


SOFTWARE RELEASE NOTICE

01. SRN Number: GHGC-SRN-168		
02. Project Title: Radionuclide Transport KTI		Project No.: 20-1402-871
03. SRN Title: NETPATH VERSION 2.0		
04. Originator/Requestor: David Turner		Date: 4/01/98
05. Summary of Actions		
<input checked="" type="checkbox"/> Release of new software <input type="checkbox"/> Release of modified software: <input type="checkbox"/> Enhancements made <input type="checkbox"/> Corrections made <input type="checkbox"/> Change of access software <input checked="" type="checkbox"/> Software Retirement		
<i>E.C.P.</i> 12/5/2001		
06. Persons Authorized Access		
Name	RO/RW	A/C/D
D. Turner	RO	A
E. Percy	RO	A
R. Pabalan	RO	A
07. Element Manager Approval: <i>E.C.P.</i>		Date: 4/6/98
08. Remarks: U.S. Geological Survey		

SOFTWARE SUMMARY FORM

01. Summary Date: 04/01/98		02. Summary prepared by (Name and phone) David Turner, (210) 522-2139		03. Summary Action:  New	
04. Software Date: 04/01/98		05. Short Title: NETPATH Version 2.0			
06. Software Title:  NETPATH Version 2.0				07. Internal Software ID:  NONE	
08. Software Type:  <input type="checkbox"/> Automated Data System <input checked="" type="checkbox"/> Computer Program <input type="checkbox"/> Subroutine/Module		09. Processing Mode:  <input checked="" type="checkbox"/> Interactive <input type="checkbox"/> Batch <input checked="" type="checkbox"/> Combination		10. APPLICATION AREA a. General: <input checked="" type="checkbox"/> Scientific/Engineering <input type="checkbox"/> Auxiliary Analyses <input type="checkbox"/> Total System PA <input type="checkbox"/> Subsystem PA <input type="checkbox"/> Other  b. Specific:	
11. Submitting Organization and Address: CNWRA 6220 Culebra Road San Antonio, TX 78228			12. Technical Contact(s) and Phone:  David Turner, (210) 522-2139 John Bradbury (NRC), (301) 415-6597		
13. Narrative: NETPATH is an interactive FORTRAN 77 computer program used to interpret net geochemical mass-balance reactions between an initial and final water along a hydrologic flowpath. NETPATH can also compute mixing proportions of 2 to 5 initial waters and net geochemical reactions that can account for the observed composition of a final water.					
14. Computer Platform  PC		15. Computer Operating System:  DOS		16. Programming Language(s):  Fortran 77	
17. Number of Source Program Statements:  N/A		18. Computer Memory Requirements:  4 MB RAM		19. Tape Drives:  N/A	
20. Disk/Drum Units:  5 MB		21. Graphics:  N/A		22. Other Operational Requirements: None	
23. Software Availability:  <input checked="" type="checkbox"/> Available <input type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY			24. Documentation Availability:  <input checked="" type="checkbox"/> Available <input type="checkbox"/> Inadequate <input type="checkbox"/> In-House ONLY		
Software Custodian:  Date: 4/6/98					

# CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

## SOFTWARE CONTROL CHECKLIST

Name of Software: NETPATH  
Primary User: David Turner

Version: 2.0

- SOFTWARE REQUIREMENTS DESCRIPTION
  - Documentation
- DESIGN AND DEVELOPMENT
  - Documentation (Scientific Notebook)
- DESIGN VERIFICATION
  - Computer runs uniquely identified
  - Software analysis tools have been applied and discrepancies resolved
  - Design Verification Report
- INSTALLATION TESTING
  - Installation test documentation
  - Discrepancy resolution
- CONFIGURATION CONTROL
  - Software Summary Form
  - User's Manual - U.S. Geological Survey Water Resources Investigation Report 94-4169
  - Technical Description ON DISKETTE
  - Source Code
  - Version Control  N/A
  - Software Release Notice
- SOFTWARE PROBLEM REPORTING AND RESOLUTION
  - Software Problem and Change Request
- SOFTWARE VALIDATION
  - Software Validation Test Plan
  - Software Validation Test Report
  - Software Validation Review
- SOFTWARE RETIREMENT
  - Software Release Notice

TO: Bruce Mabrito  
FROM: David Turner *JKT*  
SUBJECT: Installation and Testing of NETPATH, Version 2.0 Acquired Software  
DATE: April 1, 1998

The geochemical mass-balance code NETPATH, Version 2.0 was obtained as a compressed file (**netp2-13.exe**) from the U.S. Geological Survey anonymous FTP site. The FTP address is:

**brrcrftp.cr.usgs.gov**

On this site, the DOS/PC version of NETPATH is located in the **geochem/pc/netpath** subdirectory. The compressed file **netp2-13.exe** contains the executable file, the fortran 77 source code, test problem input and output files, and a postscript copy of the user's manual. This file is attached (3.5" floppy disk). The code can also be ordered from:

U.S. Geological Survey  
NWIS Program Office  
437 National Center  
Reston, VA 22092

The compressed file was expanded and NETPATH, Version 2.0 was installed on the shared drive (**G:\turner\usgscode\netpath2**), and has been tested in the DOS shell for Windows NT 4.0. No problems were encountered during installation.

The test problems provided with the NETPATH distribution file were run to test proper installation. Hardcopies and electronic files of the following are attached:

- Input Files (from USGS)
- Output Files (from USGS)
- Output Files (CNWRA-generated)

The input and output files received from the USGS are also included as electronic files on the attached disk (**netp2-13.exe**), and also on

np-1a.out

Carbon	Sulfur	+NaCl	+GYPSUM	KAOLINIT	Mixing: No
Calcium	Magnesium	Ca-MONT	CO2 GAS	CALCITE	Evaporation: No
Sodium	Chloride	SiO2	BIOTITE	+PLAGAN38	Rayleigh Calcs: No
Silica	Aluminum				
Potassium					

Warning: There is no data for Aluminum in 2 of the wells: zero will be used

Initial Well : Sierra Nevada (Ephemeral Spr.)  
 Final Well : Sierra Nevada (Perennial Spr.)

	Final	Initial
C	1.1993	0.7825
S	0.0250	0.0100
CA	0.2600	0.0780
MG	0.0710	0.0290
NA	0.2590	0.1340
CL	0.0300	0.0140
SI	0.4100	0.2730
AL	0.0000	0.0000
K	0.0400	0.0280

NaCl NA 1.0000 CL 1.0000  
 GYPSUM CA 1.0000 S 1.0000 RS 6.0000 I3 22.0000  
 KAOLINIT AL 2.0000 SI 2.0000  
 Ca-MONT CA 0.1670 AL 2.3300 SI 3.6700  
 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  
 SiO2 SI 1.0000  
 BIOTITE AL 1.0000 MG 3.0000 K 1.0000 SI 3.0000  
 PLAGAN38 CA 0.3800 NA 0.6200 AL 1.3800 SI 2.6200  
 No models found.

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np-1b.out

Initial Well : Sierra Nevada (Ephemeral Spr.)  
Final Well : Sierra Nevada (Perennial Spr.)

Constraints: 8		Phases: 9			Parameters
Carbon	Sulfur	+NaCl	+GYPSUM	KAOLINIT	Mixing: No
Calcium	Magnesium	Ca-MONT	CO2 GAS	CALCITE	Evaporation: No
Sodium	Chloride	SiO2	BIOTITE	+PLAGAN38	Rayleigh Calcs: No
Silica	Aluminum				

Warning: There is no data for Aluminum in 2 of the wells: zero will be used

	Final	Initial
C	1.1993	0.7825
S	0.0250	0.0100
CA	0.2600	0.0780
MG	0.0710	0.0290
NA	0.2590	0.1340
CL	0.0300	0.0140
SI	0.4100	0.2730
AL	0.0000	0.0000

NaCl	NA	1.0000	CL	1.0000								
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000				
KAOLINIT	AL	2.0000	SI	2.0000								
Ca-MONT	CA	0.1670	AL	2.3300	SI	3.6700						
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		
SiO2	SI	1.0000										
BIOTITE	AL	1.0000	MG	3.0000	K	1.0000	SI	3.0000				
PLAGAN38	CA	0.3800	NA	0.6200	AL	1.3800	SI	2.6200				

9 models checked  
5 models found

	MODEL	1
NaCl	+	0.01600
GYPSUM	+	0.01500
KAOLINIT		-0.03355
Ca-MONT		-0.08136
CO2 GAS		0.30296
CALCITE		0.11380
BIOTITE		0.01400
PLAGAN38	+	0.17584

	MODEL	2
NaCl	+	0.01600
GYPSUM	+	0.01500
KAOLINIT		-0.82741
Ca-MONT		0.60007
CO2 GAS		0.41676
SiO2		-0.91311
BIOTITE		0.01400

PLAGAN38 + 0.17584

MODEL 3

NaCl + 0.01600  
GYPSUM + 0.01500  
KAOLINIT 2.07993  
Ca-MONT -1.89550  
CALCITE 0.41676  
SiO2 2.43096  
BIOTITE 0.01400  
PLAGAN38 + 0.17584

MODEL 4

NaCl + 0.01600  
GYPSUM + 0.01500  
KAOLINIT -0.12833  
CO2 GAS 0.31655  
CALCITE 0.10021  
SiO2 -0.10902  
BIOTITE 0.01400  
PLAGAN38 + 0.17584

MODEL 5

NaCl + 0.01600  
GYPSUM + 0.01500  
Ca-MONT -0.11015  
CO2 GAS 0.29815  
CALCITE 0.11861  
SiO2 0.03859  
BIOTITE 0.01400  
PLAGAN38 + 0.17584

np-1c.out

Initial Well : Sierra Nevada (Ephemeral Spr.)

Final Well : Sierra Nevada (Perennial Spr.)

```

-----|-----Forced-----|-----
Carbon   Sulfur   |-KAOLINIT                      |Mixing: No
Calcium  Magnesium|-----Unforced-----|Evaporation: No
Sodium   Chloride  |+NaCl   +GYPSUM  -Ca-MONT    |Rayleigh Calcs: No
Silica   Aluminum| CO2 GAS  CALCITE  SiO2      |
          | BIOTITE +PLAGAN38          |
=====

```

Warning: There is no data for Aluminum in 2 of the wells: zero will be used

```

=====
          Final      Initial
C         1.1993     0.7825
S         0.0250     0.0100
CA        0.2600     0.0780
MG        0.0710     0.0290
NA        0.2590     0.1340
CL        0.0300     0.0140
SI        0.4100     0.2730
AL        0.0000     0.0000

```

```

KAOLINIT AL  2.0000 SI  2.0000
NaCl      NA  1.0000 CL  1.0000
GYPSUM   CA  1.0000 S   1.0000 RS  6.0000 I3  22.0000
Ca-MONT  CA  0.1670 AL  2.3300 SI  3.6700
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
SiO2     SI  1.0000
BIOTITE  AL  1.0000 MG  3.0000 K   1.0000 SI  3.0000
PLAGAN38 CA  0.3800 NA  0.6200 AL  1.3800 SI  2.6200

```

8 models checked  
2 models found

```

MODEL  1
KAOLINIT - F -0.03355
NaCl     +   0.01600
GYPSUM   +   0.01500
Ca-MONT  -  -0.08136
CO2 GAS  +   0.30296
CALCITE  +   0.11380
BIOTITE  +   0.01400
PLAGAN38 +   0.17584

```

```

MODEL  2
KAOLINIT - F -0.12833
NaCl     +   0.01600
GYPSUM   +   0.01500
CO2 GAS  +   0.31655
CALCITE  +   0.10021
SiO2     -  -0.10902
BIOTITE  +   0.01400
PLAGAN38 +   0.17584

```



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          Sulfur   | CO2 GAS  NaCl      ARAGONIT | Mixing: No
Calcium         Sodium   | MIRABILI GYPSUM   | Evaporation: Yes
Chloride        |      |      | 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-3-1.out

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

```

=====
Constraints: 3 | Phases: 3 | Parameters
-----|-----|-----
Carbon Calcium | CALCITE EXCHANGE CO2 GAS | Mixing: No
Sodium          | | | | | Evaporation: No
                | | | | | Rayleigh Calcs: No
                | | | | | Exchange: Ca/Na
=====

```

```

=====
          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  0.0000 I2  0.0000
EXCHANGE CA -1.0000 NA  2.0000 MG  0.0000
CO2 GAS  C   1.0000 RS  4.0000 I1 -25.0000 I2 100.0000

```

1 model checked  
1 model found

```

MODEL 1
CALCITE 2.01547
EXCHANGE 2.96382
CO2 GAS 0.88468

```

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np-3-2.out

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

Constraints: 4		Phases: 4	Parameters
Carbon	Calcium	CALCITE EXCHANGE+O2 GAS	Mixing: No
Sodium	Redox	+"CH2O"	Evaporation: No
			Rayleigh Calcs: No
			Exchange: Ca/Na

	Final	Initial
C	5.9742	3.0741
CA	0.0749	1.0232
NA	6.0930	0.1653
RS	23.8968	12.2962

CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2	0.0000
EXCHANGE	CA	-1.0000	NA	2.0000	MG	0.0000				
O2 GAS	RS	4.0000								
"CH2O"	C	1.0000	I1	-25.0000	I2	0.0000				

1 model checked  
1 model found

	MODEL	1
CALCITE		2.01547
EXCHANGE		2.96382
O2 GAS	+	0.88468
"CH2O"	+	0.88468

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np-3-3a.out

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

```

=====
Constraints: 5 | Phases: 5 | Parameters
-----|-----|-----
Carbon        Calcium | CALCITE +"CH2O"  GOETHITE | Mixing: No
Sodium        Redox   | FeII-Na  CO2 GAS | Evaporation: No
Iron          | | | | | Rayleigh Calcs: No
=====

```

Warning: There is no data for Iron in 1 of the wells; zero will be used

```

=====
Final      Initial
C          5.9742   3.0741
CA         0.0749   1.0232
NA         6.0930   0.1653
RS        23.8968  12.2962
FE         0.0000   0.0000
=====

```

```

CALCITE CA  1.0000 C   1.0000 RS  4.0000 I1  0.0000 I2  0.0000
"CH2O"  C   1.0000 I1 -25.0000 I2  0.0000
GOETHITE FE  1.0000 RS  3.0000
FeII-Na FE -1.0000 NA  2.0000 RS -2.0000
CO2 GAS  C   1.0000 RS  4.0000 I1 -25.0000 I2 100.0000

```

1 model checked  
1 model found

```

MODEL  1
CALCITE          -0.94835
"CH2O"  +         0.74096
GOETHITE         2.96382
FeII-Na         2.96382
CO2 GAS         3.10755

```

np-3-3b.out

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

```

=====
Constraints: 5 | Phases: 5 | Parameters
-----|-----|-----
Carbon Calcium | CALCITE EXCHANGE+"CH2O" | Mixing: No
Sodium Redox | GOETHITE MAGNETIT | Evaporation: No
Iron | | Rayleigh Calcs: No
| | | Exchange: Ca/Na
=====

```

Warning: There is no data for Iron in 1 of the wells: zero will be used

```

=====
Final Initial
C 5.9742 3.0741
CA 0.0749 1.0232
NA 6.0930 0.1653
RS 23.8968 12.2962
FE 0.0000 0.0000
=====

```

```

CALCITE CA 1.0000 C 1.0000 RS 4.0000 I1 0.0000 I2 0.0000
EXCHANGE CA -1.0000 NA 2.0000 MG 0.0000
"CH2O" C 1.0000 I1 -25.0000 I2 0.0000
GOETHITE FE 1.0000 RS 3.0000
MAGNETIT FE 3.0000 RS 8.0000

```

1 model checked  
1 model found

```

MODEL 1
CALCITE 2.01547
EXCHANGE 2.96382
"CH2O" + 0.88468
GOETHITE 10.61616
MAGNETIT -3.53872

```

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np-3-4.out

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

```

=====
Constraints: 6 | Phases: 6 | Parameters
-----|-----|-----
Carbon Calcium | CALCITE EXCHANGE+"CH2O" | Mixing: No
Sodium Redox | GOETHITE+GYPSUM -PYRITE | Evaporation: No
Iron Sulfur | | Rayleigh Calcs: No
| | | Exchange: Ca/Na
=====

```

Warning: There is no data for Iron in 1 of the wells: zero will be used

```

=====
Final Initial
C 5.9742 3.0741
CA 0.0749 1.0232
NA 6.0930 0.1653
RS 24.7092 13.4833
FE 0.0000 0.0000
S 0.1354 0.1978
=====

```

```

CALCITE CA 1.0000 C 1.0000 RS 4.0000 I1 0.0000 I2 0.0000
EXCHANGE CA -1.0000 NA 2.0000 MG 0.0000
"CH2O" C 1.0000 I1 -25.0000 I2 0.0000
GOETHITE FE 1.0000 RS 3.0000
GYPSUM CA 1.0000 S 1.0000 RS 6.0000 I3 22.0000
PYRITE FE 1.0000 S 2.0000 RS 0.0000 I3 -60.0000

```

1 model checked  
1 model found

```

MODEL 1
CALCITE 1.13821
EXCHANGE 2.96382
"CH2O" + 1.76194
GOETHITE 0.46985
GYPSUM + 0.87726
PYRITE - -0.46985

```

np-3-5.out

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

```

=====
Constraints: 4 | Phases: 4 | Parameters
-----|-----|-----
Carbon        Calcium | CALCITE EXCHANGE CH4 GAS | Mixing: No
Sodium        Redox  | +"CH2O"                   | Evaporation: No
               |                             | Rayleigh Calcs: No
               |                             | Exchange: Ca/Na
=====

```

```

=====
Final      Initial
C          5.9742  3.0741
CA         0.0749  1.0232
NA         6.0930  0.1653
RS        23.8968  12.2962
=====

```

```

CALCITE CA  1.0000 C  1.0000 RS  4.0000 I1  0.0000 I2  0.0000
EXCHANGE CA -1.0000 NA  2.0000 MG  0.0000
CH4 GAS  C  1.0000 RS -4.0000 I1 -40.0000 I2  0.0000
"CH2O"   C  1.0000 I1 -25.0000 I2  0.0000

```

1 model checked  
1 model found

```

MODEL 1
CALCITE 2.01547
EXCHANGE 2.96382
CH4 GAS -0.88468
"CH2O" + 1.76936

```

np-3-6.out

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

Constraints: 6		Phases: 6			Parameters
Carbon	Calcium	CALCITE	EXCHANGE	GOETHITE	Mixing: No
Sodium	Redox	+GYPSUM	-PYRITE	+LIGNITE	Evaporation: No
Iron	Sulfur				Rayleigh Calcs: No
					Exchange: Ca/Na

Warning: There is no data for Iron in 1 of the wells: zero will be used

	Final	Initial
C	5.9742	3.0741
CA	0.0749	1.0232
NA	6.0930	0.1653
RS	24.7092	13.4833
FE	0.0000	0.0000
S	0.1354	0.1978

CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2	0.0000
EXCHANGE	CA	-1.0000	NA	2.0000	MG	0.0000				
GOETHITE	FE	1.0000	RS	3.0000						
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000		
PYRITE	FE	1.0000	S	2.0000	RS	0.0000	I3	-60.0000		
LIGNITE	C	1.0000	RS	-0.4000	I1	-25.0000	I2	0.0000		

1 model checked  
1 model found

	MODEL	1
CALCITE		0.91086
EXCHANGE		2.96382
GOETHITE		0.58353
GYPSUM	+	1.10461
PYRITE	-	-0.58353
LIGNITE	+	1.98929



np-3-7.out

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

```

=====
Constraints: 3 | Phases: 3 | Parameters
-----|-----|-----
Carbon Calcium | CALCITE CO2 GAS H-Exch | Mixing: No
Sodium | | | Evaporation: No
| | | | Rayleigh Calcs: No
=====

```

```

=====
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 0.0000 I2 0.0000
CO2 GAS C 1.0000 RS 4.0000 I1 -25.0000 I2 100.0000
H-Exch NA 1.6000 CA -1.0000
=====

```

1 model checked  
1 model found

```

MODEL 1
CALCITE 2.75643
CO2 GAS 0.14373
H-Exch 3.70478

```

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np-4.out

Initial Well 1 : Pinal Cr. background, #404  
Initial Well 2 : Pinal Cr pH<4 plume, #51  
Final well : Pinal Cr pH 4-5, #402

Constraints: 11		Phases: 11			Parameters
Carbon	Sulfur	CALCITE	CO2 GAS	GYPSUM	Mixing: Yes
Calcium	Aluminum	+ALBITE	+O2 GAS	GIBBSITE	Evaporation: No
Magnesium	Sodium	GOETHITE+DOLOMITE	MnOOH		Rayleigh Calcs: No
Chloride	Silica	KAOLINIT	SiO2		
Iron	Manganese				
Redox					

The mixing ratio will be determined by Chloride  
Warning: There is no data for Aluminum in 1 of the wells: zero will be used

	Final	Initial 1	Initial 2
C	4.6957	3.9020	4.2204
S	34.5357	0.1875	92.8765
CA	13.5447	0.9984	11.1301
AL	0.3726	0.0000	9.3939
MG	7.8567	0.5349	16.2636
NA	4.8102	1.1749	9.2610
CL	3.9699	0.2257	9.7230
SI	1.6062	0.5328	1.6874
FE	9.7207	0.0000	50.8313
MN	1.2078	0.0018	1.3841
RS	247.9333	17.4742	678.6412

CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	0.0000	I2	0.0000
CO2 GAS	C	1.0000	RS	4.0000	I1	-25.0000	I2	100.0000		
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000		
ALBITE	NA	1.0000	AL	1.0000	SI	3.0000				
O2 GAS	RS	4.0000								
GIBBSITE	AL	1.0000								
GOETHITE	FE	1.0000	RS	3.0000						
DOLOMITE	CA	1.0000	MG	1.0000	C	2.0000	RS	8.0000	I1	0.0000
	I2	0.0000								
MnOOH	MN	1.0000	RS	3.0000						
KAOLINIT	AL	2.0000	SI	2.0000						
SiO2	SI	1.0000								

11 models checked  
3 models found

	MODEL	1
Init 1	+ F	0.60576
Init 2	+ F	0.39424
CALCITE		9.62443
CO2 GAS		-11.19810
GYPSUM		-2.19327
ALBITE	+	0.44746
O2 GAS	+	2.31576
GIBBSITE		-3.05421
GOETHITE		-10.31891

DOLOMITE	+	1.12089
MnOOH		0.66099
KAOLINIT		-0.36204

	MODEL	2	
Init 1	+ F		0.60576
Init 2	+ F		0.39424
CALCITE			9.62443
CO2 GAS			-11.19810
GYP SUM			-2.19327
ALBITE	+		0.44746
O2 GAS	+		2.31576
GIBBSITE			-3.77829
GOETHITE			-10.31891
DOLOMITE	+		1.12089
MnOOH			0.66099
SiO2			-0.72409

	MODEL	3	
Init 1	+ F		0.60576
Init 2	+ F		0.39424
CALCITE			9.62443
CO2 GAS			-11.19810
GYP SUM			-2.19327
ALBITE	+		0.44746
O2 GAS	+		2.31576
GOETHITE			-10.31891
DOLOMITE	+		1.12089
MnOOH			0.66099
KAOLINIT			-1.88915
SiO2			3.05421

np-5-1.out

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

Constraints: 6		Phases: 6			Parameters
Carbon	Calcium	CALCITE	EXCHANGE	GOETHITE	Mixing: No
Sodium	Redox	+GYPSUM	-PYRITE	+LIGNITE	Evaporation: No
Iron	Sulfur				Rayleigh Calcs: Yes
					Exchange: Ca/Na
					Init C-14 50.00 (TDC)
					(User-defined)

Warning: There is no data for Iron in 1 of the wells: zero will be used

	Final	Initial
C	5.9742	3.0741
CA	0.0749	1.0232
NA	6.0930	0.1653
RS	24.7092	13.4833
FE	0.0000	0.0000
S	0.1354	0.1978

CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	1.1000	I2	0.0000
EXCHANGE	CA	-1.0000	NA	2.0000	MG	0.0000				
GOETHITE	FE	1.0000	RS	3.0000						
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000		
PYRITE	FE	1.0000	S	2.0000	RS	0.0000	I3	-60.0000		
LIGNITE	C	1.0000	RS	-0.4000	I1	-22.0000	I2	0.0000		

1 model checked  
 1 model found

MODEL 1		Computed	Observed
CALCITE		0.91086	
EXCHANGE		2.96382	
GOETHITE		0.58353	
GYPSUM	+	1.10461	
PYRITE	-	-0.58353	
LIGNITE	+	1.98929	
Carbon-13		-13.6412	-6.2000
C-14 (% mod)		25.7278*	3.1000
Sulfur-34		66.9879	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: -13.6412

2 dissolving phases:

Phase	Delta C	Isotopic composition (o/oo)
CALCITE	0.91086	1.1000
LIGNITE	1.98929	-22.0000

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	0.91086	0.0000
LIGNITE	1.98929	0.0000

Data used for Sulfur-34

Initial Value: 0.0000 Modeled Final Value: 66.9879

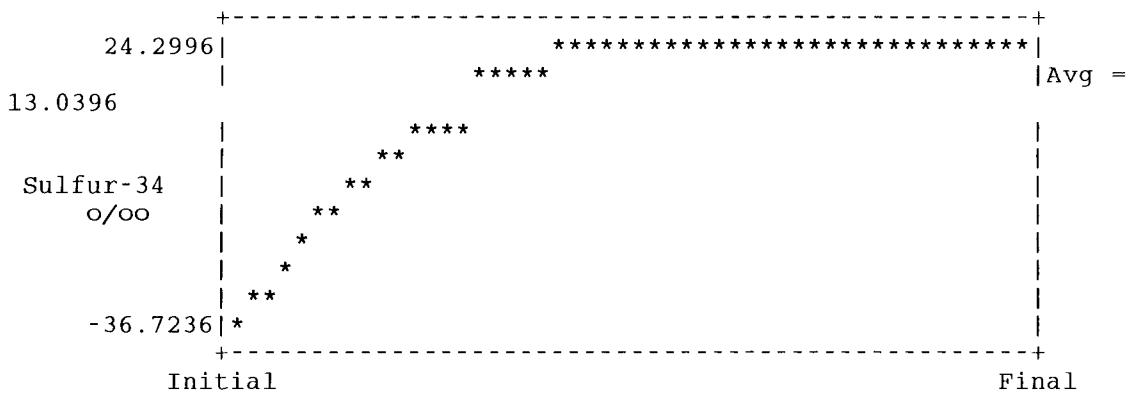
1 dissolving phases:

Phase	Delta S	Isotopic composition (o/oo)
GYP SUM	1.10461	22.0000

1 precipitating phases:

Phase	Delta S	Fractionation factor	Average Isotopic composition (o/oo)
PYRITE	-1.16705	-40.0000	13.0396

Isotopic composition of precipitating PYRITE



Data used for Strontium-87  
Insufficient data

Data used for Nitrogen-15  
Insufficient data

np-5-2.out

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

```

=====
Constraints: 6 | Phases: 6 | Parameters
-----|-----|-----
Carbon Calcium |*CALCITE EXCHANGE GOETHITE |Mixing: No
Sodium Redox |+GYPSUM -PYRITE +LIGNITE |Evaporation: No
Iron Sulfur | |Rayleigh Calcs: Yes
| | |Exchange: Ca/Na
| | |Init C-14 50.00 (TDC)
| | |(User-defined)
=====
  
```

Warning: There is no data for Iron in 1 of the wells: zero will be used

```

=====
Final Initial
C 5.9742 3.0741
CA 0.0749 1.0232
NA 6.0930 0.1653
RS 24.7092 13.4833
FE 0.0000 0.0000
S 0.1354 0.1978

CALCITE CA 1.0000 C 1.0000 RS 4.0000 I1 1.1000 I2 0.0000
EXCHANGE CA -1.0000 NA 2.0000 MG 0.0000
GOETHITE FE 1.0000 RS 3.0000
GYPSUM CA 1.0000 S 1.0000 RS 6.0000 I3 22.0000
PYRITE FE 1.0000 S 2.0000 RS 0.0000 I3 -60.0000
LIGNITE C 1.0000 RS -0.4000 I1 -22.0000 I2 0.0000
  
```

1 model checked  
 1 model found

```

MODEL 1
CALCITE 0.91086 5.200 exchanged
EXCHANGE 2.96382
GOETHITE 0.58353
GYPSUM + 1.10461
PYRITE - -0.58353
LIGNITE + 1.98929

Computed Observed
Carbon-13 -6.2068 -6.2000
C-14 (% mod) 7.8031* 3.1000
Sulfur-34 66.9879 Undefined
Strontium-87 Insufficient data
Nitrogen-15 Insufficient data
  
```

Adjusted C-14 age in years: 7631.\* \* = based on User-defined

```

-----
Model A0 Computed Observed age
(for initial A0) (initial) (no decay) (final)
-----
Original Data 33.90 5.29 3.10 4419.
Mass Balance 55.75 8.70 3.10 8531.
Vogel 85.00 13.27 3.10 12018.
Tamers 52.75 8.23 3.10 8074.
Ingerson and Pearson 50.40 7.87 3.10 7697.
Mook 34.25 5.34 3.10 4503.
  
```

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Fontes and Garnier	50.35	7.86	3.10	7688.
Eichinger	47.91	7.48	3.10	7278.
User-defined	50.00	7.80	3.10	7631.

Data used for Carbon-13

Initial Value: -12.6000      Modeled Final Value: -6.2068

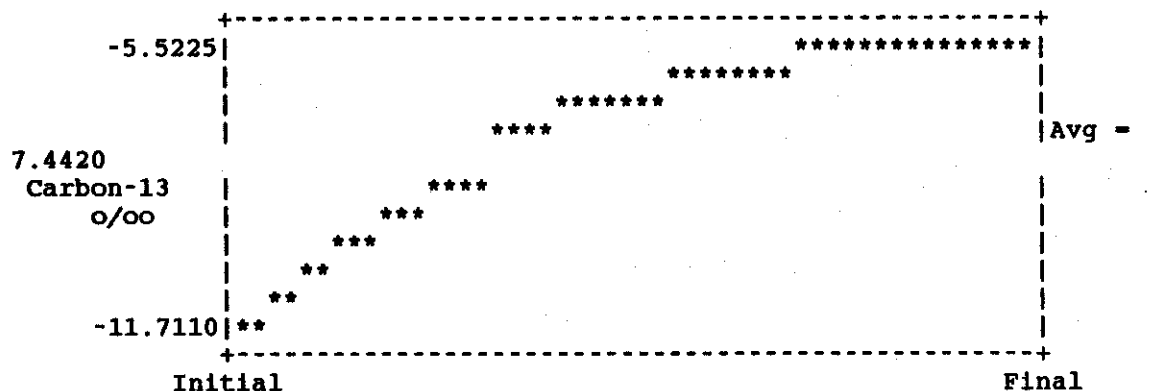
2 dissolving phases:

Phase	Delta C	Isotopic composition (o/oo)
CALCITE	6.11086	1.1000
LIGNITE	1.98929	-22.0000

1 precipitating phases:

Phase	Delta C	Fractionation factor	Average Isotopic composition (o/oo)
CALCITE	-5.20000	0.7050	-7.4420

Isotopic composition of precipitating CALCITE



Data used for C-14 (% mod)

Initial Value: 50.0000      Modeled Final Value: 7.8031

2 dissolving phases:

Phase	Delta C	Isotopic composition (% modern)
CALCITE	6.11086	0.0000
LIGNITE	1.98929	0.0000

1 precipitating phases:

Phase	Delta C	Fractionation factor	Average Isotopic composition (% modern)
CALCITE	-5.20000	1.4099	20.5975

Isotopic composition of precipitating CALCITE



7.9221| \*\*\*\*\*|  
 +-----+  
 Initial Final

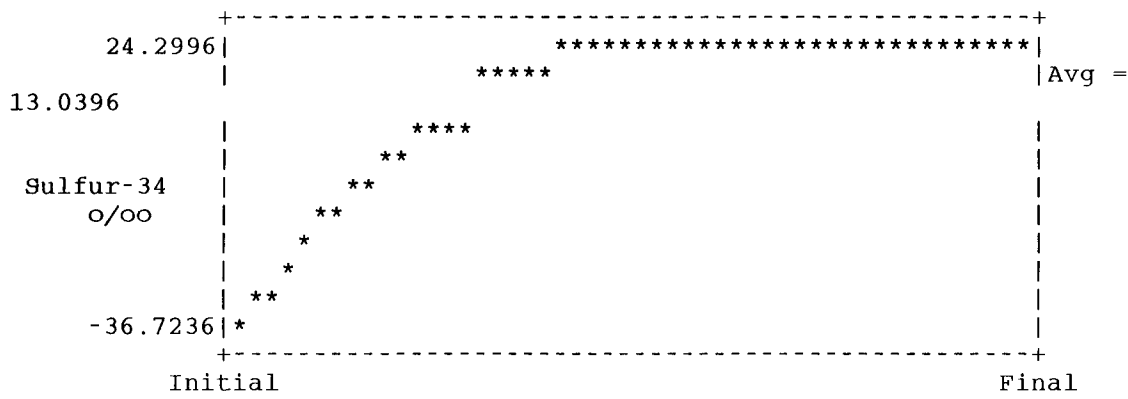
Data used for Sulfur-34

Initial Value: 0.0000 Modeled Final Value: 66.9879

1 dissolving phases:  
 Phase Delta S Isotopic composition (o/oo)  
 GYPSUM 1.10461 22.0000

1 precipitating phases: Average  
 Phase Delta S Fractionation factor Isotopic composition (o/oo)  
 PYRITE -1.16705 -40.0000 13.0396

Isotopic composition of precipitating PYRITE



Data used for Strontium-87  
Insufficient data

Data used for Nitrogen-15  
Insufficient data



np-5-3.out

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

```

=====
Constraints: 6 | Phases: 6 | Parameters
-----|-----|-----
Carbon      Calcium | CALCITE EXCHANGE GOETHITE | Mixing: No
Sodium      Redox   | +GYPSUM -PYRITE +LIGNITE  | Evaporation: No
Iron        Sulfur  | | | | | Rayleigh Calcs: Yes
            | | | | | Exchange: Ca/Na
            | | | | | Init C-14 50.00 (TDC)
            | | | | | (User-defined)
=====
  
```

Warning: There is no data for Iron in 1 of the wells: zero will be used

	Final	Initial
C	5.9742	3.0741
CA	0.0749	1.0232
NA	6.0930	0.1653
RS	24.7092	13.4833
FE	0.0000	0.0000
S	0.1354	0.1978

CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	1.1000	I2	0.0000
EXCHANGE	CA	-1.0000	NA	2.0000	MG	0.0000				
GOETHITE	FE	1.0000	RS	3.0000						
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000		
PYRITE	FE	1.0000	S	2.0000	RS	0.0000	I3	-60.0000		
LIGNITE	C	1.0000	RS	-0.4000	I1	-22.0000	I2	0.0000		

1 model checked  
 1 model found

MODEL		1
CALCITE		0.91086
EXCHANGE		2.96382
GOETHITE		0.58353
GYPSUM	+	1.10461
PYRITE	-	-0.58353
LIGNITE	+	1.98929

	Computed	Observed
Carbon-13	0.3510	-6.2000
C-14 (% mod)	0.0000	3.1000
Sulfur-34	66.9879	Undefined
Strontium-87	Insufficient data	
Nitrogen-15	Insufficient data	

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

Data used for Carbon-13

Initial Value: -12.6000      Modeled Final Value: 0.3510

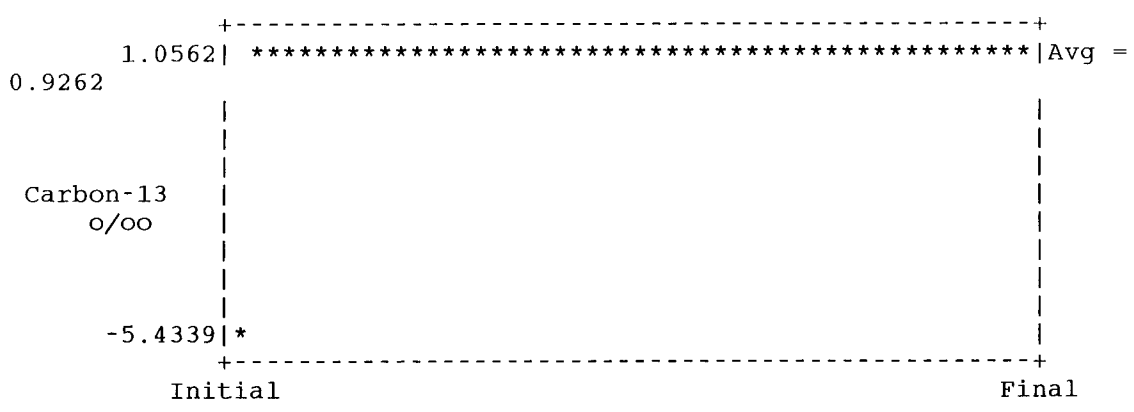
2 dissolving phases:

Phase      Delta C      Isotopic composition (o/oo)

CALCITE 1000.90986 1.1000  
 LIGNITE 1.98929 -22.0000

1 precipitating phases: Average  
 Phase Delta C Fractionation factor Isotopic composition (o/oo)  
 CALCITE -999.99900 0.7050 0.9262

Isotopic composition of precipitating CALCITE



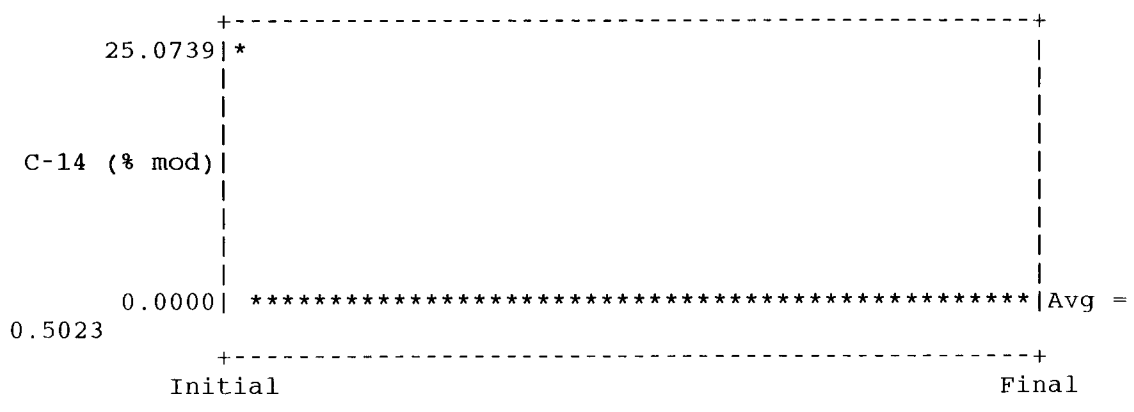
Data used for C-14 (% mod)

Initial Value: 50.0000 Modeled Final Value: 0.0000

2 dissolving phases:  
 Phase Delta C Isotopic composition (% modern)  
 CALCITE 1000.90986 0.0000  
 LIGNITE 1.98929 0.0000

1 precipitating phases: Average  
 Phase Delta C Fractionation factor Isotopic composition (% modern)  
 CALCITE -999.99900 1.4099 0.5023

Isotopic composition of precipitating CALCITE



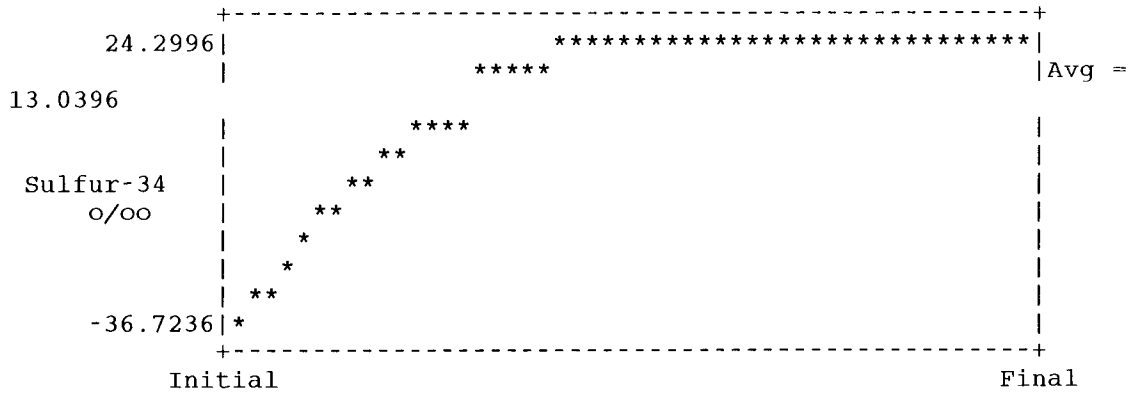
Data used for Sulfur-34

Initial Value: 0.0000 Modeled Final Value: 66.9879

1 dissolving phases:  
 Phase Delta S Isotopic composition (o/oo)  
 GYPSUM 1.10461 22.0000

1 precipitating phases:			Average
Phase	Delta S	Fractionation factor	Isotopic composition (o/oo)
PYRITE	-1.16705	-40.0000	13.0396

Isotopic composition of precipitating PYRITE



Data used for Strontium-87  
Insufficient data

Data used for Nitrogen-15  
Insufficient data

np-5-4.out

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

Constraints: 6		Phases: 6			Parameters
Carbon	Calcium	CALCITE	GOETHITE+GYPSUM	Mixing: No	
Sodium	Redox	-PYRITE	+LIGNITE	H-Exch	Evaporation: No
Iron	Sulfur				Rayleigh Calcs: Yes
					Init C-14 50.00 (TDC)
					(User-defined)

Warning: There is no data for Iron in 1 of the wells: zero will be used

	Final	Initial
C	5.9742	3.0741
CA	0.0749	1.0232
NA	6.0930	0.1653
RS	24.7092	13.4833
FE	0.0000	0.0000
S	0.1354	0.1978

CALCITE	CA	1.0000	C	1.0000	RS	4.0000	I1	1.1000	I2	0.0000
GOETHITE	FE	1.0000	RS	3.0000						
GYPSUM	CA	1.0000	S	1.0000	RS	6.0000	I3	22.0000		
PYRITE	FE	1.0000	S	2.0000	RS	0.0000	I3	-60.0000		
LIGNITE	C	1.0000	RS	-0.4000	I1	-22.0000	I2	0.0000		
H-Exch	NA	1.6000	CA	-1.0000						

1 model checked  
 1 model found

MODEL 1		Computed	Observed
CALCITE		2.70349	
GOETHITE		0.05769	
GYPSUM	+	0.05293	
PYRITE	-	-0.05769	
LIGNITE	+	0.19666	
H-Exch		3.70478	
Carbon-13		-6.7098	-6.2000
C-14 (% mod)		25.7278*	3.1000
Sulfur-34		30.4195	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: -6.7098

2 dissolving phases:

Phase	Delta C	Isotopic composition (o/oo)
CALCITE	2.70349	1.1000
LIGNITE	0.19666	-22.0000

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	2.70349	0.0000
LIGNITE	0.19666	0.0000

Data used for Sulfur-34

Initial Value: 0.0000 Modeled Final Value: 30.4195

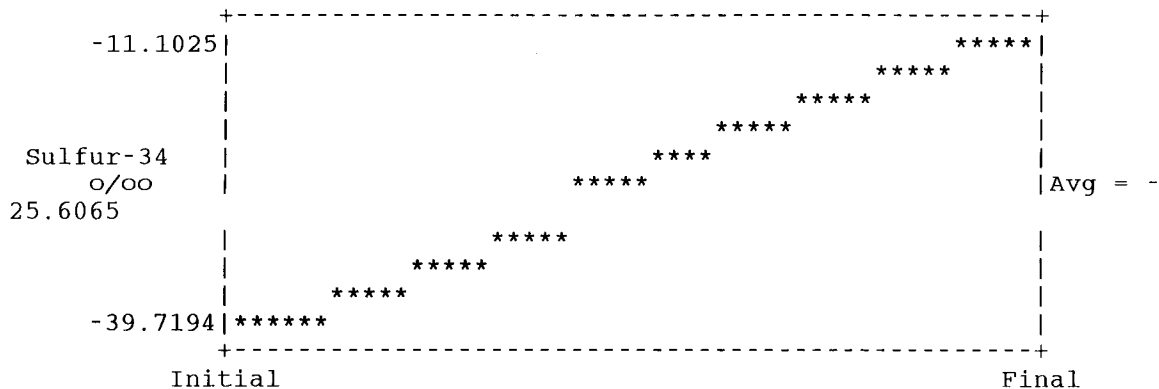
1 dissolving phases:

Phase	Delta S	Isotopic composition (o/oo)
GYP SUM	0.05293	22.0000

1 precipitating phases:

Phase	Delta S	Fractionation factor	Average Isotopic composition (o/oo)
PYRITE	-0.11537	-40.0000	-25.6065

Isotopic composition of precipitating PYRITE



Data used for Strontium-87 Insufficient data

Data used for Nitrogen-15 Insufficient data

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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 | CALCITE H-Exch CO2 GAS | Mixing: No
Sodium          |          |          | 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          A0      Computed  Observed  age
(for initial A0) (initial) (no decay) (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

```

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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
```



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

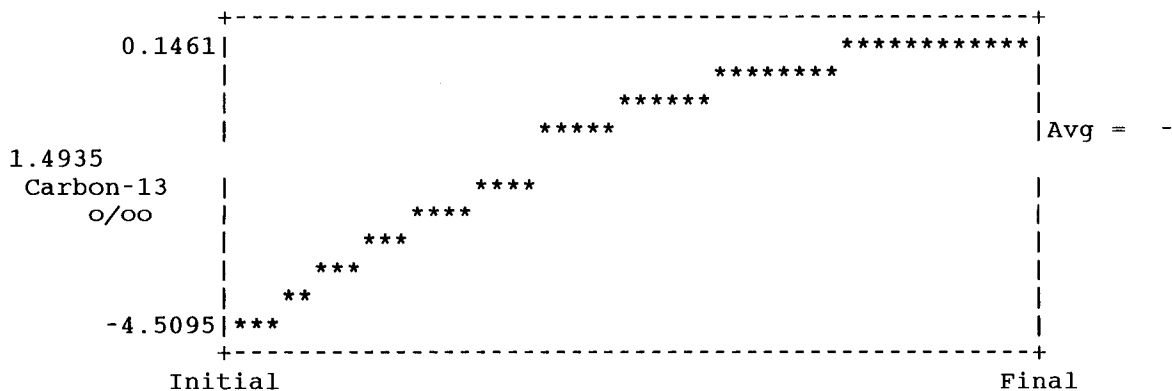
2 dissolving phases:

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

2 precipitating phases:

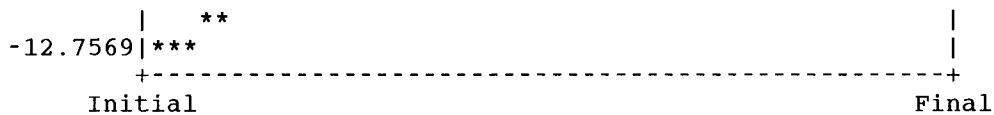
Phase	Delta C	Fractionation factor	Average Isotopic composition (o/oo)
CALCITE	-5.31723	2.3844	-1.4935
CO2 GAS	-0.04355	-5.9202	-9.7659

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

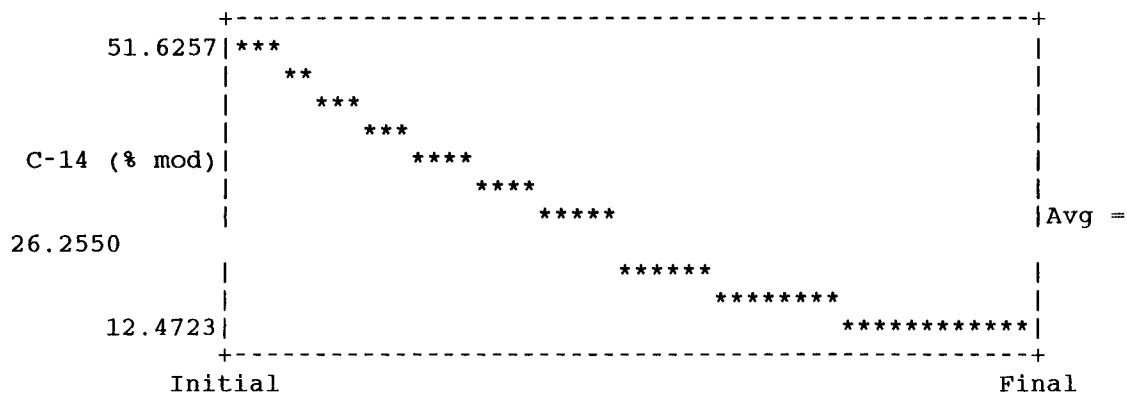
2 dissolving phases:

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

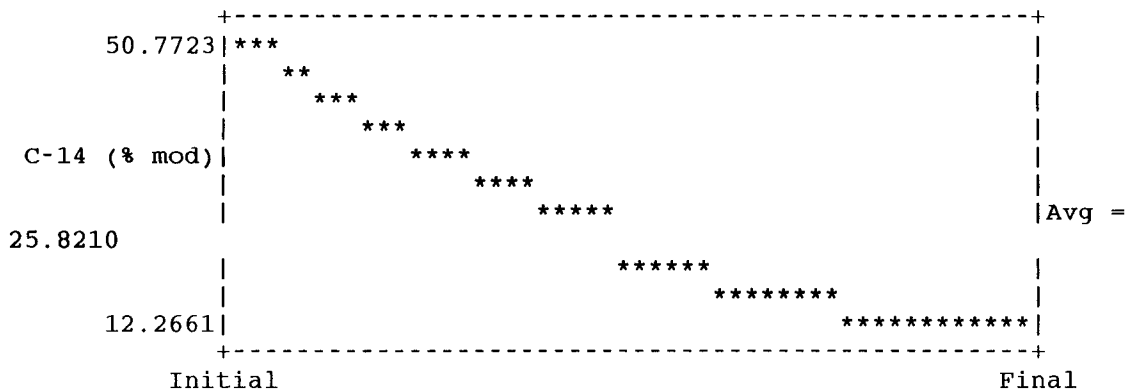
2 precipitating phases:

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

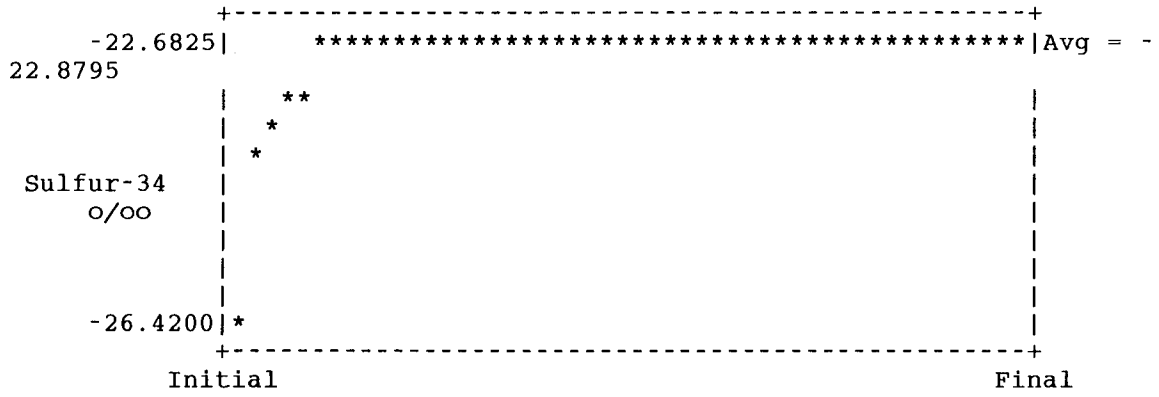
Initial Value: 9.7300 Modeled Final Value: 15.8130

1 dissolving phases:

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

1 precipitating phases:			Average
Phase	Delta S	Fractionation factor	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

np-7.out

Initial Well : Bemidjii Site AA  
 Final Well : Bemidjii Site BB

```

=====
| Constraints: 6 | Phases: 6 | Parameters | | | |
|---|---|---|---|---|---|
| Carbon        | Calcium     | MnO2       | GOETHITE  | SIDERITE  | Mixing: No |
| Iron          | Manganese  | Sorb NH4  | CO2-CH4  | CALCITE   | Evaporation: No |
| Nitrogen     | Redox       |            |           |           | Rayleigh Calcs: Yes |
|              |             |            |           |           | X CO2 in CO2-CH4: 0.14 |
|              |             |            |           |           | Init C-14 0.00 (TDC) |
|              |             |            |           |           | (Original Data) |
=====
  
```

```

=====
| Final      | Initial    | |
|---|---|---|
| C         | 12.4730   | 22.6890 |
| CA        | 3.0460    | 3.3220  |
| FE        | 0.0790    | 1.0550  |
| MN        | 0.1270    | 0.0160  |
| N         | 0.1450    | 0.1680  |
| RS        | 38.1867   | 56.9640 |

MnO2   MN   1.0000 RS   4.0000
GOETHITE FE 1.0000 RS   3.0000
SIDERITE FE 1.0000 C   1.0000 RS   6.0000 I1   0.0000 I2   0.0000
Sorb NH4 N  -1.0000 RS   3.0000
CO2-CH4 C   1.0000 RS  -2.8800 I1  -49.5540 I2   0.0000
CALCITE CA  1.0000 C   1.0000 RS   4.0000 I1   0.0000 I2   0.0000
  
```

1 model checked  
 1 model found

```

MODEL 1
MnO2           0.11100
GOETHITE       6.48751
SIDERITE      -7.46351
Sorb NH4       0.02300
CO2-CH4       -2.47649
CALCITE       -0.27600

      Computed   Observed
Carbon-13   -9.7397   -9.7385
DIC C-13    -5.9515   -5.9500
C-14 (% mod) Insufficient data
Sulfur-34   0.0000   Undefined
Strontium-87 Insufficient data
Nitrogen-15 Insufficient data
  
```

Data used for Carbon-13

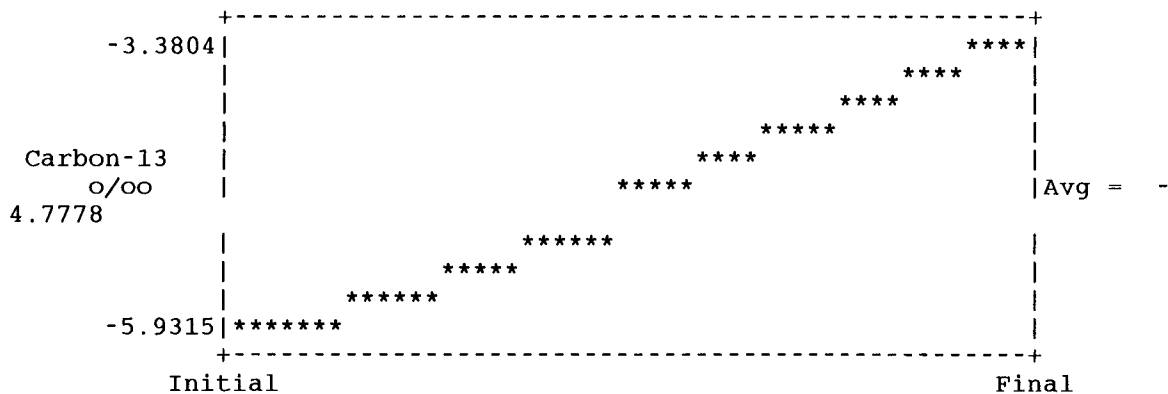
Initial Value: -12.3291      Modeled Final Value: -9.7397

```

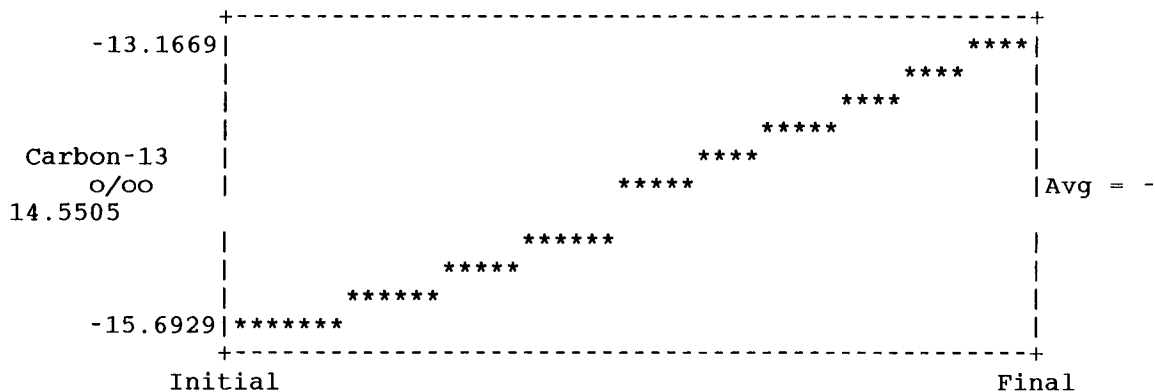
4 precipitating phases:
Phase      Delta C      Fractionation factor Isotopic composition (o/oo)
SIDERITE   -7.46351      6.4576               -4.7778
  
```

CO2 GAS	-0.34671	-3.4255	-14.5505
CH4 GAS	-2.12978	-43.9000	-54.5732
CALCITE	-0.27600	6.4576	-4.7778

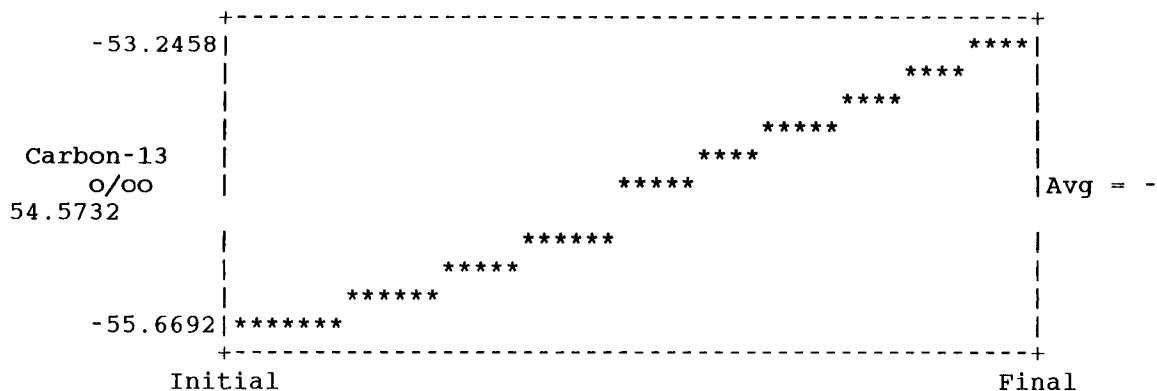
Isotopic composition of precipitating SIDERITE



Isotopic composition of precipitating CO2 GAS



Isotopic composition of precipitating CH4 GAS



Isotopic composition of precipitating CALCITE

