madison.Recharge #3
Final Well : Madison.Mysse

Constraints: 10		Phases: 10	Parameters
Carbon	Sulfur	+DOLOMITE CALCITE +ANHYDRIT	Mixing: No
Calcium	Magnesium	+"CH2O" GOETHITE-PYRITE	Evaporation: No
Sodium	Potassium	EXCHANGE+NaCl SYLVITE	Rayleigh Calcs: Yes
Chloride	Iron	CO2 GAS	Exchange: Ca/Na
Redox	Sulfur-34		Init C-14 52.33 (TDC)
			(Mass Balance)

	Final	Initial
C	6.8700	4.3000
S	20.1190	0.1600
CA	11.2800	1.2000
MG	4.5400	1.0100
NA	31.8900	0.0200
K	2.5400	0.0200
CL	17.8500	0.0200
FE	0.0004	0.0010
RS	146.1228	18.1620
I3	317.9967	1.5568

DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 8.0000
	I2	0.0000							
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	4.0000	I2 0.0000
ANHYDRIT	CA	1.0000	S	1.0000	RS	6.0000	I3	15.5000	
"CH2O"	C	1.0000	I1	-25.0000	I2	0.0000			
GOETHITE	FE	1.0000	RS	3.0000					
PYRITE	FE	1.0000	S	2.0000	RS	0.0000	I3	-44.1800	
EXCHANGE	CA	-1.0000	NA	2.0000	MG	0.0000			
NaCl	NA	1.0000	CL	1.0000					
SYLVITE	K	1.0000	CL	1.0000					
CO2 GAS	C	1.0000	RS	4.0000	I1	-16.2000	I2	100.0000	

1 model checked
1 model found

	MODEL 1
DOLOMITE	+ 3.53000
CALCITE	-5.31723
ANHYDRIT	+ 20.14723
"CH2O"	+ 0.87077
GOETHITE	0.09351
PYRITE	- -0.09411
EXCHANGE	8.28000
NaCl	+ 15.31000
SYLVITE	2.52000
CO2 GAS	-0.04355

	Computed	Observed
Carbon-13	-2.2157	-2.3400
C-14 (% mod)	12.2688*	0.8000
Sulfur-34	15.8130	15.8058
Strontium-87	Insufficient data	

7

03/13/98

Nitrogen-15 Insufficient data

Adjusted C-14 age in years: 22570.* * = based on Mass Balance

Model (for initial A0)	A0 (initial)	Computed (no decay)	Observed	age (final)
Original Data	33.05	7.75	0.80	18771.
Mass Balance	52.33	12.27	0.80	22570.
Vogel	85.00	19.93	0.80	26580.
Tamers	53.46	12.54	0.80	22747.
Ingerson and Pearson	52.33	12.27	0.80	22570.
Mook	65.91	15.45	0.80	24478.
Fontes and Garnier	52.31	12.27	0.80	22568.
Eichinger	47.57	11.15	0.80	21783.
User-defined	100.00	23.45	0.80	27924.

Data used for Carbon-13

Initial Value: -6.9900 Modeled Final Value: -2.2157

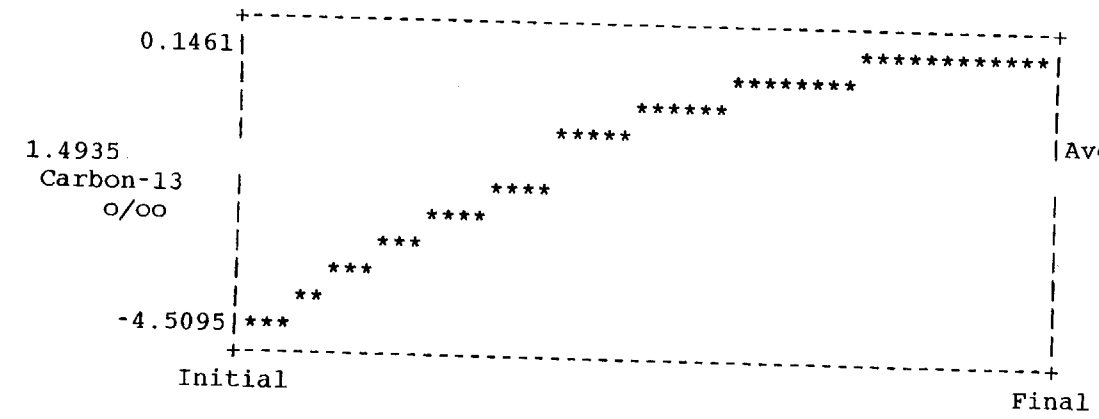
2 dissolving phases:

Phase	Delta C	Isotopic composition (o/oo)
DOLOMITE	7.06000	4.0000
"CH2O"	0.87077	-25.0000

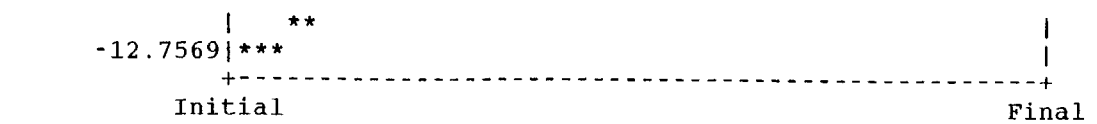
2 precipitating phases:

Phase	Delta C	Fractionation factor	Average Isotopic composition (o/oo)
CALCITE	-5.31723	2.3844	-1.4935
CO2 GAS	-0.04355	-5.9202	-9.7659

Isotopic composition of precipitating CALCITE



Isotopic composition of precipitating CO2 GAS



Data used for C-14 (% mod)

Initial Value: 52.3256 Modeled Final Value: 12.2688

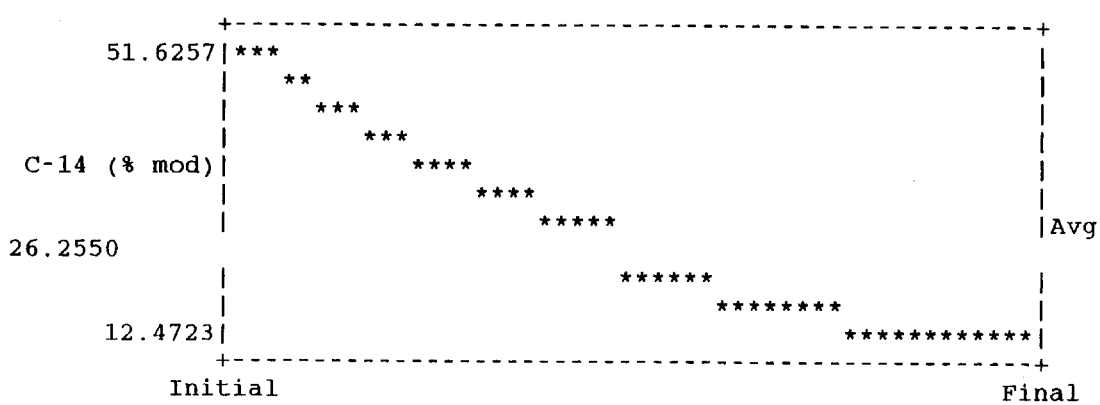
2 dissolving phases:

Phase	Delta C	Isotopic composition (% modern)
DOLOMITE	7.06000	0.0000
"CH2O"	0.87077	0.0000

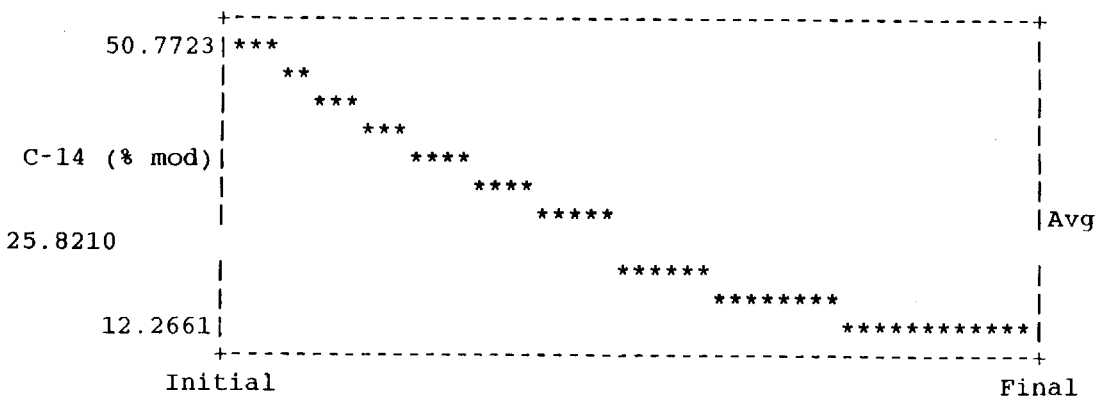
2 precipitating phases:

Phase	Delta C	Fractionation factor	Average Isotopic composition (% modern)
CALCITE	-5.31723	4.7687	26.2550
CO2 GAS	-0.04355	-11.8403	25.8210

Isotopic composition of precipitating CALCITE



Isotopic composition of precipitating CO2 GAS



Data used for Sulfur-34

Initial Value: 9.7300 Modeled Final Value: 15.8130

1 dissolving phases:

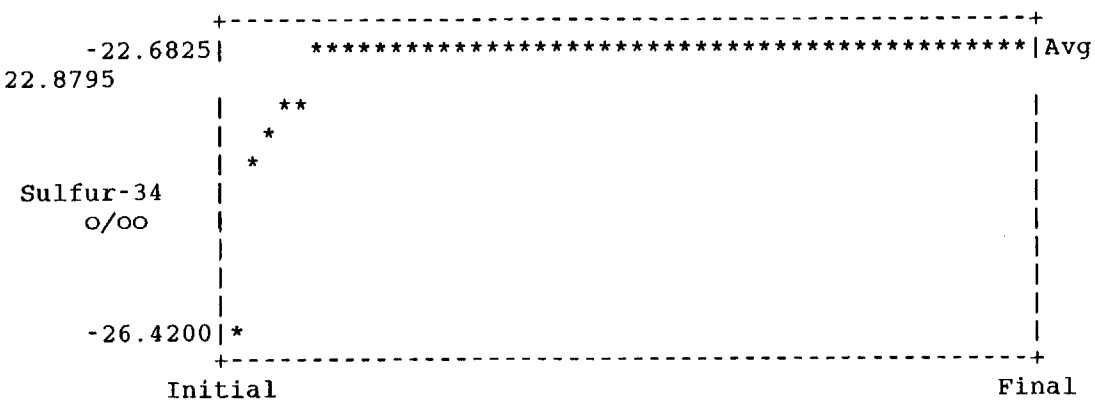
Phase	Delta S	Isotopic composition (o/oo)
ANHYDRIT	20.14723	15.5000

8/4/130

1 precipitating phases:

Phase	Delta S	Fractionation factor	Average Isotopic composition (o/oo)
PYRITE	-0.18823	-37.8958	-22.8795

Isotopic composition of precipitating PYRITE



Data used for Strontium-87
Insufficient data

Data used for Nitrogen-15
Insufficient data

4/8/98.

Refer to Disc 1 at the back for all relevant files of models described below.

Tested various routes down the "Western Route." (passing through VH1/VH2 then down to 16S/49E-05ACC.
- with available well data, this route is not feasible.

Also tested "Southern Route" (from G4/#1, or I-5 to #3 or 16S/49E/05ACC).
- this is an unlikely route due to the precipitation out of NaCl & Dolomite.

Also tested "Eastern Route" (from #1+G4 → J13, J12, 16S/49E-05ACC or 15S/49E-22A1.
- this is a good route until water passes from J12 → two lower wells.

- further testing + the addition of other wells to the Netpath Database is necessary to find how to make it so that does not precipitate out.

- Summaries on following page (attachment) explain the above findings.

April 8, 1998 Project# 20-1402-871

Western Route
Flow from H5→VH1 or VH2→16s/49e-05acc

Constraints: C, S, Ca, Al, Mg, Na, K Cl, Si, Fe
Phases: CO2, Calcite, +Gypsum, +Dolomite, +Mg/Na Exchange, SiO2, +Kspar, Kaolinite, Goethite, +NaCl, -Ca-Mont.

H5→VH1
Everything is ok except Kspar precipitates instead of dissolving.

H5→VH2
Six models are all found to be ok.

VH1→16s/49e-05acc
With the chosen constraints and phases shown on the model, water cannot originate at H5 and travel to VH1. The Netpath models say that gypsum, dolomite, Mg/Na exchange, and NaCl all precipitate. Since the original water is undersaturated in gypsum and dolomite, these would not precipitate out.
If 1) S, Mg, and Fe are removed as constraints; and, 2) dolomite, goethite, Mg/Na exchange, and gypsum are removed as phases, it is not until dolomite and Mg, goethite and Fe, and Mg/Na are added back in the model that Netpath finds any possible models. The resulting models all show NaCl precipitating.

VH2→16s/49e-05acc
Using the same original constraints and phases, gypsum, dolomite, Mg/Na exchange, NaCl, and Kspar all precipitate.

MIXING
H5+VH2→16s/49e-05acc
Using the same phases and constraints, three models resulted. All required that dolomite, Mg/Na exchange, and NaCl precipitate.

H5+VH1→16s/49e-05acc
The two resulting models required that dolomite, Mg/Na exchange, and NaCl precipitate.

Summary:
Given the available well data, it is unlikely that water travels down the western route of Yucca Mountain since, of the forced dissolving phases, at least NaCl would have to precipitate.

Dolomite, Mg/Na exchange

H1→J13
Good.

H1+G4→J13 (mixing)
Good.

J13→J12
Two models: both show a minute amount of Kspar precipitating instead of dissolving.

J12→16s/49e-05acc or 15s/49e-22a1
Both codes show NaCl precipitating. J12-16s/49e-05acc also shows dolomite precipitating.

H5, P1 →J12
G4, P1 →J12
H1, H5 →J12
H1, G4
H1, C2

Dolomite, Mg/Na (-)
"
"

4/6/96 cont.

Direct South Route
Flow from: G4, H1, or H5
to: H3 or 16s/49e-05acc

Constraints: C, S, Ca, Al, Mg, Na, K Cl, Si, Fe
Phases: CO2, Calcite, +Gypsum, +Dolomite, +Mg/Na Exchange, SiO2, +Kspar, Kaolinite, Goethite, +NaCl, -Ca-Mont.

G4→16s/49e-05acc
Using the above constraints and phases, dolomite precipitated in all resulting models. Since dolomite is undersaturated, only dissolution should occur.

G4→H3
Kspar and NaCl precipitate.

H1→16s/49e-05acc
Using the above constraints and phases, dolomite precipitated in all resulting models.

H1→H3
Both Kspar and NaCl precipitated.

H5→H3
Both Kspar and NaCl precipitated.

H5→16s/49e-05acc
Dolomite, Mg/Na exchange, and NaCl precipitate.

Summary:
Given available well data, it is unlikely that water flows in a direct southerly route since phases such as NaCl and dolomite precipitate instead of dissolve.

4/15/98.

- further testing on Eastern Route.
- presently using model file "East Route" ~~(constraints 'ea')~~.
- This contains constraints: C, Ca, Mg, K, Si, S, Al, Na, Cl, Fe.
  phases: CO_2 gas, ~~$CaCO_3$~~ Calcite, +Gypsum, +Dolomite, +Mg/Na Ex., SiO_2, +Kspar, Kaolinite, Goethite, +NaCl, -Ca-Mont.
  (same phases & constraints as on 4/8/98.)

Wells: Initial: C#2, p#1, b#1, J-12, J-13
Final: 15s/49e.22a1.
- 55 models found (file East 1.)

→ replace J13 w/ G4 = 55 models.
→ replace G4 w/ H1 (572-687) = 55 models
→ replace #1 (above) w/ H1 (687-1829) = 55 models
→ by deleting it altogether & leaving 4 initial wells = no good models.
→ add in #5 = 55 models.

→ w/out C#2 = no good models
→ w/ C#2 but w/out p#1 = no good models.
→ w/ p#1 but w/out b#1 = no good models.
→ w/ b#1 but now w/out J12 = 12 poss. models (all have (-) dolomite, Mg/Na Ex.)

MODEL "East c14"

- Using wells: Initial C#2, J-12, b#1, J-13, p#1
  Final: ~~15s/49e-05acc.ao~~
  (or ~~16s/49e-05 22 ao~~
  → 15s/49e-22a1
  or 16s/49e-05acc

- Use same phases, constraints, but add in (C14) as a constraint. - also don't ~~con~~ force dolomite, Mg/Na exchange.

4/15/98. (cont.)

With the addition of C14 as a constraint, 11 models result (files East2, East2b)

4/16/98. Since plausible models (based on chemical reactions) saved in files East2 + East2b all had some negative value for an initial well, they were all rejected.

-By altering the model to use well "15s/49c-22dcc" as the final well one good model results. Since for this model only 3 of the 5 initial wells are used, I deleted the other 2 wells from the list so it is:

Initial: UE-25 c#2
UE-25 J12
UE-25 p#1 (0-1200m)
Final: 15S/49E-22dcc.

} Corrected C-14 age = 13,248.

These results are saved in file East 3.

≈

Returning to West side w/ more well data:
Mixing Beatty well (neco) + VH1 or VH2 (Initial Wells).
to 16s/49e-05acc, 15s/49e-22a1 or 15s/49e-22dcc (Final wells)

* None of these are possible as NaCl precipitates in all of the models.

File is "westmix (neco+vh1)"

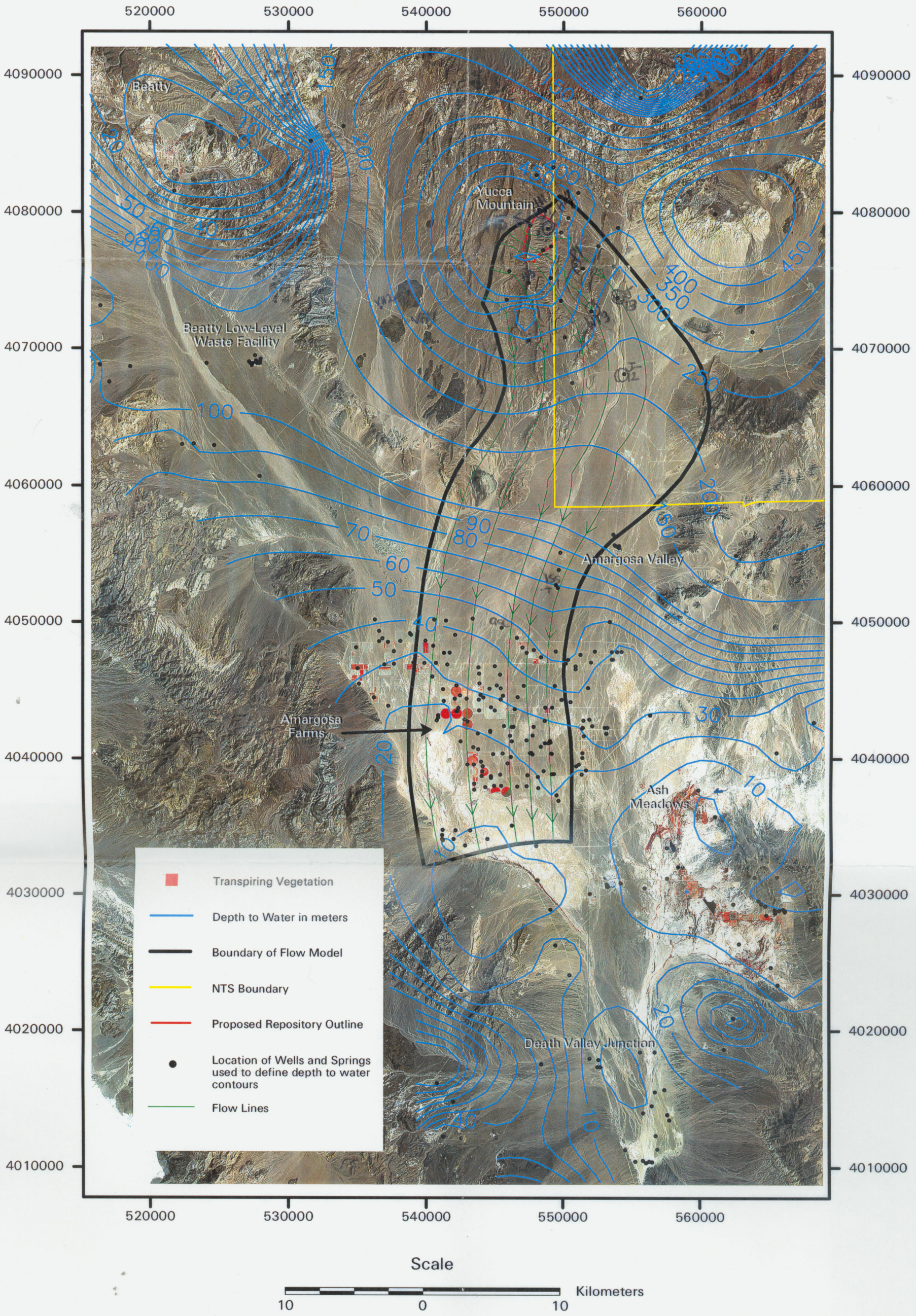
Aerial photograph of Yucca Mtn Nevada.

[redacted] - inside red circle @ top.
H-1
G-4 - little below, right.
J-13
J-12
acc → ~40,50 Depth to water, 3rd flow path

G4 further right northwestern.

Aerial photograph of Yucca Mtn Nevada.

Vegetation Map and Depth to Water: Yucca Mountain Region



4/30/98.

Disk contains:

files: ① west route summary (initial printout of west, south, east routes shown here earlier).

② Excel - Results, Results 2, 3, 4, 5 are the tables used in the final write up.
Results → has all info for these wells.
Results 2 → first draft in final paper
" 3 → 2nd " " " "
" 4 → 3rd " " " "
" 5 → 4th " " " "

③ write up - summary document produced @ end.

④ all data files for NETPATH including info in DB - Netpath Database.

CEN

April 22, 1998

Project #20-1402-871

Radionuclide transport in the Yucca Mountain area using NETPATH 2.0

Background

The Yucca Mountain, Nevada region is the proposed location of a national nuclear waste repository. The area consists of a thick sequence of volcanic rocks of Tertiary age that overlay Paleozoic carbonate rocks and contains three aquifers and two confining layers in the saturated zone. The uppermost volcanic aquifer consists of the densely welded section of the Topopah Spring Tuff of the Paintbrush Group, mainly alluvium and pyroclastic rocks of Miocene age. The confining unit of this aquifer consists of the lowermost part of the Topopah Spring Tuff, the Calico Hills Formation, and the uppermost part of the Crater Flat Group. The lower volcanic aquifer consists of most of the Crater Flat Group. Its confining unit consists of the Lithic Ridge Tuff and older tuffs, flows, and lavas. The carbonate aquifer consists of a thick sequence of Paleozoic carbonate rocks that may be confined locally by an overlying clastic unit, the Eleana Formation of Mississippian and Late Devonian age (Luckey et al, 1996).

This study attempts to determine possible groundwater flowpaths from the proposed Yucca Mountain repository using computer modeling of well data. NETPATH 2.0 is a modeling program that determines geochemical mass balance reactions between selected waters so as to assess various possible flowpaths. From the resultant models an adjusted C-14 age of the final water can be determined.

CEN

Description of NETPATH 2.0

NETPATH is a Fortran 77 computer program used to interpret net geochemical mass-balance reactions between an initial water and a final water along a hydrologic flow path. NETPATH allows up to five initial waters to be employed in each model; and, it will calculate the mixing proportions of the initial waters and the net geochemical reactions that can account for the observed composition of the final water. NETPATH uses previously defined chemical and isotopic data for a hydrochemical system that has been entered into DB, the NETPATH database. For a set of mineral and (or) gas phases believed to be the reactive phases in the system, NETPATH calculates the mass transfers in every possible combination of the selected phases that accounts for the observed changes in the selected chemical and (or) isotopic compositions observed along the flow path. The net geochemical mass-balance reaction model consists of the masses (per kilogram of water) of minerals and gases that must enter or leave the initial water(s) along the flow path to produce the composition of a selected set of chemical and isotopic observations in the final water. NETPATH can also calculate radiocarbon dating using Rayleigh distillation calculations applied to the mass balance models (Plummer, Prestemon, and Parkhurst, 1994).

CEN

CEN

Well data

The following wells were used in various flow paths down Yucca Mountain.

Table 1a. Location of wells.

Site Name	UTM-x	UTM-y	Lat DD	Lat DMS	Long DD	Long DMS	Site Elev.
	meters	meters					meters
16S/49E-05acc	546664.5	4049439	36.591	363528	116.478	1162842	746
15S/49E-22dcc	549672.5	4053523	36.628	363740	116.444	1162638	784
15S/49E-22a1	550086.3	4054974	36.641	363827	116.440	1162623	796
UE-25 J-12	554435.8	4068767	36.765	364554	116.390	1162324	953
UE-25 J-13	554004.4	4073550	36.808	364829	116.395	1162341	1011
UE-25 p#1 (0-1200 m)	551508.7	4075663	36.827	364938	116.422	1162521	1114
USW H-3	547537.0	4075762	36.828	364942	116.467	1162801	1483
USW VH-1	539986.2	4071718	36.792	364732	116.552	1163307	963
USW VH-2	537737.6	4073222	36.806	364821	116.577	1163437	974
USW H-1 (572-687 m)	548721.8	4079944	36.866	365158	116.453	1162712	1303
USW H-1 (687-1829 m)	548721.8	4079944	36.866	365158	116.453	1162712	1303
USW G-4	548938.0	4078590	36.854	365114	116.451	1162704	1270
UE-25 c#2	550944.0	4075867	36.829	364945	116.429	1162543	1132
USW H-4	549195.0	4077322	36.842	365032	116.448	1162654	1249
UE-25 b#1 (0-1220 m)	549954.5	4078422	36.852	365108	116.440	1162623	1201
USW H-5	547665.5	4078838	36.856	365122	116.465	1162755	1477
NECO #1 13S/47E-35b				364600		1164130	850

CEN

CEN

Table 1b. Well properties.

Site Name	Well Depth	WT Depth	Aquifer	Temp	pH	Charge
	meters	meters		oC		Balance
16S/49E-05acc	87	21	Qal		7.8	4.5
15S/49E-22dcc	148	78	Qtal	29.5	7.8	0.8
15S/49E-22a1	174	90	Qal	27.8	8.0	-0.9
UE-25 J-12	347	226	Tv	26.2	7.6	-0.9
UE-25 J-13	1063	283	Tpt	30.5	7.3	-0.3
UE-25 p#1 (0-1200 m)	1805	382	Tcp	57.0	6.7	-3.0
USW H-3	1219	751	Tct	26.5	9.0	-2.7
USW VH-1	762	184	Tcb	35.4	7.6	0.8
USW VH-2	1219	164	Tv	32.8	7.1	-1.3
USW H-1 (572-687 m)	1829	572	Tcp	33.0	7.7	-1.8
USW H-1 (687-1829 m)	1829	572	Tcb	34.7	7.5	1.4
USW G-4	915	541	Tct	35.6	7.7	3.7
UE-25 c#2	914	401	Tcb	40.5	7.9	-3.0
USW H-4	1219	519	Tcb/Tct	34.8	7.4	3.8
UE-25 b#1 (0-1220 m)	1220	470	Th/Tct	36.0	7.5	-0.9
USW H-5	1219	704	Tcb/Tct	35.9	7.9	2.7
NECO #1 13S/47E-35b	175	86	QTal	27.5	7.6	

CEN

Table 1c. Major ion concentrations.

Site Name	Ca	Mg	Na	K	Cl	SO_4	HCO_3	SiO_2	TDS calc
	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
16S/49E-05acc	29	2	35	5.2	6.0	26	135	62	235
15S/49E-22dcc	28	2.1	41	4.8	7.6	33	148	49	240
15S/49E-22a1	25	2.4	41	5.2	8.0	33	145	52	243
UE-25 J-12	14	2.4	42	5.0	12	21	118	48	206
UE-25 J-13	13	2.1	44	5.0	7.2	20	124	55	215
UE-25 p#1 (0-1200 m)	94	31	150	12	26	78	753	44	811
USW H-3	0.80	0.02	120	1.1	5.5	31	274	43	342
USW VH-1	10	1.5	76	1.9	10	43	160	50	274
USW VH-2	79	30	71	8.1	16	143	392	26	566
USW H-1 (572-687 m)	4.5	0.00	51	2.4	5.7	18	122	47	190
USW H-1 (687-1829 m)	6.2	0.00	51	1.6	5.8	19	115	40	181
USW G-4	13	0.20	57	2.1	5.9	19	139	45	213
UE-25 c#2	12	0.35	54	2.1	7.1	22	143	54	226
USW H-4	17	0.29	73	2.6	6.9	26	173	46	262
UE-25 b#1 (0-1220 m)	17	0.59	46	3.5	8.5	22	134	52	221
USW H-5	2.0	0.01	60	2.1	6.4	16	124	48	197
NECO #1 13S/47E-35b	55	14	170	10	79	190	328	70	792

Table 1d. Isotope data.

Site Name	δ^2H	$\delta^{18}O$	$\delta^{13}C$	^{14}C	U	$^{234}U/^{238}U$	Sr	$^{87}Sr/^{86}Sr$	$\delta^{87}Sr$
	permil	permil	permil	PMC	ug/L		mg/L		permil
16S/49E-05acc	-103.0	-13.20	-7.10	19.3					
15S/49E-22dcc	-102.0	-12.80	-10.20	15 .6					
15S/49E-22a1									
UE-25 J-12	-96.8	-12.88	-7.90	32.2	0.30	5.5		0.71151	3.3
UE-25 J-13	-96.8	-13.00	-7.30	29.2	0.56	6.7	0.0409	0.71145	3.2
UE-25 p#1 (0-1200 m)	-107.0	-13.80							
USW H-3	-101.0	-13.90	-4.90	10.5					
USW VH-1	-106.5	-14.10	-7.75	10.8	3.4	5.5		0.71079	2.5
USW VH-2					3.0	3.1		0.71300	5.4
USW H-1 (572-687 m)	-103.0	-13.40		19.8					
USW H-1 (687-1829 m)	-101.0	-13.50	-11.40	22.4					
USW G-4	-103.0	-13.80	-9.10	22.0					
UE-25 c#2	-101.0	-13.40	-7.00	15.3					
USW H-4	-104.0	-14.00	-7.40	11.8					
UE-25 b#1 (0-1220 m)	-101.0	-13.40	-10.40	16.7					
USW H-5	-101.5	-13.60	-10.30	19.8					
NECO #1 13S/47E-35b									

Using NETPATH

In running the code in NETPATH, specific constraints and phases were chosen to limit the amount of resultant models calculated by NETPATH, and to reflect expected chemical reactions along the chosen flow paths. As a result, models were more closely related to the characteristics of the Yucca Mountain region.

Constraints

Constraints were included in the code to constrain the masses of selected phases (minerals and gases) that could enter or leave the aqueous solution. Chosen constraints for the codes run here included: carbon, sulfur, calcium, aluminum, magnesium, sodium, potassium, chloride, silicon, and iron. After finding models with plausible chemical mass balance reactions, C-14 (pmc) was added as a constraint to the code.

#1) mixing with VH1 or VH2, NaCl still precipitated in all resulting models, yielding no possible flowpaths. An example of the NETPATH results from the western route can be found in Appendix A.

It has also been proposed that water could flow due south. Given NETPATH results, this path is unlikely since all of the resulting NETPATH models precipitated out dolomite, and several also precipitated out NaCl and K-spar. Since dolomite is undersaturated in all of the initial and final wells used in the southern route, it should not precipitate. Results from the southern route can be found in Appendix B.

The eastern route was originally calculated using only one initial well, with various wells being tested. NETPATH was not able to compute models that stayed within the forcing constraints assigned to the phases. Thus, in East (a), mixing was incorporated into the model and NETPATH calculated 55 models of mass balance reactions yielding the final water chemistry for 16S/49E-05acc. Since NETPATH reports all possible models, even if they ignore forcing constraints, only a percentage of the 55 models were actually plausible. Some of the reasons not all 55 models were plausible in this environment include ignored constraints on forced phases and negative amounts of initial waters. Upon adding C-14 as a constraint, none of the resultant models were possible. In fact, in some models, water in the final well was found to be younger than the initial waters (shown in NETPATH by a negative age). That the selected final water is younger than the selected initial water is unlikely since the groundwater is expected to flow from Yucca Mountain to the valley below, and not in the reverse direction.

In East (b), the final well was changed to 15S/49E-22dcc, which actually appeared to be closer to the flowpaths on aerial photographs than 16S/49E-05acc. This well was also chosen since isotopic data was available, which was not the case for many wells. NETPATH was able to generate one mass balance model that did not ignore forcing constraints, even with C-14 added in as a constraint. Using this model, NETPATH calculated an adjusted C-14 age of 13,248 years for the final water. The C-14 age of the final water represents the travel time between the initial and the final wells. The unadjusted C-14 age is 15,400 years[2]. It should be noted that the plausible flowpaths concluded from the geochemical mass balancing done by NETPATH modeling support the flowpaths currently used in the Total Performance Assessment. NETPATH results from the eastern route can be found in Appendix C.

Future work

While these results may appear fairly conclusive, it is important to remember that by acquiring more data, results can be more soundly supported. In this study, only a few wells were able to be final wells due to the lack of isotope data. Therefore, more water sampling analysis of wells would be helpful in deriving more plausible flowpaths than just the one computed here.

[2]Unadjusted age = (-8270) * ln(pmc/100). The pmc for this well is 15.6.

these got misplaced. p.21 should be before p.20

Phases

NETPATH allows users to determine whether particular phases should precipitate, dissolve, or both. Due to the subsurface geology and chemistry of the waters in the flow paths, we chose to force some phases to only dissolve, or only precipitate. Others were allowed to do either. NETPATH checks 455 models (combinations of plausible phases) that can satisfy the mass balance equations. From that, it returns all possible models, including those that ignore dissolution or precipitation forcing. Models that ignored these added constraints were not considered as possible models for this study.

Phases chosen for the code included: NaCl (d), K-feldspar (d), gypsum (d), Ca-mont (p), calcite, kaolinite, SiO_2, goethite, dolomite, Mg/Na exchange, and CO_2 gas. Due to the high solubility of NaCl, it is unlikely that it would precipitate out of the water along the selected flowpaths. For this reason, NETPATH is forced to produce models with NaCl dissolving. However, as noted above, NETPATH will also show models that are plausible if forcing constraints are ignored.

Possible flowpaths

Several routes down Yucca Mountain were selected as possible groundwater flowpaths.

1. West route:
   a) USW H-5 ⇒USW VH-1 **or** USW VH-2⇒16S/49E-05acc

   b) NECO Well #1 13S/47E-35b + USW VH1 **or** USW VH2 (mixing)⇒16S/49E-05acc **or** 15S/49E-22a1 **or** 15S/49E-22dcc

2. Southern route:
   USW G-4 **or** USW H-1 (572-687m) **or** USW H-5 ⇒USW H-3 **or** 16S/49E-05acc

3. East route:
   a) UE-25 c#2 + UE-25 J-12 + UE-25 p#1 + UE-25 J-13 + UE-25 b#1 (mixing)⇒16S/49E-05acc

   b) UE-25 c#2 + UE-25 J-12 + UE-25 p#1 (0-1200m) (mixing)⇒15S/49E-22dcc

Results

Given the available well data[1], it is unlikely that groundwater travels down the western route (a) of Yucca Mountain. Of the forced dissolving phases, at least NaCl precipitates, and depending on which of the above wells are chosen, and whether mixing is invoked, K-feldspar precipitates also. As mentioned above, the high solubility of NaCl makes it unlikely that it would precipitate out of the water. The precipitation of K-spar is contrary to the observed mineralogy; therefore, models that include K-spar precipitating were discarded. On the western route (b), with the Beatty well (NECO

[1] It should be noted that due to limited well data, possible paths may not have been found by NETPATH.

References Cited

Luckey, R.R., Tucci, P., Faunt, C.C., Ervin, E.M., Steinkampf, W.C., D'Agnese, F.A., and Patterson, G.L., 1996, Status of understanding of the saturated-zone ground-water flow system at Yucca Mountain, Nevada as of 1995:U.S. Geological Society Water-Resources Investigations Report 96-XXXX, 77p.

Plummer, L.N., Prestemon, E.C., and Parkhurst, D.L., 1994, An interactive code (NETPATH) for modeling NET geochemical reactions along a flow PATH Version 2.0: U.S. Geological Survey Water-Resources Investigations Report 94-4169, 130p.

West Route.

Initial Well : USW H-5
Final Well : USW VH-1

	Final	Initial
C	2.6231	2.0327
S	0.4478	0.1666
CA	0.2496	0.0499
AL	0.0000	0.0000
MG	0.0617	0.0004
NA	3.3070	2.6105
K	0.0486	0.0537
CL	0.2822	0.1806
SI	0.8325	0.7991
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			

11 models checked
3 models found
(Ignoring 1 dissolution/precipitation constraints)

MODEL 1			
CO2 GAS		0.31316	
CALCITE		-0.44025	
GYPSUM	+	0.28119	
DOLOMITE	+	0.35874	
Mg/Na EX	+	0.29743	
SiO2		0.04359	
K-SPAR	+	-0.00511	(Constraint ignored)
KAOLINIT		0.00255	
GOETHITE		0.00000	
NaCl	+	0.10159	

MODEL 2			
CO2 GAS		-0.12709	
GYPSUM	+	0.28119	
DOLOMITE	+	0.35874	
Mg/Na EX	+	0.29743	
SiO2		3.57613	
K-SPAR	+	-0.00511	(Constraint ignored)
KAOLINIT		3.07376	
GOETHITE		0.00000	
NaCl	+	0.10159	
Ca-MONT	-	-2.63623	

CAV

MODEL 3			
CALCITE		-0.12709	
GYPSUM	+	0.28119	
DOLOMITE	+	0.35874	
Mg/Na EX	+	0.29743	
SiO2		2.55637	
K-SPAR	+	-0.00511	(Constraint ignored)
KAOLINIT		2.18717	
GOETHITE		0.00000	
NaCl	+	0.10159	
Ca-MONT	-	-1.87521	

CAV

Initial Well : USW H-5
Final Well : USW VH-2

	Final	Initial
C	6.4293	2.0327
S	1.4898	0.1666
CA	1.9726	0.0499
AL	0.0000	0.0000
MG	1.2349	0.0004
NA	3.0907	2.6105
K	0.2073	0.0537
CL	0.4517	0.1806
SI	0.4331	0.7991
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			

11 models checked
6 models found

MODEL 1

CO2 GAS		2.45807
CALCITE		-0.73954
GYPSUM	+	1.32317
DOLOMITE	+	1.33903
Mg/Na EX	+	0.10454
SiO2		-0.67321
K-SPAR	+	0.15359
KAOLINIT		-0.07680
GOETHITE		0.00000
NaCl	+	0.27108

MODEL 2

CO2 GAS		2.37417
CALCITE		-0.65564
GYPSUM	+	1.32317
DOLOMITE	+	1.33903
Mg/Na EX	+	0.10454
SiO2		0.00000
K-SPAR	+	0.15359
KAOLINIT		0.50850
NaCl	+	0.27108
Ca-MONT	-	-0.50240

MODEL 3

CO2 GAS		2.44706
CALCITE		-0.72853
GYPSUM	+	1.32317
DOLOMITE	+	1.33903
Mg/Na EX	+	0.10454
SiO2		-0.58488
K-SPAR	+	0.15359
GOETHITE		0.00000
NaCl	+	0.27108
Ca-MONT	-	-0.06592

MODEL 4

CO2 GAS		2.37417
CALCITE		-0.65564
GYPSUM	+	1.32317
DOLOMITE	+	1.33903
Mg/Na EX	+	0.10454
K-SPAR	+	0.15359
KAOLINIT		0.50850
GOETHITE		0.00000
NaCl	+	0.27108
Ca-MONT	-	-0.50240

MODEL 5

CO2 GAS		1.71853
GYPSUM	+	1.32317
DOLOMITE	+	1.33903
Mg/Na EX	+	0.10454
SiO2		5.26082
K-SPAR	+	0.15359
KAOLINIT		5.08227
GOETHITE		0.00000
NaCl	+	0.27108
Ca-MONT	-	-4.42838

MODEL 6

CALCITE		1.71853
GYPSUM	+	1.32317
DOLOMITE	+	1.33903
Mg/Na EX	+	0.10454
SiO2		19.05023
K-SPAR	+	0.15359
KAOLINIT		17.07082
GOETHITE		0.00000
NaCl	+	0.27108
Ca-MONT	-	-14.71898

Initial Well : USW VH-1
Final Well : 16S/49E-05acc

	Final	Initial
C	2.2132	2.6231
S	0.2707	0.4478
CA	0.7238	0.2496
AL	0.0000	0.0000
MG	0.0823	0.0617
NA	1.5229	3.3070
K	0.1330	0.0486
CL	0.1693	0.2822
SI	1.0322	0.8325
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			

11 models checked
2 models found
(Ignoring 4 dissolution/precipitation constraints)

MODEL 1

CO2 GAS		-0.24616	
CALCITE		1.46628	
GYPSUM	+	-0.17705	(Constraint ignored)
DOLOMITE	+	-0.81505	(Constraint ignored)
Mg/Na EX	+	-0.83562	(Constraint ignored)
SiO2		0.03089	
K-SPAR	+	0.08442	
KAOLINIT		-0.04221	
GOETHITE		0.00000	
NaCl	+	-0.11287	(Constraint ignored)

MODEL 2

CO2 GAS		-0.25221	
CALCITE		1.47233	
GYPSUM	+	-0.17705	(Constraint ignored)
DOLOMITE	+	-0.81505	(Constraint ignored)
Mg/Na EX	+	-0.83562	(Constraint ignored)
SiO2		0.07944	
K-SPAR	+	0.08442	
GOETHITE		0.00000	
NaCl	+	-0.11287	(Constraint ignored)
Ca-MONT	-	-0.03623	

Initial Well : USW VH-2
Final Well : 16S/49E-05acc

	Final	Initial
C	2.2132	6.4293
S	0.2707	1.4898
CA	0.7238	1.9726
AL	0.0000	0.0000
MG	0.0823	1.2349
NA	1.5229	3.0907
K	0.1330	0.2073
CL	0.1693	0.4517
SI	1.0322	0.4331
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			

11 models checked
1 model found
(Ignoring 5 dissolution/precipitation constraints)

MODEL 1

CO2 GAS		-2.39107	
CALCITE		1.76557	
GYPSUM	+	-1.21903	(Constraint ignored)
DOLOMITE	+	-1.79534	(Constraint ignored)
Mg/Na EX	+	-0.64273	(Constraint ignored)
SiO2		0.74769	
K-SPAR	+	-0.07428	(Constraint ignored)
KAOLINIT		0.03714	
GOETHITE		0.00000	
NaCl	+	-0.28236	(Constraint ignored)

Appendix B - Southern Route

Initial Well : USW G-4
Final Well : 16S/49E-05acc

	Final	Initial
C	2.2132	2.2787
S	0.2707	0.1979
CA	0.7238	0.3244
AL	0.0000	0.0000
MG	0.0823	0.0082
NA	1.5229	2.4801
K	0.1330	0.0537
CL	0.1693	0.1665
SI	1.0322	0.7492
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					

11 models checked
4 models found
(Ignoring 1 dissolution/precipitation constraints)

MODEL 1

CO2 GAS		0.01398	
CALCITE		0.73239	
GYPSUM	+	0.07289	
SiO2		0.12441	
K-SPAR	+	0.07931	
KAOLINIT		-0.03966	
GOETHITE		0.00000	
NaCl	+	0.00283	
DOLOMITE	+	-0.40595	(Constraint ignored)
Mg/Na EX		-0.48001	

MODEL 2

CO2 GAS		0.00830	
CALCITE		0.73807	
GYPSUM	+	0.07289	
SiO2		0.17002	
K-SPAR	+	0.07931	
KAOLINIT		0.00000	
NaCl	+	0.00283	
Ca-MONT	-	-0.03404	
DOLOMITE	+	-0.40595	(Constraint ignored)
Mg/Na EX		-0.48001	

```
                MODEL   3
CO2 GAS                      0.00830
CALCITE                      0.73807
GYPSUM          +            0.07289
SiO2                         0.17002
K-SPAR          +            0.07931
GOETHITE                     0.00000
NaCl            +            0.00283
Ca-MONT         -           -0.03404
DOLOMITE        +           -0.40595    (Constraint ignored)
Mg/Na EX                    -0.48001

                MODEL   4
CALCITE                      0.74637
GYPSUM          +            0.07289
SiO2                         0.23658
K-SPAR          +            0.07931
KAOLINIT                     0.05787
GOETHITE                     0.00000
NaCl            +            0.00283
Ca-MONT         -           -0.08371
DOLOMITE        +           -0.40595    (Constraint ignored)
Mg/Na EX                    -0.48001
```

```
Initial Well : USW H-1 (572-687m)
Final Well   : 16S/49E-05acc

          Final      Initial
C        2.2132       1.9999
S        0.2707       0.1874
CA       0.7238       0.1123
AL       0.0000       0.0000
MG       0.0823       0.0000
NA       1.5229       2.2189
K        0.1330       0.0614
CL       0.1693       0.1608
SI       1.0322       0.7824
FE       0.0000       0.0000

CO2 GAS   C    1.0000 RS   4.0000 I1 -25.0000 I2 100.0000
CALCITE   CA   1.0000 C    1.0000 RS   4.0000 I1   0.0000 I2   0.0000
GYPSUM    CA   1.0000 S    1.0000 RS   6.0000 I3  22.0000
SiO2      SI   1.0000
K-SPAR    K    1.0000 AL   1.0000 SI   3.0000
KAOLINIT  AL   2.0000 SI   2.0000
GOETHITE  FE   1.0000 RS   3.0000
NaCl      NA   1.0000 CL   1.0000
Ca-MONT   CA   0.1670 AL   2.3300 SI   3.6700
DOLOMITE  CA   1.0000 MG   1.0000 C    2.0000 RS   8.0000 I1   0.0000
          I2   0.0000
Mg/Na EX  NA   2.0000 MG  -1.0000

                11 models checked
                 3 models found
        (Ignoring  1 dissolution/precipitation constraints)
```

```
                MODEL   1
CO2 GAS                     -0.04496
CALCITE                      0.79814
GYPSUM          +            0.08331
SiO2                         0.10648
K-SPAR          +            0.07164
KAOLINIT                    -0.03582
GOETHITE                     0.00000
NaCl            +            0.00847
DOLOMITE        +           -0.26997    (Constraint ignored)
Mg/Na EX                    -0.35226

                MODEL   2
CO2 GAS                     -0.05010
CALCITE                      0.80327
GYPSUM          +            0.08331
SiO2                         0.14768
K-SPAR          +            0.07164
KAOLINIT                     0.00000
NaCl            +            0.00847
Ca-MONT         -           -0.03075
DOLOMITE        +           -0.26997    (Constraint ignored)
Mg/Na EX                    -0.35226
```

		MODEL 3	
CO2 GAS		-0.05010	
CALCITE		0.80327	
GYPSUM	+	0.08331	
SiO2		0.14768	
K-SPAR	+	0.07164	
GOETHITE		0.00000	
NaCl	+	0.00847	
Ca-MONT	-	-0.03075	
DOLOMITE	+	-0.26997	(Constraint ignored)
Mg/Na EX		-0.35226	

GW

Initial Well : USW H-5
Final Well : USW H-3

	Final	Initial
C	4.4927	2.0327
S	0.3229	0.1666
CA	0.0200	0.0499
AL	0.0000	0.0000
MG	0.0008	0.0004
NA	5.2222	2.6105
K	0.0281	0.0537
CL	0.1552	0.1806
SI	0.7160	0.7991
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000 I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000
SiO2	SI	1.0000						
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000		
KAOLINIT	AL	2.0000	SI	2.0000				
GOETHITE	FE	1.0000	RS	3.0000				
NaCl	NA	1.0000	CL	1.0000				
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700		
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000 I1 0.0000
	I2	0.0000						
Mg/Na EX	NA	2.0000	MG	-1.0000				

11 models checked
4 models found
(Ignoring 2 dissolution/precipitation constraints)

GW

		MODEL 1	
CO2 GAS		1.32721	
CALCITE		-1.50512	
GYPSUM	+	0.15626	
SiO2		-0.03192	
K-SPAR	+	-0.02558	(Constraint ignored)
KAOLINIT		0.01279	
GOETHITE		0.00000	
NaCl	+	-0.02536	(Constraint ignored)
DOLOMITE	+	1.31892	
Mg/Na EX		1.31851	

		MODEL 2	
CO2 GAS		1.32323	
CALCITE		-1.50114	
GYPSUM	+	0.15626	
K-SPAR	+	-0.02558	(Constraint ignored)
KAOLINIT		0.04054	
GOETHITE		0.00000	
NaCl	+	-0.02536	(Constraint ignored)
Ca-MONT	-	-0.02382	
DOLOMITE	+	1.31892	
Mg/Na EX		1.31851	

GW

```
                MODEL    3
CO2 GAS                    -0.17791
GYPSUM          +           0.15626
SiO2                       12.04509
K-SPAR          +          -0.02558    (Constraint ignored)
KAOLINIT                   10.51258
GOETHITE                    0.00000
NaCl            +          -0.02536    (Constraint ignored)
Ca-MONT         -          -9.01269
DOLOMITE        +           1.31892
Mg/Na EX                    1.31851

                MODEL    4
CALCITE                    -0.17791
GYPSUM          +           0.15626
SiO2                       10.61755
K-SPAR          +          -0.02558    (Constraint ignored)
KAOLINIT                    9.27147
GOETHITE                    0.00000
NaCl            +          -0.02536    (Constraint ignored)
Ca-MONT         -          -7.94737
DOLOMITE        +           1.31892
Mg/Na EX                    1.31851
```



```
Initial Well : USW H-1 (572-687m)
Final Well   : USW H-3

             Final      Initial
C           4.4927      1.9999
S           0.3229      0.1874
CA          0.0200      0.1123
AL          0.0000      0.0000
MG          0.0008      0.0000
NA          5.2222      2.2189
K           0.0281      0.0614
CL          0.1552      0.1608
SI          0.7160      0.7824
FE          0.0000      0.0000

CO2 GAS   C    1.0000 RS   4.0000 I1 -25.0000 I2 100.0000
CALCITE   CA   1.0000 C    1.0000 RS   4.0000 I1   0.0000 I2   0.0000
GYPSUM    CA   1.0000 S    1.0000 RS   6.0000 I3  22.0000
SiO2      SI   1.0000
K-SPAR    K    1.0000 AL   1.0000 SI   3.0000
KAOLINIT  AL   2.0000 SI   2.0000
GOETHITE  FE   1.0000 RS   3.0000
NaCl      NA   1.0000 CL   1.0000
Ca-MONT   CA   0.1670 AL   2.3300 SI   3.6700
DOLOMITE  CA   1.0000 MG   1.0000 C    2.0000 RS   8.0000 I1   0.0000
          I2   0.0000
Mg/Na EX  NA   2.0000 MG  -1.0000

          11 models checked
           3 models found
(Ignoring  2 dissolution/precipitation constraints)

                MODEL    1
CO2 GAS                     1.21525
CALCITE                    -1.73302
GYPSUM          +           0.13543
SiO2                        0.00008
K-SPAR          +          -0.03325    (Constraint ignored)
KAOLINIT                    0.01663
GOETHITE                    0.00000
NaCl            +          -0.00561    (Constraint ignored)
DOLOMITE        +           1.50526
Mg/Na EX                    1.50444

                MODEL    2
CO2 GAS                    -0.51777
GYPSUM          +           0.13543
SiO2                       13.90571
K-SPAR          +          -0.03325    (Constraint ignored)
KAOLINIT                   12.10622
GOETHITE                    0.00000
NaCl            +          -0.00561    (Constraint ignored)
Ca-MONT         -          -10.37734
DOLOMITE        +           1.50526
Mg/Na EX                    1.50444
```

		MODEL 3	
CALCITE		-0.51777	
GYPSUM	+	0.13543	
SiO2		9.75115	
K-SPAR	+	-0.03325	(Constraint ignored)
KAOLINIT		8.49423	
GOETHITE		0.00000	
NaCl	+	-0.00561	(Constraint ignored)
Ca-MONT	-	-7.27692	
DOLOMITE	+	1.50526	
Mg/Na EX		1.50444	

Initial Well : USW G-4
Final Well : USW H-3

	Final	Initial
C	4.4927	2.2787
S	0.3229	0.1979
CA	0.0200	0.3244
AL	0.0000	0.0000
MG	0.0008	0.0082
NA	5.2222	2.4801
K	0.0281	0.0537
CL	0.1552	0.1665
SI	0.7160	0.7492
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000		
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2	0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000		
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1	0.0000
	I2	0.0000								
Mg/Na EX	NA	2.0000	MG	-1.0000						
SiO2	SI	1.0000								
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000				
KAOLINIT	AL	2.0000	SI	2.0000						
GOETHITE	FE	1.0000	RS	3.0000						
NaCl	NA	1.0000	CL	1.0000						
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700				

11 models checked
3 models found
(Ignoring 2 dissolution/precipitation constraints)

		MODEL 1	
CO2 GAS		1.27419	
CALCITE		-1.79876	
GYPSUM	+	0.12501	
DOLOMITE	+	1.36928	
Mg/Na EX	+	1.37669	
SiO2		0.01801	
K-SPAR	+	-0.02558	(Constraint ignored)
KAOLINIT		0.01279	
GOETHITE		0.00000	
NaCl	+	-0.01125	(Constraint ignored)

		MODEL 2	
CO2 GAS		-0.52457	
GYPSUM	+	0.12501	
DOLOMITE	+	1.36928	
Mg/Na EX	+	1.37669	
SiO2		14.45117	
K-SPAR	+	-0.02558	(Constraint ignored)
KAOLINIT		12.56103	
GOETHITE		0.00000	
NaCl	+	-0.01125	(Constraint ignored)
Ca-MONT	-	-10.77102	

		MODEL 3	
CALCITE		-0.52457	
GYPSUM	+	0.12501	
DOLOMITE	+	1.36928	
Mg/Na EX	+	1.37669	
SiO2		10.24205	
K-SPAR	+	-0.02558	(Constraint ignored)
KAOLINIT		8.90160	
GOETHITE		0.00000	
NaCl	+	-0.01125	(Constraint ignored)
Ca-MONT	-	-7.62988	

GW

Initial Well : USW H-5
Final Well : 16S/49E-05acc

	Final	Initial
C	2.2132	2.0327
S	0.2707	0.1666
CA	0.7238	0.0499
AL	0.0000	0.0000
MG	0.0823	0.0004
NA	1.5229	2.6105
K	0.1330	0.0537
CL	0.1693	0.1806
SI	1.0322	0.7991
FE	0.0000	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			

11 models checked
3 models found
(Ignoring 3 dissolution/precipitation constraints)

		MODEL 1	
CO2 GAS		0.06700	
CALCITE		1.02603	
GYPSUM	+	0.10414	
DOLOMITE	+	-0.45631	(Constraint ignored)
Mg/Na EX	+	-0.53819	(Constraint ignored)
SiO2		0.07448	
K-SPAR	+	0.07931	
KAOLINIT		-0.03966	
GOETHITE		0.00000	
NaCl	+	-0.01128	(Constraint ignored)

		MODEL 2	
CO2 GAS		0.06132	
CALCITE		1.03171	
GYPSUM	+	0.10414	
DOLOMITE	+	-0.45631	(Constraint ignored)
Mg/Na EX	+	-0.53819	(Constraint ignored)
SiO2		0.12009	
K-SPAR	+	0.07931	
GOETHITE		0.00000	
NaCl	+	-0.01128	(Constraint ignored)
Ca-MONT	-	-0.03404	

		MODEL 3	
CALCITE		1.09303	
GYPSUM	+	0.10414	
DOLOMITE	+	-0.45631	(Constraint ignored)
Mg/Na EX	+	-0.53819	(Constraint ignored)
SiO2		0.61208	
K-SPAR	+	0.07931	
KAOLINIT		0.42774	
GOETHITE		0.00000	
NaCl	+	-0.01128	(Constraint ignored)
Ca-MONT	-	-0.40120	

Appendix C - East Route

East 3
w/carbon 14
good!

Initial Well 1 : UE-25 c#2
Initial Well 2 : UE-25 J-12
Initial Well 3 : UE-25 p#1 (0-1200m)
Final well : 15S/49E-22dcc

	Final	Initial 1	Initial 2	Initial 3
C	2.4181	2.3361	1.9344	12.3555
S	0.3436	0.2291	0.2187	0.8129
CA	0.6863	0.2995	0.3494	2.3481
AL	0.0000	0.0000	0.0000	0.0000
MG	0.0844	0.0165	0.0987	1.2766
NA	1.7840	2.3496	1.8274	6.5324
K	0.1215	0.0537	0.1279	0.3073
CL	0.2144	0.1989	0.3358	0.7342
SI	0.8158	0.8824	0.7991	0.7332
FE	0.0000	0.0000	0.0000	0.0000
I2	37.7225	35.7423	62.2877	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000	
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000	
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1 0.0000
	I2	0.0000							
Mg/Na EX	NA	2.0000	MG	-1.0000					
SiO2	SI	1.0000							
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000			
KAOLINIT	AL	2.0000	SI	2.0000					
GOETHITE	FE	1.0000	RS	3.0000					
NaCl	NA	1.0000	CL	1.0000					
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700			

11 models checked
1 model found

	MODEL 1
Init 1	+ F 0.91024
Init 2	+ F 0.08161
Init 3	+ F 0.00815
CO2 GAS	0.00105
CALCITE	0.48736
GYPSUM	+ 0.11064
DOLOMITE	-0.22764
Mg/Na EX	-0.27854
SiO2	-0.14361
K-SPAR	+ 0.05968
KAOLINIT	0.00000
GOETHITE	0.00000
Ca-MONT	- -0.02561

	Computed	Observed
Carbon-13	-5.7636	-10.2000
C-14 (% mod)	77.4667*	15.6000
Sulfur-34	7.0833	Undefined
Strontium-87	0.063287	Undefined
Nitrogen-15	0.0000	Undefined

Adjusted C-14 age in years: 13248.* * = based on Mass Balance

Model (for initial A0)	A0 (initial)	Computed (no decay)	Observed	age (final)

Original Data	15.77	12.90	15.60	-1569.
Mass Balance	94.94	77.47	15.60	13248.
Vogel	85.00	69.36	15.60	12334.
Tamers	51.82	42.30	15.60	8246.
Ingerson and Pearson	27.06	22.11	15.60	2881.
User-defined	100.00	81.59	15.60	13677.

Data used for Carbon-13

Initial Value: -6.7640 Modeled Final Value: -5.7636

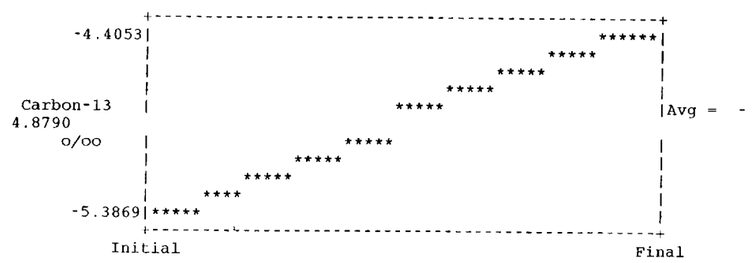
2 dissolving phases:

Phase	Delta C	Isotopic composition (o/oo)
CO2 GAS	0.00105	-25.0000
CALCITE	0.48736	0.0000

1 precipitating phases:

Phase	Delta C	Fractionation factor	Average Isotopic composition (o/oo)
DOLOMITE	-0.45528	1.3753	-4.8790

Isotopic composition of precipitating DOLOMITE



Data used for C-14 (% mod)

Initial Value: 94.9389 Modeled Final Value: 77.4667

2 dissolving phases:

Phase	Delta C	Isotopic composition (% modern)
CO2 GAS	0.00105	100.0000
CALCITE	0.48736	0.0000

1 precipitating phases:

Phase	Delta C	Fractionation factor	Average Isotopic composition (% modern)
DOLOMITE	-0.45528	2.7505	86.1224

Isotopic composition of precipitating DOLOMITE

Data used for Sulfur-34

Initial Value: 0.0000 Modeled Final Value: 7.0833

1 dissolving phases:

Phase	Delta S	Isotopic composition (o/oo)
GYPSUM	0.11064	22.0000

Data used for Strontium-87

Initial Value: 0.0633 Modeled Final Value: 0.0633

No incoming or outgoing phases

Data used for Nitrogen-15

Initial Value: 0.0000 Modeled Final Value: 0.0000

No incoming or outgoing phases

Initial Well 1 : UE-25 c#2
Initial Well 2 : UE-25 J-12
Initial Well 3 : UE-25 b#1
Initial Well 4 : UE-25 J-13
Initial Well 5 : UE-25 p#1 (0-1200m)
Final well : 16S/49E-05acc

	Final	Initial 1	Initial 2	Initial 3	Initial 4	Initial 5
C	2.2132	2.3361	1.9344	2.1967	2.0328	12.3555
S	0.2707	0.2291	0.2187	0.2291	0.2083	0.8129
CA	0.7238	0.2995	0.3494	0.4243	0.3244	2.3481
AL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MG	0.0823	0.0165	0.0987	0.0243	0.0864	1.2766
NA	1.5229	2.3496	1.8274	2.0015	1.9144	6.5324
K	0.1330	0.0537	0.1279	0.0895	0.1279	0.3073
CL	0.1693	0.1989	0.3358	0.2398	0.2031	0.7342
SI	1.0322	0.8824	0.7991	0.8657	0.9156	0.7332
FE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
I2	42.7138	35.7423	62.2877	36.6854	58.9500	0.0000

CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000
CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000 I2 0.0000
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000 I1 0.0000
	I2	0.0000						
Mg/Na EX	NA	2.0000	MG	-1.0000				
SiO2	SI	1.0000						
K-SPAR	K	1.0000	AL	1.0000	SI	3.0000		
KAOLINIT	AL	2.0000	SI	2.0000				
GOETHITE	FE	1.0000	RS	3.0000				
NaCl	NA	1.0000	CL	1.0000				
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700		

11 models checked
10 models found

		MODEL 1	
Init 1	+ F	0.00000	
Init 2	+ F	0.00000	
Init 3	+ F	0.00000	
Init 4	+ F	0.96983	
Init 5	+ F	0.03017	
CO2 GAS		-0.14458	
CALCITE		0.57456	
GYPSUM	+	0.04424	
DOLOMITE	+	-0.28052	(Constraint ignored)
Mg/Na EX	+	-0.24050	(Constraint ignored)
SiO2		0.12265	
K-SPAR	+	-0.00029	(Constraint ignored)
KAOLINIT		0.00015	
GOETHITE		0.00000	
NaCl	+	-0.04987	(Constraint ignored)

		MODEL 2
Init 1	+ F	1.08298
Init 2	+ F	-0.03714

Init 3	+ F	0.00000	
Init 4	+ F	0.00000	
Init 5	+ F	-0.04584	
CO2 GAS		0.06319	
CALCITE		0.65926	
GYPSUM	+	0.06802	
DOLOMITE	+	-0.20054	(Constraint ignored)
Mg/Na EX	+	-0.32719	(Constraint ignored)
SiO2		0.00641	
K-SPAR	+	0.09369	
KAOLINIT		0.00000	
GOETHITE		0.00000	
Ca-MONT	-	-0.04021	

MODEL 3

Init 1	+ F	0.00000	
Init 2	+ F	0.00000	
Init 3	+ F	0.00000	
Init 4	+ F	0.96983	
Init 5	+ F	0.03017	
CO2 GAS		-0.14457	
CALCITE		0.57454	
GYPSUM	+	0.04423	
DOLOMITE	+	-0.28053	(Constraint ignored)
Mg/Na EX	+	-0.24050	(Constraint ignored)
SiO2		0.12248	
K-SPAR	+	-0.00029	(Constraint ignored)
KAOLINIT		0.00000	
NaCl	+	-0.04988	(Constraint ignored)
Ca-MONT	-	0.00013	(Constraint ignored)

MODEL 4

Init 1	+ F	0.00000	
Init 2	+ F	0.00000	
Init 3	+ F	0.00000	
Init 4	+ F	0.96983	
Init 5	+ F	0.03017	
CO2 GAS		-0.14457	
CALCITE		0.57454	
GYPSUM	+	0.04423	
DOLOMITE	+	-0.28053	(Constraint ignored)
Mg/Na EX	+	-0.24050	(Constraint ignored)
SiO2		0.12248	
K-SPAR	+	-0.00029	(Constraint ignored)
GOETHITE		0.00000	
NaCl	+	-0.04988	(Constraint ignored)
Ca-MONT	-	0.00013	(Constraint ignored)

MODEL 5

Init 1	+ F	0.00842	
Init 2	+ F	0.00000	
Init 3	+ F	0.00000	
Init 4	+ F	0.95954	
Init 5	+ F	0.03203	
CO2 GAS		-0.14152	
CALCITE		0.56429	
GYPSUM	+	0.04293	
DOLOMITE	+	-0.28780	(Constraint ignored)

Mg/Na EX	+	-0.24615	(Constraint ignored)
SiO2		0.00000	
KAOLINIT		-0.10666	
GOETHITE		0.00000	
NaCl	+	-0.05083	(Constraint ignored)
Ca-MONT	-	0.09156	(Constraint ignored)

MODEL 6

Init 1	+ F	0.00000	
Init 2	+ F	0.00000	
Init 3	+ F	0.00000	
Init 4	+ F	0.96736	
Init 5	+ F	0.03264	
CO2 GAS		-0.14312	
CALCITE		0.56358	
GYPSUM	+	0.04274	
DOLOMITE	+	-0.28850	(Constraint ignored)
Mg/Na EX	+	-0.24554	(Constraint ignored)
K-SPAR	+	-0.00073	(Constraint ignored)
KAOLINIT		-0.10742	
GOETHITE		0.00000	
NaCl	+	-0.05118	(Constraint ignored)
Ca-MONT	-	0.09252	(Constraint ignored)

MODEL 7

Init 1	+ F	-0.91897	
Init 2	+ F	1.81040	
Init 3	+ F	0.00000	
Init 4	+ F	0.00000	
Init 5	+ F	0.10857	
CO2 GAS		-0.37206	
CALCITE		0.32843	
GYPSUM	+	-0.00288	(Constraint ignored)
DOLOMITE	+	-0.21995	(Constraint ignored)
SiO2		0.43435	
K-SPAR	+	-0.08251	(Constraint ignored)
KAOLINIT		0.00000	
GOETHITE		0.00000	
NaCl	+	-0.33548	(Constraint ignored)
Ca-MONT	-	0.03541	(Constraint ignored)

MODEL 8

Init 1	+ F	0.00000	
Init 2	+ F	0.00000	
Init 3	+ F	1.29435	
Init 4	+ F	-0.25256	
Init 5	+ F	-0.04179	
CO2 GAS		0.10118	
CALCITE		0.29836	
GYPSUM	+	0.06079	
Mg/Na EX	+	-0.12605	(Constraint ignored)
SiO2		0.08482	
K-SPAR	+	0.06228	
KAOLINIT		0.00000	
GOETHITE		0.00000	
NaCl	+	-0.05913	(Constraint ignored)
Ca-MONT	-	-0.02673	

This notebook appears to comply with QAP-001.

E. C. Pierce

2/3/2000

	MODEL 9		
Init 1	+ F	-0.83778	
Init 2	+ F	1.73547	
Init 3	+ F	0.00000	
Init 4	+ F	0.00000	
Init 5	+ F	0.10231	
CO2 GAS		-0.35440	
CALCITE		0.34185	
DOLOMITE	+	-0.21916	(Constraint ignored)
Mg/Na EX	+	-0.01327	(Constraint ignored)
SiO2		0.41699	
K-SPAR	+	-0.07537	(Constraint ignored)
KAOLINIT		0.00000	
GOETHITE		0.00000	
NaCl	+	-0.32187	(Constraint ignored)
Ca-MONT	-	0.03235	(Constraint ignored)

	MODEL 10		
Init 1	+ F	0.00000	
Init 2	+ F	0.00000	
Init 3	+ F	2.69263	
Init 4	+ F	-1.57310	
Init 5	+ F	-0.11953	
CO2 GAS		0.36668	
GYPSUM	+	0.07867	
DOLOMITE	+	0.30306	
Mg/Na EX	+	-0.00240	(Constraint ignored)
SiO2		0.04414	
K-SPAR	+	0.12987	
KAOLINIT		0.00000	
GOETHITE		0.00000	
NaCl	+	-0.06913	(Constraint ignored)
Ca-MONT	-	-0.05574	

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