

**Electronic Scientific Notebook  
858E**

**Sensitivity of Repository Thermal-  
Hydrological-Chemical Simulations to Choice  
of Numerical Algorithm**

**Project # 20.06002.01.212**

**Lynn Sabido**

Notebook 858E  
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10/17/06

## **Sensitivity of Repository Thermal-Hydrological-Chemical Simulations to Choice of Numerical Algorithm**

**By** Lynn Sabido LS

**Objective:** To test the differences of the thermal-hydrological-chemical output of the near field environment of the potential repository at Yucca Mountain, Nevada among codes that use different split-operator algorithms at the reactive transport step.

**Training:** In order to perform said mentioned work one needs to be familiar with Multiflo and Toughreact computer programs and have a basic understanding of various aqueous systems and graphs and tools to interpret such systems. I personally read the instruction manuals and became acquainted with the program by performing examples from the books.

**Hypothesis:** Although the Global implicit algorithm (transport and chemical reactions solved simultaneous) is more accurate and computational demanding, the goal is to see how various split-operator algorithms (decoupled transport and chemical reactions) measure up and save time in comparison to the Global algorithm.

**Approach:** To use the same set of input files and run them through the various split-operator and Global implicit algorithms to compare the required run times, chemistry of seepage water, and volume fractions of precipitated minerals.

**Mathematical and other model assumptions:** The user is referred to the instruction manuals that accompany the program to determine theory and assumptions employed by the program.

**Input Files:** The input files were originally created by Scott Painter and were based on the TableC-1 in DST and TH Seepage report Rev 01 and Updated using Tptpl1 data from DSHT and THC Rev03 of the DOE report labeled MDL-NBS-HS-000001.

**File Location:** original files from S painter D:\originals\THC2006  
The working directory \\spock\home\lsabido\THC2006

**LS**

10/17/06

The original Multiflo files acquired from S Painter were modified to include F- and Fluorite that was in the DOEs report. The concentration and reaction rates came from revision 2 of the DST THC report.

I had previously put together a spreadsheet with the hydrogeology-thermal-chemical properties of the DOE case from revision 2 and compared it with S painters input files. This spreadsheet is in D:\THC and is named input\_details\_MF.xls

LS

10/25/06

I had planned on using the volumes and surface areas from the Toughreact sample problem number 3. However, I couldn't correlate the rock units, rather figure out why all the rock units were not present. I used the appendix of the Doe THC paper to figure out the volumes and SA of the Fluorite that was being added, some calculations were performed in excel (the file is found at D:\THC). However, these are the SA of a whole mineral, not just a fraction that would be exposed in the matrix or fracture.

LS

10/26/06

There was mention of a formula in the multiflo manual that could formulate the surface area that was needed from the whole mineral surface area. This involves some information I do not currently have, so I was planning on using a small arbitrary SA for the units that has 0 volume and for those units with a small volume (.0001) I will multiple the volume times the whole mineral surface area. Even though the conversion formula isn't linear, the estimates of surface area should work well enough.

LS

10/27/06

Altering the Fi.INP file for the THC to update the fluorite data, however, the numbers are still off.

LS

10/30/06

I couldn't find Specific surface area information on Silica, Fluorite, or Burkeite on Google or ask.com. The SA is needed to make sure the comparison is accurate, because we will use the SA for one mineral to use as fluorites SA in zones where there is no volume fraction of Fluorite. Using the equations in Multiflo, tried to gather the data needed, however, we don't know grain size.

LS

11/8/06

Looked on SWRI library resources and found some references to fluorite and Silica specific surface area, none were found for burkeite. Fluorite oxides with a grain size up to 3 microns have a SA of 10m<sup>2</sup>/g and amorphous silica for grain sizes 7-17 microns have a SA of 100-300m<sup>2</sup>/g. I was looking to convert the data in the THC file to do a density calculation; the data is in log form and then needs to be converted to mg/L for comparison to THC revision 2. This data then can be used in the conversion formula for Surface area. Density was ultimately assumed to be 1. D:\THC\fluorite1.xls This conversion shows that the chemistry for the problem is off from either sample listed in THC rev 2. Using the Matrix porosity from the file D:\THC\Input Details\_MF.xls, the

SA was calculated. The calculations are in the file seen D:\THC\fluorite1.xls . The fracture porosity needs to be extracted from the THC files to perform a similar calculation.

LS

11/9/06

There are no fracture porosity data listed in the THC files I was given. Not sure what at this point to use. The matrix surface area calculations were compared against other minerals in the fi.inp file, however, its not an accurate comparison because the volume fractions listed, do not match those of any of the various revisions of the drift-scale Coupled reports. So I do not know what mineral SA was used for the calculations. For amorphous silica whose volume fraction is zero, they took the mineral reactive surface values from the DOE report and divided by  $10^6$ . Not sure how the other values came about. For Glass the Volume fraction for the fractures match those of the DOE report (although the values have been divided by 100), however the matrix values do not. If the SA formula from multiflo is used to calculate the SA for the fraction portion of the glass, the calculated values for SA do not match those in the file. The same is true for quartz, tridymite, and cristobalite.

LS

11/10/06

The formula I used is incorrect. In Multiflo the Volume fracture is multiplied by 1-porosity, so in order to calculate the Surface area the formula is  $SA = SA^{DOE} \cdot (VF^{DOE} \cdot (1-\theta))$ . For fractures the porosity is 0.99, due to the large amount of void space, little is left for surface. I used the Porosity from the DOE report for the matrix, see calculations in D:\THC file fluorite1.xls

LS

11/21/06

Entered the new fracture and surface area for fluorites fracture and matrix into the multiflo input file and began the run.

LS

12/6/06

The file is still running and not converging, it is up to 1316 years; however the run should go out to 10,000 years. Adjustments will be made.

LS

12//8/06

The file had reached 1420 years, so the run was aborted. The output files indicate difficulty reaching convergence for each step this is what increased the run time.

LS

12/14/06

I recopied the original files given to me by S Painter and then reentered F into the chemistry and Fluorite information into the mineral section. I did this to ensure that all previous changes were corrected back to the original file. The delthH I found on the

internet was 47.7kj/mole. Other than that change all the data used is what had been discussed above. The THC run was initiated again.

LS

12/15/06

The run was stopped in order to make a few adjustments. I looked up a different delta H value from the PHREEQC database and converted it to the proper units. (19.623 KJ). It was suggested that the istepdt value be increased back to 3, the dtcutf lowered to 0.3 or 0.5. Also two separate runs will be started, one with a implicit time stepping algorithm, method 1, and one with the split operator algorithm, method 2. The first will be run with IOPS = 0, the second with IOPS=2. These runs were started out with the dtcuttf of 0.5.

LS

12/18/06

Method 1 run had been moving along over the weekend; however method 2 stopped because it exceeded its ihalv number. When I tried to alter the method 2 fi.inp file, the file wouldn't run and kept getting an error message. So I altered the file one parameter at a time, and it still wouldn't run. I intend to change the dtcutf to 0.3 and then alter other parameters as needed. However, I keep getting the same error message.

LS

12/19/06

It was pointed out to me that when updating the file from Lisa's old computer, wordpad is a dos editor and filled the file with odd characters that are not readable in unix. So I fixed the file on textpad at my computer, changed the dtcutf, and if that doesn't work, I'll make option adjustments.

LS

12/21/2006

The files seem to be moving along, however, the output files haven't been written to in 2 days but the run is progressing. There is a warning/error message "Notice max possible qw is less than the specified QBC. The next line states the IBC, qwmx, and qbc. After looking into this, the qwmx is computed internally and altering the qbc wouldn't make the run any faster. This error directly relates to the metra boundary condition file. There is a specified qbc, different than whats reported in the warning message. I believe it has something to do with equation e-16. However, no changes will be made at this time.

LS

12/27/06

The method one run had completed after 136 hours, however the method 2 run was still at 1620 years after 176 hour of run time.

LS

1/8/07

The F- value was wrong in the input file and is the reason why the file failed. I originally took the log of Mg/L instead of mol/mg, so hopefully the run will go faster. Scott also

suggested the QBC for the matrix be reduced in order to eliminate a continuing warning message that just increases the file size. There are now three runs set up method 1 (option 0-doesn't matter), Method 2 option 1, and method 2 option 2. After less than an hour the three files ranged from 70-282 years with M2O2 being the fastest.

LS

1/9/07

I made the changes to the runs and selected 3 different operator styles. As of this morning, one had properly completed, another had made it to 1600 yrs, and the last only to 840yrs.

So I'm going to try to pull the chemistry from the completed run (28 time step printouts-I'll pull (6-7) then evaporate them in Phreeqc. There is another mathematica script (concentrations, various 2 and 3 d models) I will work with to graph major changes to the various aspects of the system. The Mathematica notebooks will be located in the various method folders on spock. Similar notebooks will be created for each the fracture and matrix.

LS

1/10/07

Completed the Mathematica Notebooks, (note: when file is reopened the cursor to the right of the preliminary box needs to be re-run in order make changes or before any other cursor is used). I made a spreadsheet for Method 2 opt 2 and pulled 10 of the 28 seepage chemistries that started from 0 distances from the drift wall (or center) to 164m back to 0 distance at a few thousand years. I then included the time, seepage number, and temperature from the temp file for each. These will then be put into Phreeqc in order to evaporate them water to look at the mineral precipitation. Upon setting up the initial files for Phreeqc, I was unsure how to incorporate HCO<sub>3</sub><sup>-</sup> and CO<sub>2</sub>(g) based on the THC input file. Turns out that the value entered for HCO<sub>3</sub><sup>-</sup>, even though listed as type 4 and dependent on CO<sub>2</sub>(g), was the concentration and not the SI for CO<sub>2</sub>(g). The type 4 for HCO<sub>3</sub><sup>-</sup> was changed to type 7 and the M2-2 was restarted. The other two were corrected, but not started due to time restraints.

LS

1/11/07

The M2-2 completed and the mathematica notebooks were adjusted and the excel spreadsheet was corrected, the Phreeqc files created and run, and then graphs were made from the Phreeqc output.

LS

1/15/07

I started two new runs for the THC2006 modified files Scott Painter gave me (multi.dat and multi.phk). Two runs were started using method 1 and Method 2 option 2.

LS

1/17/07

The M1 completed and the mathematica notebooks were adjusted and the excel spreadsheet was constructed, the Phreeqc files created and run, and then graphs were made from the Phreeqc output. Also the modified THC runs were restarted using different files provided by Scott (multi.dat and multi.pck). Three versions were run using method 1, method 2 option 1, and method 2 option 2.

LS

1/18/07

Two versions of the modified THC files completed, method 1 and method 2 option 2. Seepchem was run and only two note book files were created for each, one for the matrix and one for fractures.

LS

1/29/07

The seepchem information was pulled for dryout zones starting at 0 distance from the drift (wall-center-Scotts not sure) at 50 years selecting important times that indicate the movement of the dryout zone boundary. This data was added to a spreadsheet then the chemistry, pH, and temperature values were used to create Phreeqc files. Phreeqc was used to evaporate the water in order to see the resultant SI of all possible minerals

LS

1/30/07

The capturing of data for the modified methods continued..

LS

1/31/07

The data pulled was then put into another spreadsheet to construct graphs to compare the chemistries, saturation indexes for method 1 and method 2-2, method 1 modified with method two modified, and then the original files with the modified files.

LS

2/2/07

Fixed a glitch with the chemistry used in the seepchem files (copy error), I also added the data for 1 and 10 years throughout the various files.

LS

2/5/07

The graphs for all chemistry comparisons were pulled, and overall SI for each model. I started pulling data for porosity, but will use the mathematica notebooks to cut and paste 2-d graphs.

LS

2/6/07

Tried to run THC problems on Coyote, but gave an error message (do not have access). Put in IT ticket.

LS

2/26/07

Received two revisions to the unmodified (without VPL) runs, the wtkin will be changed to 0.5 instead of 1 (for method 1 and Method 2-2). These will be run in Dos and on Coyote to compare run times and the THC2-2 will be run as is to compare run times between Coyote and Texas. Scott P needed to recompile the multiflo program in order to have it run properly on Coyote, also the cshrc file needed to be modified (my unix account) in order to run the program and access the right directories and libraries.

LS

2/27/07

Texas took 3 hrs to run THC2-2, Coyote took 6.8 hours. The Dos runs also completed successfully and ran the THC2-2 in 1.6hrs, THC2-2 wtkin=.5 in 1.6hrs, and the THCwtkin = .5 in 7.2 hours. Coyote is set up to run both files in which the wtkin was altered.

The Dos runs will be set up in Mathematica notebooks to mainly look at porosity.

LS

2/28/07

I put the porosity notebooks for the Wtkin=0.5 runs in my Spock folder (THCDos). There are a separate notebook for matrix and fracture in both the method 1 and method 2 folders. The Fracture graphs look the same; however there is a variation between the matrix predictions. In method 1 the matrix porosity increases slightly and decreases in method 2. The same plot coordinates, data range, and color scheme are used for both. The variance is so small (range .145 to .5) it shouldn't be significant.

LS

3/1/07

The modified (with VPL) runs were completed, and all the fracture and matrix notebooks were separated out and put into a separate folder for comparison on the spock drive. Below are inserts of the run times of the problems between Dos and Texas along with a brief comparison between runs-meaning wtkin 1 and 0.5, and Methods one and two.

Run times	Texas	Dos	coyote
THCM1-Wtkin=1	21		
THCM2-2-Wtkin=1	3	1.6	6.8
THC_mod_M1-Wtkin=1	16		
THC_mod_M2-2-Wtkin=1	2.4		
THCM1-Wtkin=0.5		7.2	didn't finish
THCM2-2-Wtkin=0.5		1.6	6.8
THC_mod_M1-Wtkin=0.5		5.9	
THC_mod_M2-2-Wtkin=0.5		1.2	



## Porosity comparison

<b>Matrix</b>	notebooks	
specifications (0,30), (-25,25) range (0.14-0.15)		
Runs	type	comments
M2-2 wtkin=1	Very Similar	Off a bit - predictions of area where ultimately porosity is affected'
M2-2 wtkin=0.5	to eachother	
Modmeth2 wtkin=0.5	same	Doesn't reach as high porosity as others just below 0.14
Modmeth2 wtkin=1	same	Doesn't reach as high porosity as others just below 0.15
Mod2-1 wtkin=1	oddball	porosity off and at 100 yrs all same throughtout
M1 wtkin = 1	similar	
M1 wtkin = 0.5	similar	
Modmeth1 wtkin = 0.5	similar	higher porosities closer to the drift
Modmeth1 wtkin=1	similar	0.15 predicted close to drift varies further out
mod meth wtkin 0.5+1	same	
<b>Fracture</b>	notebooks	
specifications (0,30), (-15,15) range (0.7-1)		
Runs	type	comments
M1 Wtkin=1	similar	More area with lower porosity right at drift in M1 wtkin 1
M2-2 wtkin=1		
Mod2-1 wtkin=1	oddball	Porosity starts off at 1 and then at 100yrs all is 0.7
M1 wtkin = 0.5	same	These two are the same
M2-2 wtkin=0.5	same	
Modmeth2 wtkin=1	similar	Porosity slightly higher at drift at end of run
Modmeth1 wtkin=1	similar	Porosity slightly lower at drift at end of run and encompasses larger area
Modmeth1 wtkin=1	same	
Modmeth1 wtkin=0.5		
Modmeth2 wtkin=1	same	
Modmeth2 wtkin=.05	same	
M2-2 wtkin=.05	silmilar	Slightly lower porosities for longer periods of time

LS

3/5/07

A few more runs were set up. One with the original THC method 1 wtkin=1, however Calcite and Gypsum were suppressed due to the fact of higher than normal precipitation and total plug effects. Method 2-2 and 2-1 were run with wtkin=0. In some of the runs it appears that amorphous Silica doesn't dissolve as fast as it should upon re-wetting. The Doe used  $7.32 \times 10^{-13}$  (MF  $7.32 \times 10^{-17}$ ) for the dissolution of Am Silica; however in Tough react they used  $1 \times 10^{-10}$  for the precipitation of Am Silica. That is how the mineral section is set up-separate entries for the dissolution and precipitation of individual minerals In Tough react. I'm not sure if you can enter it in twice With a fkin as  $1 \times 10^{-20}$  for the reaction constant of  $7.32 \times 10^{-17}$ , and a separate entry for fkin=1 and a reaction constant of  $1 \times 10^{-14}$ . I wasn't sure about Nrxn under the mineral section pg 2-113 of the manual. I assume it meant how many reactions present that will produce Am Silica.

So far the porosity values I found in the DOE report (which are few-summation table) match that of the fracture (multi.dcm) and Matrix (multi.phk) files. I haven't seen anything yet to suggest the reaction constants are pH dependant.

LS

3/6/07

The run in which Calcite and Gypsum were suppressed was still running and after 12 hours had only reached 1822 years. This was run on Cheryl Pattons computer along with the Meth2-2 wtkin=0 (2.7 hours to complete). I also ran Meth2-2 wtkin=0 which completed in only 1.7 hours and was run along with Meth2-1 Wtkin=0 that took 2 hours. The following files were used for a Cl- vs time comparison and will be further used for other chemical and evaporate comparisons.

A few more runs will be set up that have a delcmax of 2 instead of 10 and all with a wtkin=0. Method 1, Method 2-2, and Method 2-1 all without VPL.

LS

3/7/07

The Method 2-2, and Method 2-1 with a delcmax of 2 with a wtkin=0 finished running in 4.6 and 3 hours respectively. The seepchem was extracted for both and added to the Cl vs time spreadsheet.

It appears that the calculation of the reaction rate is not dependant on pH. The Doe2003 Paper states [by neglecting the effect of pH or other aqueous species activities on reaction rates...]

Method 1 W0 Delcmax 2 will be set to run tonight.  
LS

3/8/07

The Method 1 W0 Delcmax 2 run failed at 5198 years the number of tries was exceeded so the program aborted the run. The Delmax was increased to 5 and rerun on my computer.

I was trying to show the effect of Amorphous Silica dissolution/precipitation above the drift upon heating and rewetting. I used the seepchem data (step 14) and entered it into Phreeqc, evaporated as much water as possible (55.4moles) and then added water back and used 145 134 128 118 103 88 for the reaction temperature which come from the seepchem files 14-19. This was done to see how much and how quickly the Am silica and quartz would dissolve. For the time frame, I'm not getting the infiltration correct.  
LS

2/6/08

Work on this project has halted; the notebook will be closed and handed in to QA. If the project is to be resumed in the future a new notebook will be created.

LS

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