

**Electronic Scientific Notebook
898E**

**Evaluating the DOE's Near field process as
discussed in TDR-TDIP-NF-000005.**

Project # 20.06002.01.212

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8/13/07

Evaluating the DOE's Near field process as discussed in TDR-TDIP-NF-000005.

By Lynn Sabido LS

Objective: The DOE will be releasing a new Physical and chemical environment report that summarizes the new approach to modeling the near field flow and chemistry that feeds into the total system performance assessment. To create a similar plug flow model that represents the system above the potential nuclear repository at Yucca Mountain. To assess if modeling flow and chemistry separately accurately depicts the system.

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 aqueous systems and carbonate processes. I personally read the instruction manual and became acquainted with the programs by performing examples from the books.

Hypothesis: Some details discussed in TDR-TDIP-NF-000005, in which a plug flow model is set up and chemistry is modeled separately. The four units above the repository were averaged, the run was made into a single continuum and the values were weighted based on thickness of each unit. For this project a similar model system will be created to evaluate the effectiveness of separating flow from reaction and the results should be comparable to those performed by the DOE. Further, then the potential seepage chemistries and resultant evaporation products will also be evaluated.

Approach: Set up Multiflo and Toughreact input file that mimics the steps followed to create the plug flow experiment that simulates flow and chemical reactions separately which is in turn feed into the TSPA model. This will be done by pulling the various input parameters from the TSPA March, 2007 report and the documentation referenced within. The sample problem 3 from the Toughreact Manual will also be used to gather data. This will be compared to DOE results and dual continuum results. If the separation of the processes seems reasonable, then extra efforts will be made to validate the possible seepage chemistries and the evaporation products. Any further adjustments will be noted.

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

Input Files: The input files will be generated based on the referenced documentation and will be summarized in an inputs.xls spreadsheet.

File Location: D:\Nearfield, however at the conclusion of this project all files will be transferred to a cd that will accompany this notebook.

LS

8/13/07

I have created a spreadsheet that will accompany this notebook that details the specific inputs required to run a plug flow model using Multiflo and toughreact programs. The spreadsheet contains several pages including, but not limited to a list of parameters, a page of calculations, a reference page, and a file excerpt page.

A few notes about the calculation worksheet. The matrix saturation, porosity, and mineral abundances used the values provided in the DOE report and were averaged using a weighted method based on unit thickness. Many parameter values were extracted from the Problem 3 that accompanies the Toughreact program. To account for the fracture and matrix averages for parameters such as grain density, permeability, Van-Genuchten properties the volume fraction of the fracture and matrix portions of each unit was used to weight the values for each unit. These averaged values were then weighted accordingly based on unit thickness. Based on the lithostratigraphic and UZ model layers, TSW33, is made up of two units the Tptrl and Tptpul. This isn't a problem, because all the values reported apply to both those units. The Tptpln layer is made up of two UZ sublayers (TSW 36 and TSW 37). Where these two reported the same values, no changes to the calculations were performed. When the values differed for TSW 36+37, the values were averaged between the two, then that averaged value was used to factor the weighted average of the Tptpln unit as a whole.

	UZ
	model
Lithostratigraphic	layer
Tptrl	TSW33
Tptpul	TSW33
Tptpmn	TSW34
Tptpll	TSW35
	TSW36
Tptpln	TSW37

For other needed parameters not mentioned in detail within the provided reports will have a best fit value or commonly accepted value used and will also be documented in the above mentioned worksheet. The initial pore water chemistry, Group2, was selected because it had the highest Ca concentration, and reported all the essential concentrations including SiO₂ and HCO₃. These values have begun being feed into input files for both programs.

LS

8/17/07

Multiflo will be set up to demonstrate they separation of flow and reactive transport, until further notice in which a input file for Toughreact will be modified/created. The Gem file was updated using the information from the input.xls. The list of secondary species was initially taken from another Yucca mountain example and in addition other possible

salt species were added. In order to make the number reactions and number of equations equal some unnecessary secondary species were eliminated. The time scheme was taken from this same Yucca (THC) problem that specifies the times, and steps up to 10,000 years. The minerals were adjusted, but still data is missing, however SiO₂ (am) and calcite should be in equilibrium with the system. The file will be later tweaked to add k-spar, but the database must be altered first. The Metra file was begun, however the qbc, needs to be pinned down and there is a problem with the time step cuts exceeded the maximum.

LS

9/6/07

The metra file is now running since adjusting the limit parameters and decreasing the gas saturation to .99. Some of the parameters that were averaged for the 3 units were adjusted because the weight average of TSW6 and TSW7 that make up unit Tptpln was not properly calculated based on volume. (Tsw6 = 66.6% and Tsw7 = 33.3% both the fracture and matrix of unit Tptpln. The infiltration rate was calculated based on 0.5L per day. These calculations can be seen in the Inputs spreadsheet on the calculation tab.

LS

9/7/07

The input parameters for both the Gem and Metra files of the Multiflo program were altered based on yesterdays corrections. Some of the incomplete data has been based on the Toughreact example 3 (Yucca Mt.) problems. There are a few loose ends, such as a few calculations for mineral surface area and initial volume. Right now both files are running, but need to be updated.

LS

9/10/07

The files were both run separately while altering one parameter at a time, (such as saturation, temperature, system pressure, diffusion coefficients, and flow properties). The default gas diffusion parameter from the multiflo manual was used and the liquid diffusion coefficient should be on an order of 4 times smaller. The mineral surface areas and fractions will be calculated from the problem 3 file; however the setup needs to be understood first.

LS

9/11/07

The original Toughreact example 3 (Yucca Mt.) problems was cut down to include only the four units of interest which correlate to TWS3-7. The problem was run as a dual continuum with infiltration and without infiltration. The option in Solute.inp to allow feedback affects from changes in porosity, permeability, and capillary pressure was turned on. The original TR file specifies the aqueous diff coeff as 2e-9 m²/s and it allowed for the gas diff coeff to be calculated. I changed the gas diff coeff to 2e-5 now both the TR and MF files match for diff coefficients. The print options, writing controls, and mineral pointers were also altered. The nodes selected for print were picked randomly through the column, but grouped closer to the top and bottom.

The mineral section (chemical.inp) was altered; gypsum and glass were deleted and SiO2am and calcite are to be equilibrium with the system.

NOTE: When deleting or editing the mineral section of chemical.inp, all minerals in equilibrium must come before those under kinetic constraints.

In the TR Flow.inp file the Gener keyword was updated to actually allow infiltration at a rate of .5L/day. The activation energy (A_e) was changed to the default found in MF of 12.6 or $7e5$ J/Kg. There was little change when using the original and new A_e value. The run time was bumped from 100 to 10000years. The saturations of the selected cells do show a small glitch towards the bottom of the column. The liquid saturation in the bottom most cells is slightly increased to those directly above. There may be an issue with the lower boundary.

The Multiflo files were re-run after matching up the target times between the gem and metra files. The TR printouts will need to produce the same target times as MF, however if the files become too large, TR will automatically abort the run. This must be adjusted within the solute.inp file.

LS

9/12/07

The mineral section for both codes still need to be updated. The Toughreact dual run will also be pared down to a single continuum once all the properties are weighted, and the initial mineral content is decided and averaged. The Dual TR run file runs without error for 1000yrs, but will not complete a run of 10000yrs. The single TR file was set up, but calculations still need to be performed on the initial mineral section of example problem 8. The Mineral volume fraction needs to be calculated and averaged (based on volume fractions of the matrix or fraction volume that make up the whole system). Also the reactive surface in problem 3 is defined as cm^2/g and for multiflo it needs to be $1/\text{cm}$.

LS

9/21/07

After pulling information from the original TR manual (and DST THC seepage model, 2001) and the Multiflo manual it was decided how to proceed with the averaging of the rock properties.

Porosity and Volume fraction as defined in the Multiflo manual (b-36) and Toughreact manual (F.1). The volume fracture for both refer to the $V_{\text{mineral}}/V_{\text{medium}}$ (total volume of rock including pore space.). So the volume fractions are interchangeable, but in order to be averaged from the example file calculations based on the matrix/fracture volume need to be considered. So

$V_f(\text{fracture}) * \text{Volume \%}(\text{fracture/matrix+fracture}) + V_f(\text{fracture}) * \text{Volume \%}(\text{matrix/matrix+fracture}) = \text{total } V_f \text{ of that unit.}$ The Volume % was calculated in the inputs spreadsheet. The V_f given for the matrix and fractures in the sample 3 problem are the volume % of just the matrix and fracture respectively.

Porosity and mineral volume fractions are related by the equation

$$\phi = 1 - \sum_{m=1}^{N_m} \phi_m \quad (\text{B-36})$$

The porosity of the medium (fracture or matrix) is given by

$$\phi = 1 - \sum_{m=1}^{N_m} f_m - f_n \quad (\text{F.1})$$

where N_m is the number of minerals, f_m is the volume fraction of mineral m in the rock ($V_{\text{mineral}}/V_{\text{medium}}$, including porosity), and f_n is the volume fraction of nonreactive rock. As the f_m of each mineral changes, the porosity is recalculated at each time step. The porosity is not allowed to go below zero.

.....

The Surface area calculations from toughreact to Multiflo as follows
 $Sa \text{ (cm}^2/\text{g in TR)} * Vf * \text{Density} * \text{volume \% (inputs spreadsheet)} = Sa \text{ 1/cm}$
 The Surface areas can then just be added up for each unit TSW3-7.
 LS

9/25/07
 After reading a paper by L Browning (year?), I realized that the Activation energy values I pulled from the Toughreact problem 3, I had entered into the Multiflo model which uses Activation enthalpies. The conversion equation is
 $He = Ae - RT$
 Where He = Activation enthalpy, Ae = Activation energy, and $R = .008314 \text{ KJ/mol K}$, and T is temperature in Kelvin (298.15). These changes were made in the "Inputs" spreadsheet. The Volume fraction averaging using the above equations was added to the inputs spreadsheet.

LS

9/26/07
 The Surface area calculations have been added to the Input spreadsheet. Two different calculations, one to average the parameters in the units entered into toughreact, so eventually the file can be run as one averaged rock unit, and secondly averaging and converting the SA from cm^2/g to $1/\text{cm}$. To convert to units of $1/\text{cm}$ the following equation was use.
 $SA \text{ (1/cm)} = SA \text{ (cm}^2/\text{g)} * Vf * \%VofRock * \text{density}$

where
 $\%VofRock = \text{vol frac/total volume or } V \text{ matrix/total volume}$

The other mineral parameters that were missing such as Activation enthalpy and reaction constant were taken from another multiflo run used to perform THC modeling. The Multiflo and

Toughreact files were updated. However, there are still problems with the saturation and mineral precipitation/dissolution. I had added gypsum to the multiflo file as being in equilibrium, but excluded it from the toughreact files. Also the reaction constants may need to be adjusted to get the desired results.

LS

9/27/07

Gypsum will be incorporated back into the tough file in equilibrium (as seen in TR sample problems 3+4), also initially albite will be added to represent the feldspar component. Any missing rock parameters will be taken from the example 3 files, if this is not satisfactory, then the information will be pulled from example 4 (including the albite data).

LS

10/1/07

The Albite data was calculated in the "inputs" spreadsheet. The volume fraction was equal to 1- (total of all other minerals). The Surface area was calculated the same as with the other minerals, but assuming the area listed in each unit was the same for albite. Gypsum has been added to the toughreact file and when the albite_low was added AlO₂ needed to be added to the chemistry composition (0.6e-9 from example 4). For the multiflo database Al will have to be entered in order to add Albite_low as a mineral.

LS

10/2/07

Albite is kinetically controlled and therefore needs to be placed at the bottom of the mineral list in the chemical file of toughreact. In multiflo even after the Al aqueous species is added, an error message arises "Warning: possibly skip reaction, i nam(i) = 3 al+3".

Not sure what the error exactly means, but if any secondary al species are entered then there are too many unknowns versus equations.

LS

10/18/07

I tried to extend the length of the toughreact run to 1000 years; however the file only ran to about 587 yrs. There are no error messages in the dump files.

LS

10/19/07

The multiflo gem file is working and the error (syntax error) was discovered and changed. The simulation ran through 10,000 yrs without errors. The single continuum tough file has yet to be altered and depends on the final setup used for the dual continuum.

LS

10/22/07

Changing “Param” parameters in order to successfully complete 1,000 years, but the run is getting no further than before. I’m looking into the file for possible causes, and making comparisons to the Multiflo single continuum for compatibility.

LS

10/24/07

I noticed that in the mesh file, the x, y cell sizes were 0.5 rather than 1, which really affects the infiltration amount. If I change the mesh maker to get an x, y cell of 1.

NX 1 2.0

NY 1 2.0

NZ 400 0.5

The toughreact file completed until 2,290 years.

LS

10/25/07

I unsuccessfully tried to delete the additional boundary layers in the flow file, thinking that would alter the files progression.

LS

10/29/07

For the time being, I will compare and update the files to run only to 1000 years. This way the time for each run is shorter and file modification should be easier. Once some of the bugs are worked out the files will be bumped up to 10,000 years. While comparing the Toughreact file to Multiflo, it appears both precipitate calcite on the order of $0.5e-6$ and TR shows dissolution of Albite on the order of $1e-10$. Albite dissolution wasn’t noticeable in MF because the output reports current mineral volumes, while TR reports changes in mineral volumes. When comparing the concentrations, I noticed discrepancies in the input files, TR hadn’t been fully updated and NO₃ was added and the database used was changed from therm208 to therm1.01 which was updated for version 3 and up. This database was found in example problem #4 folder, where as the previous came from example 3 folder (calcite problem). However, when the TR file was re-run the calcite mineral volume didn’t increase as it did before.

LS

10/30/07

In order to compare output files they need report similar types of data and a format in which to compare those needs to be the same. I tried plotting various graphs on tecplot for both TR and MF, however, being a 1-D model, the choices are limited and for some reason the files loaded, but the data wouldn’t graph or show correctly. According to the spreadsheet created “inputs” there are specific minerals in equilibrium, allowed to dissolve only, and those allowed to dissolve and precipitate. The MF gem file was altered to $1e20$ for the Ikin value to prevent precipitation of certain minerals.

LS

10/31/07

In the TR file several writing control values in the solute file were changed. The aqueous species changed to molality to match that of MF, the aqueous species concentration, rather than total aqueous component concentrations, and mineral reporting was changed to current mineral abundance in volume fraction. The print out frequency was changed to 10, as was the mcypr in the param keyword. In order to make a comparison between MF and TR easier, the data reported for both were adjusted to the same cells (within the programs such as TR solute and flow files). Also in TR Flow file a time keyword allows you to specify the output times for the cells selected. However, the printout options didn't perform as the manual stated. Specific times were entered but not observed in the TR output files.

The MF file run yesterday that specified 1e20 for the Ikin value had no mineral volumes for any listed mineral. After changing back the values, there was still an error within the file and the previous untouched file from the beginning of yesterday was used. The TR file showed no value for fluorite even though it was initially present; all minerals with a volume fraction of 0 within the chemical file were changed to .0001.

LS

11/1/07

The MF file was corrected since some of the rock properties were switched since fluorite was significantly off. Also, it allows anything to precipitate and dissolve, which may not be the case, so this was changed mineral by mineral (ikin = 1e20).

LS

11/2/07

The initial mineral volumes in the TR and MF output files are similar now that the kinetic controls have been matched (although Albite is allowed to precipitate and dissolve in both codes, even though initially it was meant to dissolve only). Upon comparison of the aqueous species, the basis components are similar. The TR output is not reported all the minerals specified in the solute input file, to remedy this, some species were deleted from the writing list. The porosity is correctly specified in both codes; however multiflo has an initial porosity (.0023) that is far off from that reported by TR (.154) and entered into the input file. Not sure what the problem is looking at the output.

LS

11/05/07

For the Multiflo input files the gem file looks to be correct. However, I'm looking into other options for the porosity.

LS

11/7/07

For the gem MF file I wasn't sure of the output files produced, however only the total aqueous concentrations will be pulled to match that of TR. The BRKP data block was added to print a separate file that can be uploaded to excel.

PLTFiles

:iplot a s t m si sf v z b in e ex ti g itex

1 0 0 1 0 0 0 1 0 2 0 0 0 0 1 2

Since the gem and metra portions of Multiflo are run separately the couple keyword shouldn't make a difference. However, the gas velocity isn't specified and the liquid velocity is converted from the infiltration rate, but I'm not sure that accounts for the infiltration, in metra the infiltration is specified (QBC) at the boundary conditions.

LS

11/8/07

The gem file was changed to isothermal (o-in the isys keyword), this shouldn't affect the run because for know it's at a constant 25 C. I can't find a gas flow measurement and I'm not sure how that affects the run.

Currently the isys keyword specifies the systems porosity and permeability, not the matrix, which should be fine since this is a single continuum.

```
: isat isothrm iread phir por0 sat porm satm lambda toldelt tolpor  
ISYSstem 0 0 0 1. 0.1393 0.7 0. 0. 0.28987 1.e-3 1.e-3
```

LS

11/9/07

After speaking with J Myers, the run will be converted to a 2-D problem to help with potential future problems when the heat is added. The toughreact sample 4 problem will be scaled down to the four units of concern. From this the actual depth TR 4 will be cut down to the 4 significant units, and the horizontal distance will be kept as is for now. Eventually a single averaged continuum file for the TR code may be made. For MF, a file from a former project, THC, will be used to model the dual continuum. The existing averaged data will then be used in MF to create an averaged single continuum model.

LS

11/19/07

After spending some time trying to cut down the original THC files to only the four units of interest, Scott suggested either cutting off the units above the Tsw units, or changes the mineral properties to those units to burkeite. By changing the overlying units to the non-reactive mineral burkeite, the infiltration water will be unaffected when passing through these layers. Burkeite volume + porosity = 1 for each unit. Initially changing the above units to burkeite will be made, eventually cutting down the file to eliminate the above units may be implemented.

LS

11/27/07

The gem file was changed according to the equation above (data in spreadsheet labeled burkeite), however this method replaces all the minerals with burkeite and all mineral is in the matrix fraction. Using the same spreadsheet, I added all the volume fractions and surface areas for both the matrix and fractures, separately, for each unit. The gem file will slowly be altered to make the change for the top few layers to consist of only burkeite.

LS

11/29/07

After the volume fractions and surface areas were added to the gem file, the chemistry was altered to reflect that of the one used in the total system performance assessment data input package for EBS-P+C environment (March 2007) paper that starts with the water composition from the Tsw33 layer. The file was run as non-isothermal.

LS

11/30/07

The same file from yesterday was also run as an isothermal run. The previous non-isothermal run will be compared to the original THC file make sure the porosity has remained the same. Then the seepchem files will be extracted for comparison to the THC file and they should be comparable.

LS

12/3/07

I have been having problems running the Seepchem files. Mathematica 5.1 on sun solaris may be set up wrong. IT can't find the "home" directory, not sure if the file knows the home is now Texas and not spock. I'm running a script that scott made, it worked before the switch over. Its running, It just can't write. It's supposed to create files named seepchem1 through #, and write data to them. Here is the error message below see where it points to usr/bin/test I think that's invalid and it performs Openwrite to Home.....Maybe it can't find Home (aka texas). I tried it with my two unix accounts same results for both, I checked my profile for mathematica (the old and new accounts) and there is nothing to change, it's the same files we only changed the tecplot info. Is there a mathematica file that points to the correct files, I know we had to change the command to access some programs since texas is home. I was figuring this is the same kind of thing.

Error messages

```
$ math < seepchem.m  
/usr/bin/test: /dev/null: cannot create  
/usr/bin/test: /dev/null: cannot create  
Mathematica 5.1 for Sun Solaris (UltraSPARC)  
Copyright 1988-2004 Wolfram Research, Inc.  
■ Motif graphics initialized –
```

OpenWrite::noopen:

Cannot open /home/lmsabido/nearfield/MF-Dual/heat/seepchem1.dat.

General::openx: seepchem1.dat is not open.

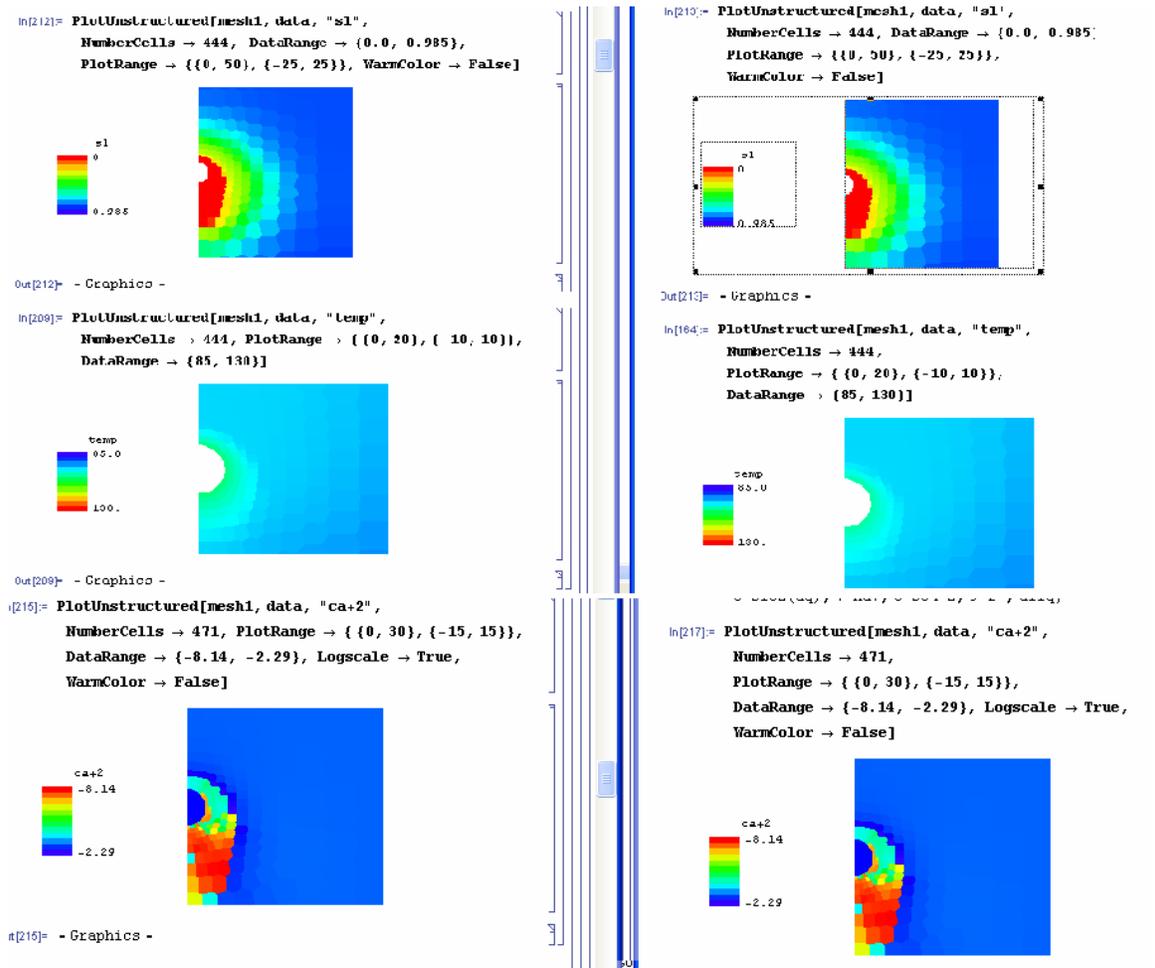
OpenAppend::noopen: Cannot open seepchem1.dat.

After running the mathematica graphing scripts, the porosity of the near field versus the original THC files are not the same. The burkeite needs to be set to 0 for the reaction rate and also the surface area set to 0. Then the total volume fraction of the minerals plus porosity should add up to 1. I know one unit where the volume fraction alone is over 1.

LS

12/04/07

The porosity taken from the phk file was used as originally planned (see Burkeite spreadsheet). Only the first 3 of 6 layers differed when adding up the volume fractions as opposed to using Porosity + Volume rock (fractions added) = 1. The burkeite Volume fraction was relatively high for these units. The porosity of the fractures is around 0.99% so the mineral fraction is .01. I used the values from the burkeite spreadsheet. Below is a comparison of the results. The nearfield graphs are on the left and the original THC graphs are on the right.

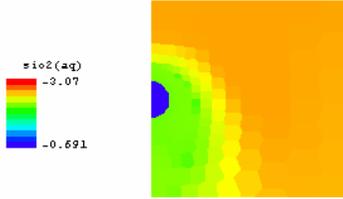


Saturation of liquid, Temperature, and Calcium (aq) comparison. Near field run on the left, original THC run on the right.

```

In[222]= PlotUnstructured[mesh1, data, "sio2(aq)",
  NumberCells → 471,
  PlotRange → {{0, 30}, {-15, 15}}, Logscale → True,
  WarmColor → False]

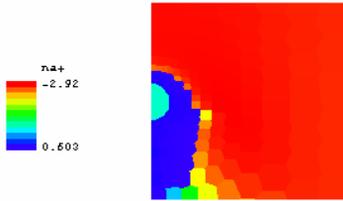
```



```

In[231]= PlotUnstructured[mesh1, data, "na+",
  NumberCells → 471,
  PlotRange → {{0, 30}, {-15, 15}}, Logscale → True,
  WarmColor → False]

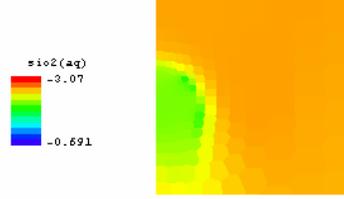
```



```

In[225]= PlotUnstructured[mesh1, data, "sio2(aq)",
  NumberCells → 471, DataRange → {-3.07, -0.691},
  PlotRange → {{0, 30}, {-15, 15}},
  Logscale → True, WarmColor → False]

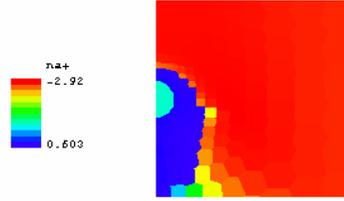
```



```

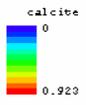
In[233]= PlotUnstructured[mesh1, data, "na+",
  NumberCells → 471, DataRange → {-2.92, 0.603},
  PlotRange → {{0, 30}, {-15, 15}},
  Logscale → True, WarmColor → False]

```



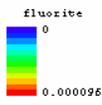
SiO₂ (aq) and Na⁺ aqueous species comparison. Near field run on the left, original THC run on the right

```
In[247]= PlotUnstructured[mesh1, data, "calcite",  
DataRange -> {0.0, 0.923}, NumberCells -> 444,  
PlotRange -> {{0, 30}, {-15, 15}}]
```

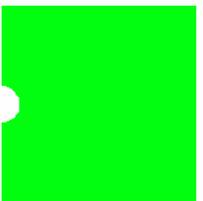
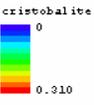


Out[247]= - Graphics -

```
In[248]= PlotUnstructured[mesh1, data, "fluorite",  
NumberCells -> 444, PlotRange -> {{0, 30}, {-15, 15}}]
```

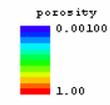


```
In[257]= PlotUnstructured[mesh1, data, "cristobalite",  
DataRange -> {0.0, 0.310}, NumberCells -> 444,  
PlotRange -> {{0, 30}, {-15, 15}}]
```



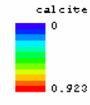
Out[257]= - Graphics -

```
In[258]= PlotUnstructured[mesh1, data, "porosity",  
NumberCells -> 444, PlotRange -> {{0, 30}, {-15, 15}}]
```



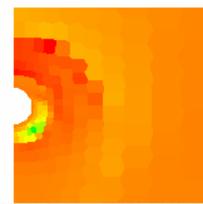
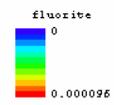
Out[258]= - Graphics -

```
In[242]= PlotUnstructured[mesh1, data, "calcite",  
NumberCells -> 444, DataRange -> {0.0, 0.923},  
PlotRange -> {{0, 30}, {-15, 15}}]
```

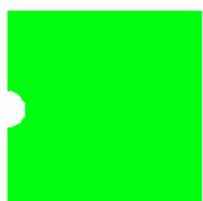
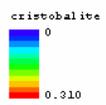


Out[242]= - Graphics -

```
In[243]= PlotUnstructured[mesh1, data, "fluorite",  
NumberCells -> 444,  
PlotRange -> {{0, 30}, {-15, 15}}]
```

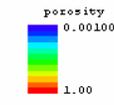


```
In[249]= PlotUnstructured[mesh1, data, "cristobalite",  
NumberCells -> 444,  
PlotRange -> {{0, 30}, {-15, 15}}]
```



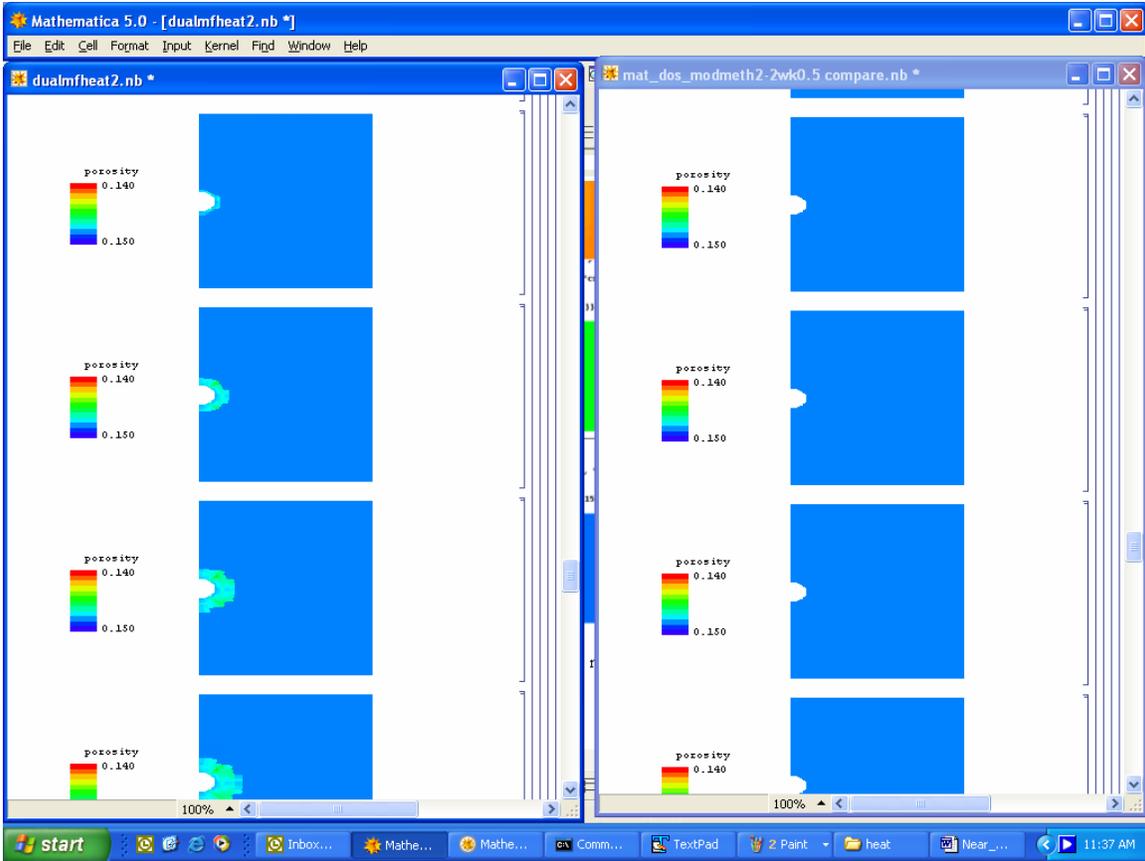
Out[249]= - Graphics -

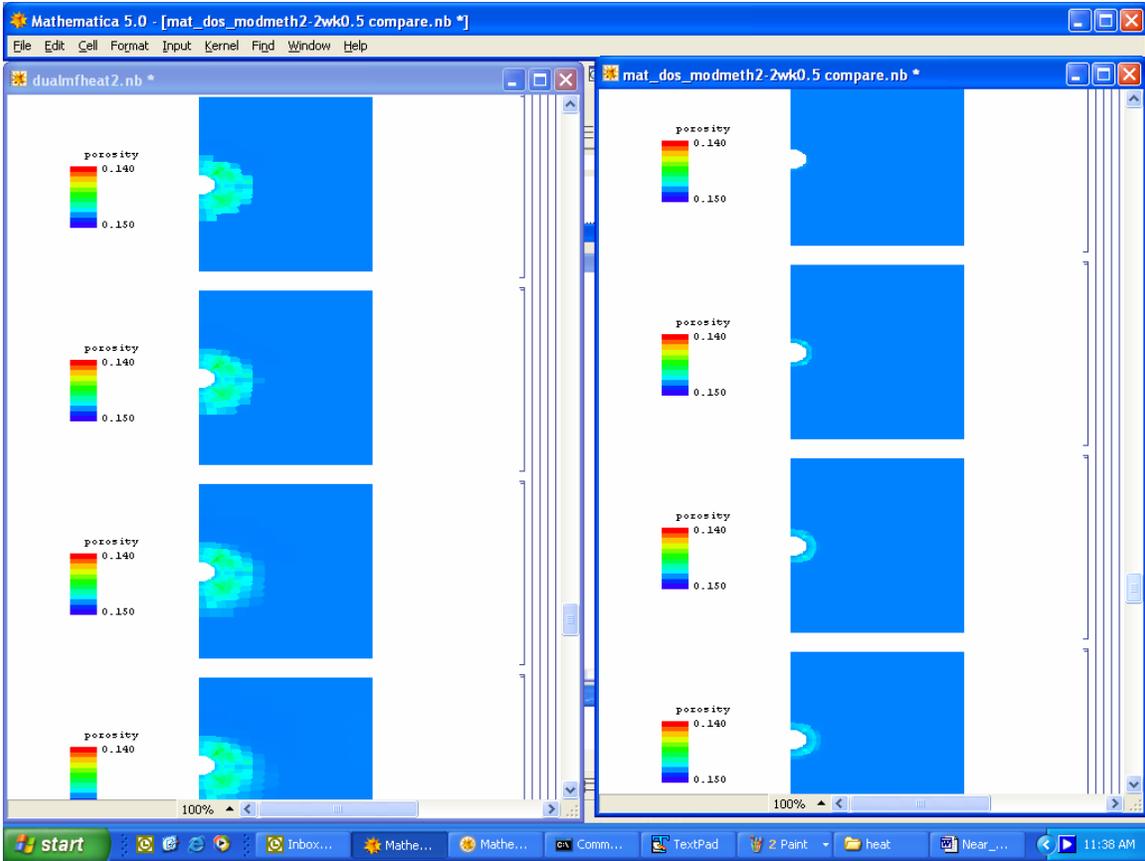
```
In[250]= PlotUnstructured[mesh1, data, "porosity",  
NumberCells -> 444,  
PlotRange -> {{0, 30}, {-15, 15}}]
```



Out[250]= - Graphics -

Mineral comparison of Calcite, fluorite, cristobalite, and porosity. Near field run on the left, original THC run on the right. I would expect these to be slightly different, especially at the top where all minerals were replaced by Burkeite.





Porosity starting at step 7 (20 years) to step 14 (100 years). The results vary greatly and both sets of data have the same data range. This should not be the case.

LS

12/06/07

The file will be cut down to eliminate the top few layers (as a trial) as opposed to changing those layers to inactive burkeite. Initially the blocks from 405 to 446 were cut leaving the drift area (cells 447-471). However, because not in sequence the numbering system had to be altered. Since the top few layers were removed (405-446) there is a new top layer (363-404). The drift was renumbered to begin at 405-429). The Connection file and all other input files needed to be altered.

In drift #s	New drift #s
447	405
448	406
449	407
450	408
451	409
452	410
453	411
454	412

Deleted Sequence	replaced with
446	404
445	403
444	402
443	401
442	400
441	399
440	398

LS

12/10/07

I found two errors in the DAT file where corrections for the new number system hadn't been made. The file still showed error messages, appearing from the phk file, something to do with format. Once corrected the file advanced what appears to be the first half of the DAT file without errors accepting the pckr, conn, phik, and init files. Then after the next 14 lines a call out to the dcmp file is made an error arise. I'm not sure if its in the actual dcmp file of the DAT file. I copied and pasted all the files to a separate folder and began to cut out the drift sections cells 447-441 which had been converted to cell numbers 405-429.

LS

12/11/07

After deciding to cut all cells above 404, which include the drift, the files were again altered cutting out the drift cells. There still appeared to be a problem with the thermal data being out of range. I cut down the pck file to reflect the curve (van G, tabular) numbers listed for each cell according to the new phk file. The phk file lists for each cell what pck curve, THERmal curve are used among other data. IF a pck curve wasn't used I cut it from the file. This didn't work. I thought the problem had something to do with re-numbering the Thermal -properties from the multi.dat file, which I had deleted some and renumbered. I created a new folder and copied the original files where burkeite replaced all other minerals. I then went through and altered the files just as above to cut out cells 405-446, and renumber the drift from 447-471 to 405-429. This time I didn't change the numbering of the THERMAL properties, curves or the corresponding numbers listed in the phk file. The file ran with a few adjustments. Fi2, has the chemistry from the input data report and completed within an hour. Fi has the original THC chemistry and is running fast. Both runs will be compared to the original THC output for accuracy.

LS

12/12/07

The near field file that incorporated the original THC chemistry ran within 44 minutes. In order to compare both cut near field files with the output of the THC run, the mathematica script and accompanying files needed to be modified. A quick comparison shows that the approximate porosity in the nearfield runs looks ok, but until a graphical comparison is done, the comparison between the files over the range can't be accessed. The Segment file was updated to reflect the new numbering system. The cells 405-446 were cut and the drift cells were renumbered.

LS

12/13/07

When the altered segment file was used with the mathematica script one of the near field output files worked and the other produced error messages. The chemistry used in the new PBSsystem didn't work, but the gem file appears to be the same. The gem file with the original chemistry was copied, chemistry was updated and the run was restarted. The

file with the THC chemistry worked in the mathematica file, but the results seem off. The porosity is constant as are the mineral volumes and aqueous species. There may be a problem with either how the segment/mathematic files were altered, or the problem lies within the cutting of the original THC files to exclude the top few layers.

LS

12/14/07

The run that ran over night worked fine in mathematica, as did the file that initially didn't work (incorrect file location), however, there is still the problem of the graphs being wrong which is most likely due to the alteration of the segment file. Below is a partial copy of the original segment file where I had initially replaced the deleted top layer cell #s with corresponding lower numbers. I decided that these 6 lines should be deleted because cells 399-404 are no longer connected to anything above them. I also reevaluated the other files I had altered. Only the connection file was further changed and may be changed again. Cells 399-404 initially were connected to overlying cells, so replacing them with the chart above (12/6/07-table) was incorrect. I'm not sure if the connections of the drift cells be further altered. So the drift was connected to deleted cells which their numbers were replaced by the table above (12/6/07), but when the original drift cells were connected to cell #s that remained the same (ie 404), I left the cell number (404) as is instead of converting it to the equivalent further down the unit. The question is on how to handle the drift cell connections, by changing them to cells in TSW 33 and 34, the drift is being shifted down.

First inserted page – original segment file showing the cutoff and the 6 cells highlighted above the cutoff line were deleted for the reasons mentioned above.

Second page, maps out the cells of the model. I believe that left side starts with cell 446- to 441 on the right. This shows the arrangement of cells before and after the cut.

segmt	0	155.41	5.125	155.41	0	399	393
	5.125	177.2	0	177.2	1	399	405
	0	177.2	0	155.416667	0	399	* 87
	10.125	155.416667	10.125	155.416667	0	400	395
	10.125	155.416667	10.125	177.2	1	400	401
	10.125	177.2	5.125	177.2	1	400	406 364
	5.125	177.2	5.125	155.416667	0	400	399
	5.125	155.416667	10.125	155.416667	0	400	394
	10.125	155.416667	15.75	155.416667	0	401	395
	15.75	155.416667	15.75	155.416667	0	401	396
	15.75	155.416667	15.75	177.2	1	401	402
	15.75	177.2	10.125	177.2	1	401	407 365
	10.125	177.2	10.125	155.416667	0	401	400
	10.125	155.416667	10.125	155.416667	0	401	394
	15.75	155.416667	22.25	155.416667	0	402	396
	22.25	155.416667	22.25	177.2	1	402	403
	22.25	177.2	15.75	177.2	1	402	408 366
	15.75	177.2	15.75	155.416667	0	402	401
	15.75	155.416667	15.75	155.416667	0	402	395
	22.25	155.416667	22.25	155.416667	0	403	396
	22.25	155.416667	29.875	155.416667	0	403	397
	29.875	155.416667	29.875	177.2	1	403	404
	29.875	177.2	22.25	177.2	1	403	409 367
	22.25	177.2	22.25	155.416667	0	403	402
	29.875	155.416667	29.875	155.416667	0	404	397
	29.875	155.416667	40.5	155.416667	0	404	398
	40.5	155.416667	40.5	177.2	0	404	* 88
	40.5	177.2	29.875	177.2	1	404	410 368 → delete
	29.875	177.2	29.875	155.416667	0	404	403
	0	177.2	5.125	177.2	0	405	399
	5.125	177.2	5.125	198.25	1	405	406
	5.125	198.25	0	198.25	1	405	411
	0	198.25	0	177.2	0	405	* 89
	5.125	177.2	10.125	177.2	0	406	400
	10.125	177.2	10.125	198.25	1	406	407
	10.125	198.25	5.125	198.25	1	406	412
	5.125	198.25	5.125	177.2	0	406	405
	10.125	177.2	15.75	177.2	0	407	401
	15.75	177.2	15.75	198.25	1	407	408
	15.75	198.25	10.125	198.25	1	407	413
	10.125	198.25	10.125	177.2	0	407	406
	15.75	177.2	22.25	177.2	0	408	402
	22.25	177.2	22.25	198.25	1	408	409
	22.25	198.25	22.25	198.25	1	408	415
	22.25	198.25	15.75	198.25	1	408	414
	15.75	198.25	15.75	177.2	0	408	407
	15.75	177.2	15.75	177.2	0	408	401
	22.25	177.2	22.25	177.2	0	409	402
	22.25	177.2	29.875	177.2	0	409	403
	29.875	177.2	29.875	198.25	1	409	410
	29.875	198.25	22.25	198.25	1	409	415
	22.25	198.25	22.25	177.2	0	409	408
	29.875	177.2	40.5	177.2	0	410	404
	40.5	177.2	40.5	198.25	0	410	* 90
	40.5	198.25	29.875	198.25	1	410	416
	29.875	198.25	29.875	177.2	0	410	409
	0	198.25	5.125	198.25	0	411	405
	5.125	198.25	5.125	198.25	0	411	406
	5.125	198.25	5.125	221.3	1	411	412
	5.125	221.3	0	221.3	1	411	417
	0	221.3	0	198.25	0	411	* 91
	5.125	198.25	10.125	198.25	0	412	406
	10.125	198.25	10.125	198.25	0	412	407
	10.125	198.25	10.125	221.3	1	412	413
	10.125	221.3	5.125	221.3	1	412	418

Larger Z#
higher it is in order
Z → 0

P105 TOP units
~~0, 395~~
 441 - 446
 0, 361
 435 - 440
 0, 313
 429 - 434
 0, 273
 423 - 428
 0, 245
 417 - 422
 0, 221
 411 - 416
 0, 198
 405 - 410

 0, 177
 399 - 404 New top
 0, 155
 393 - 398
 0, 131
 387 - 392
 0, 108
 381 - 386
 0,

left side
 447
 448-439
 drift connections
 cut

X=0 indicates Right side
 Z = height larger # closer to Top of Model

405	406	407	408	409	410
399	400	401	402	403	404

change
 Segment →
 curm → keep cell & exchange to connect drift #s to new top #s
 DCM → didn't change
 INT → no change
 PCK → no change
 PH K → no change

LS

12/16/07

I started with a new segment file and made the changes mentioned above. The connection file was also redone. This was done because an error message for the run

occurred. IT still has not been decided what to do with the connections for the drift cells. The files will be run with both chemistries.

LS

12/18/07

The runs completed without error, but when the output files were used in Mathematica, there still was a problem. It still shows no change in porosity. Looking at the files comparing the original THC output for time step 28, matrix, the porosity is variable between 0.14 and .0.15 while the porosity for the near field run remains constant.

LS

12/20/07

The connection file was once again redone using the original THC file. The drift was not attached to the deleted cells, I read the file incorrectly. Row one of the file lists the cell number, row two the cell its connected to, and row three the distance-how many cells away the two connected are. If you add row 1 and 3 they should equal row 2. Previously when I was renumbering the deleted sequence with the corresponding new top layer, I had stopped altering column 3 when I came across numbers that were not deleted, because I had initially thought these were cell numbers not distance. This should fix the connectivity, but when the file ran these didn't fix the porosity. The temperature was constant rather than a gradient. The source file was the only file not changed from drift cell 471 to 429. For the segment file I put back in the 6 lines I had deleted. Those connection lines close the polygons that now make up the top row. They do not really indicate that the former row above is still present, just closes the box (polygon). The file ran successfully and there are changes in porosity and temperature gradient. The files will be compared using mathematica, for both chemistries of the near field files to the original THC method 2-2 wtkin 0.5.

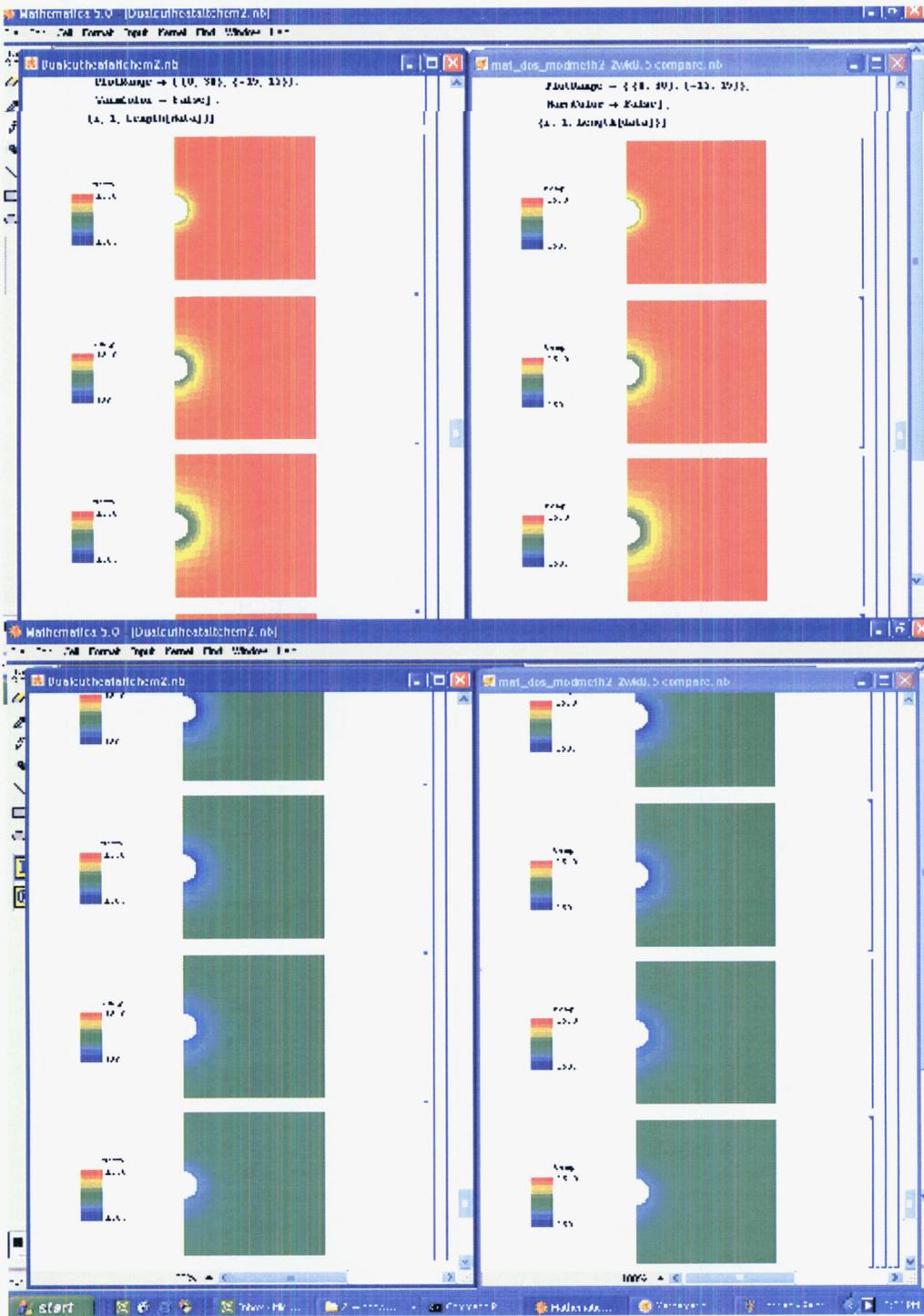
LS

12/21/07

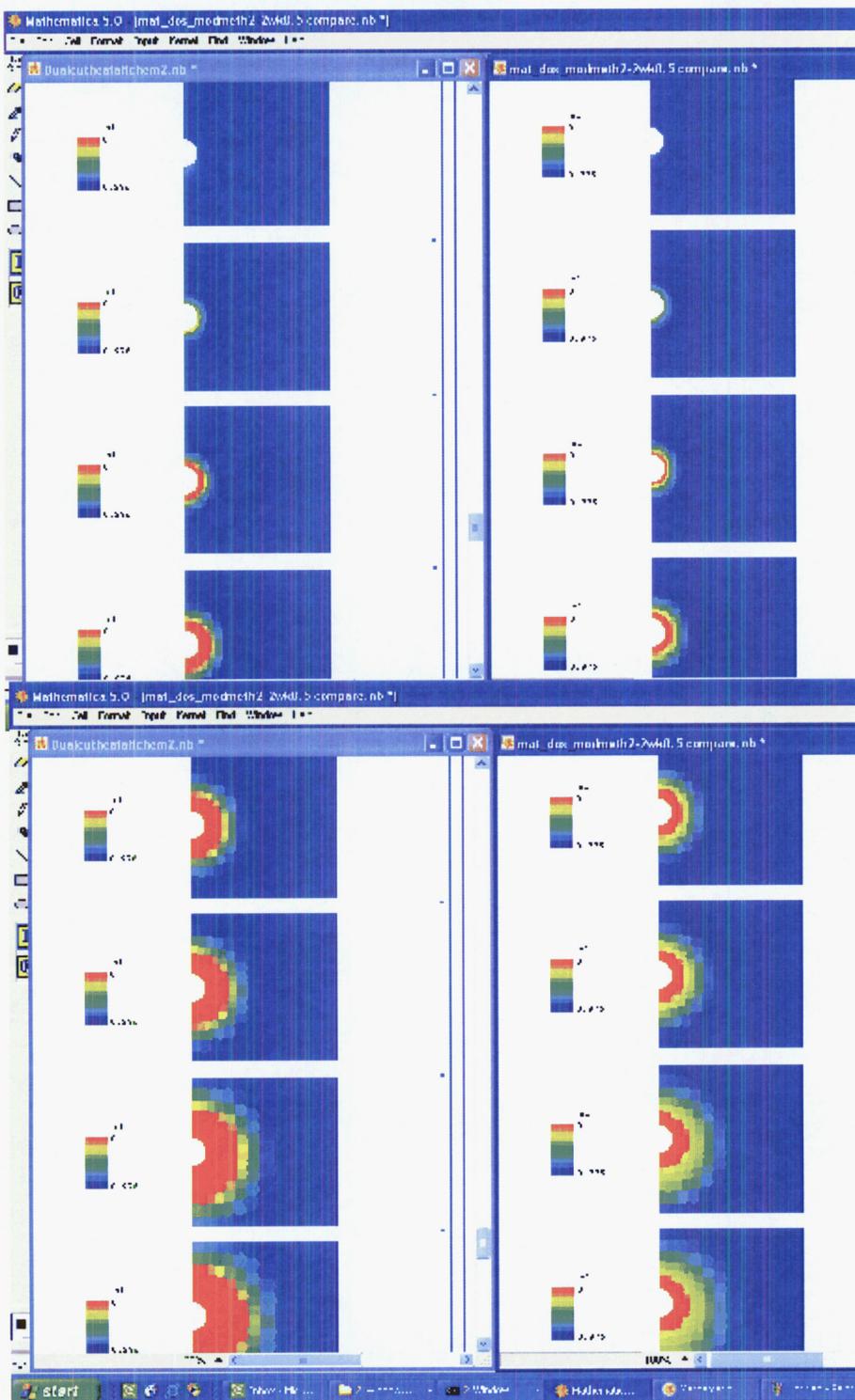
The run with group 2 chemistry from the TDR paper took 4 hours and the original chemistry (simple) took 1.3 hours.

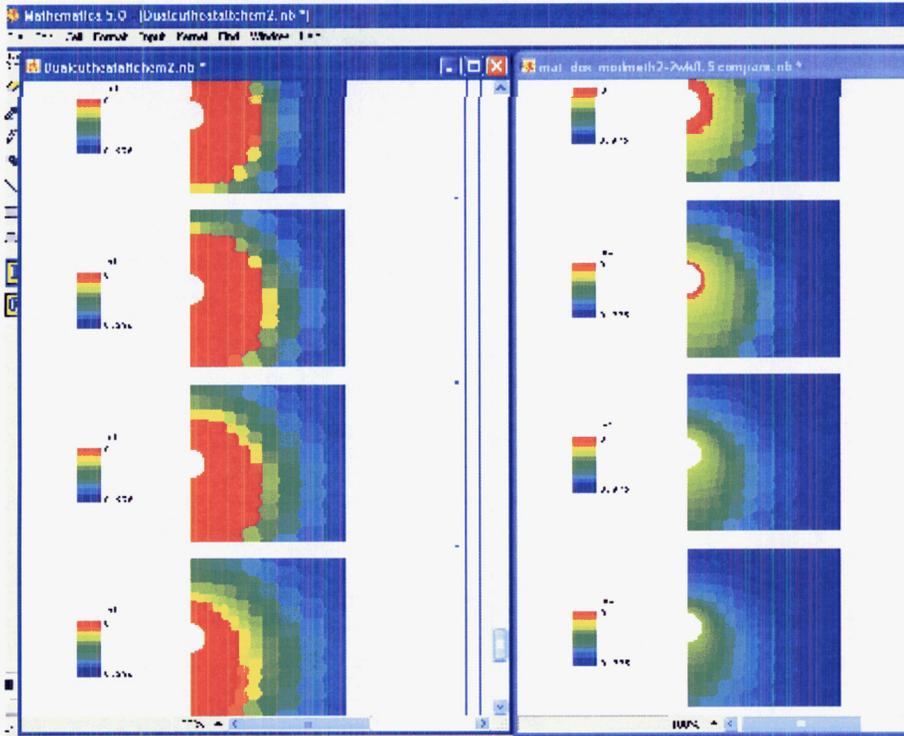
Below is a comparison of the near field run, group 2 chem, and the original THC run, which is on the right.

Temperature (top pics up to 1 year, bottom 150-500yrs)

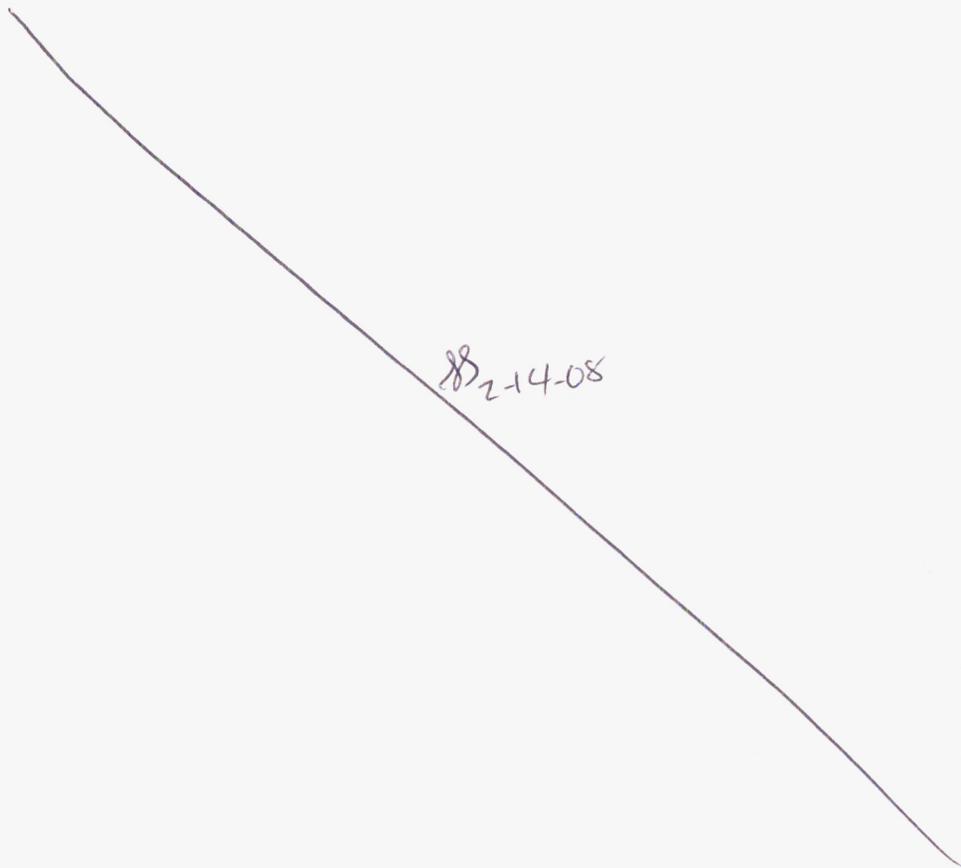


Liquid saturation (55-1000 years) - next figure
 8/2/14-08

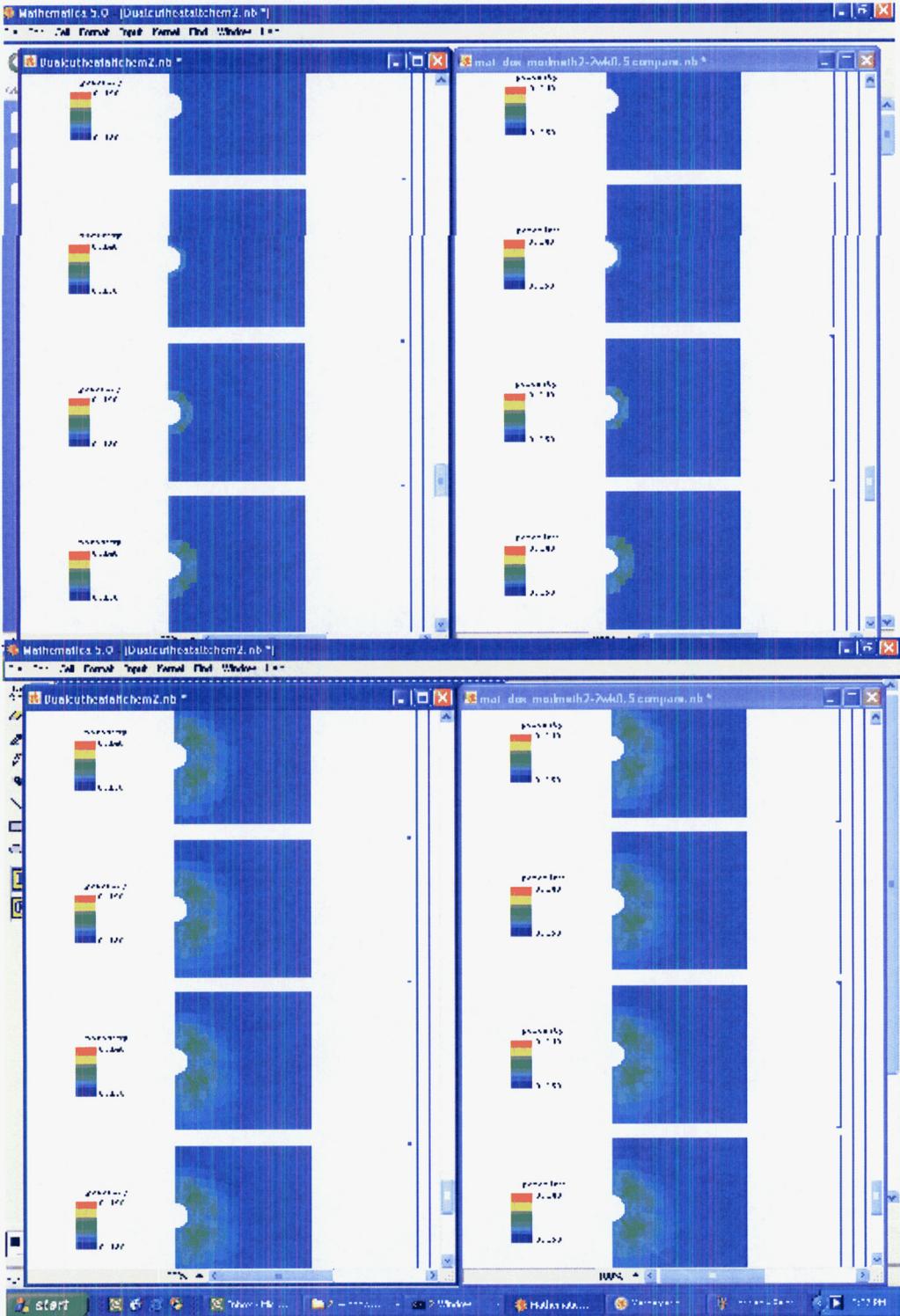


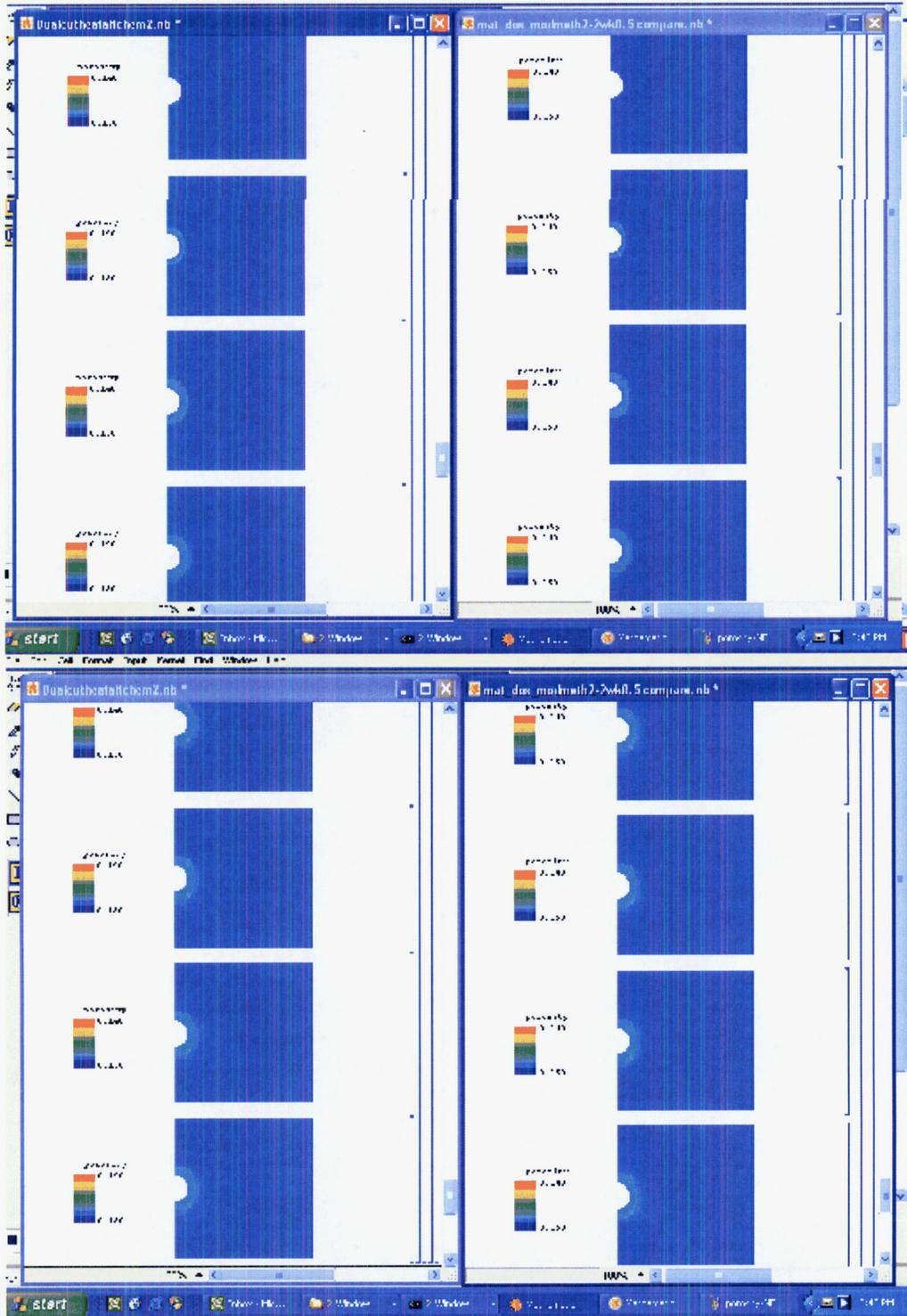


Porosity (55-1000 years) There are two sets, I think there is a glitch with regraphing data in mathematica. Both sets are taken from the same output data and redrawn show two different graphs. *NYT figure LS 2-14-08*



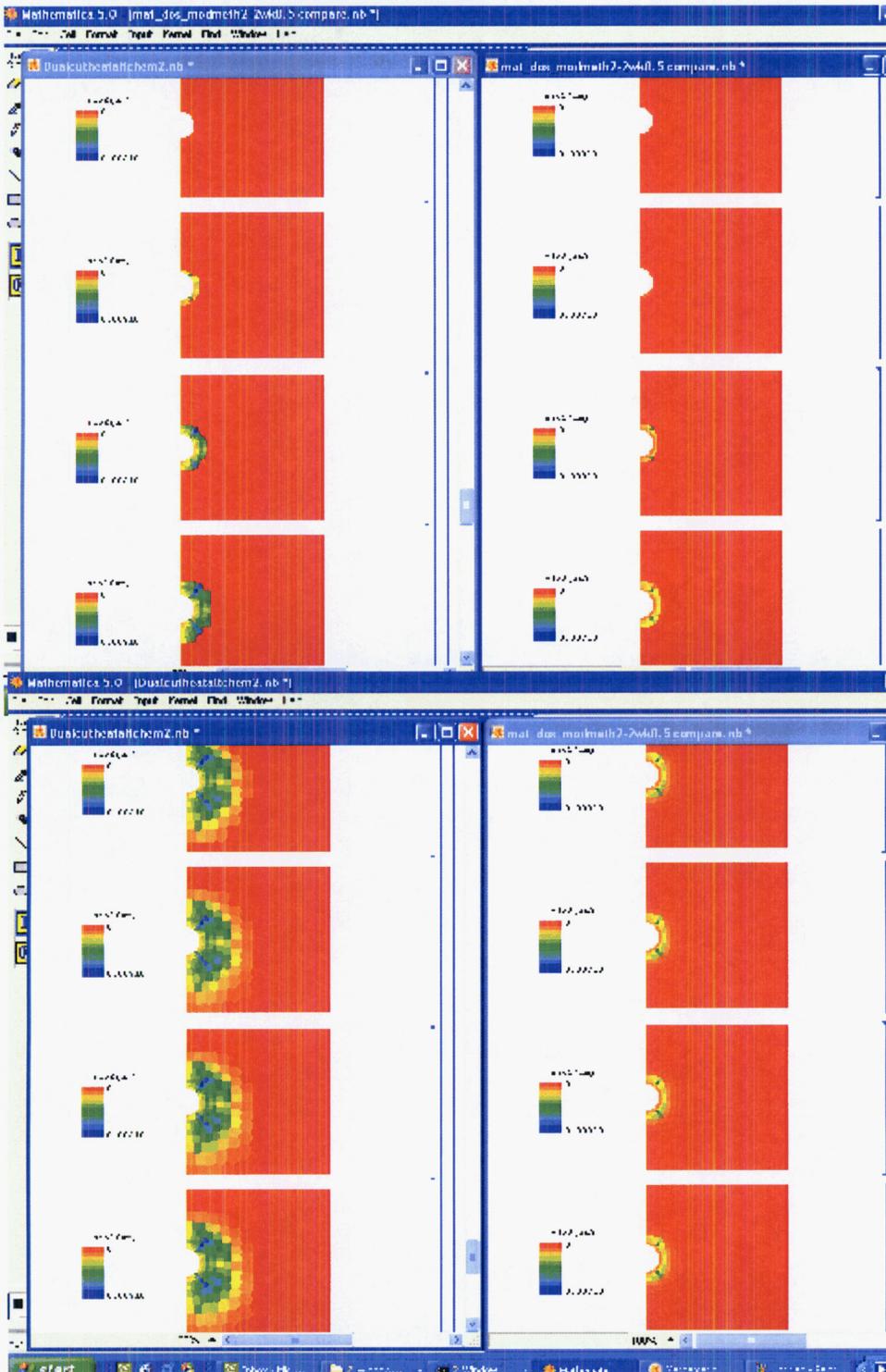
88 2-14-08





Sio2am concentration, The difference may not be as significant as shown. Actual data should be extracted for comparison.

Next Figure AS 2-14-08



LS

1/2/08

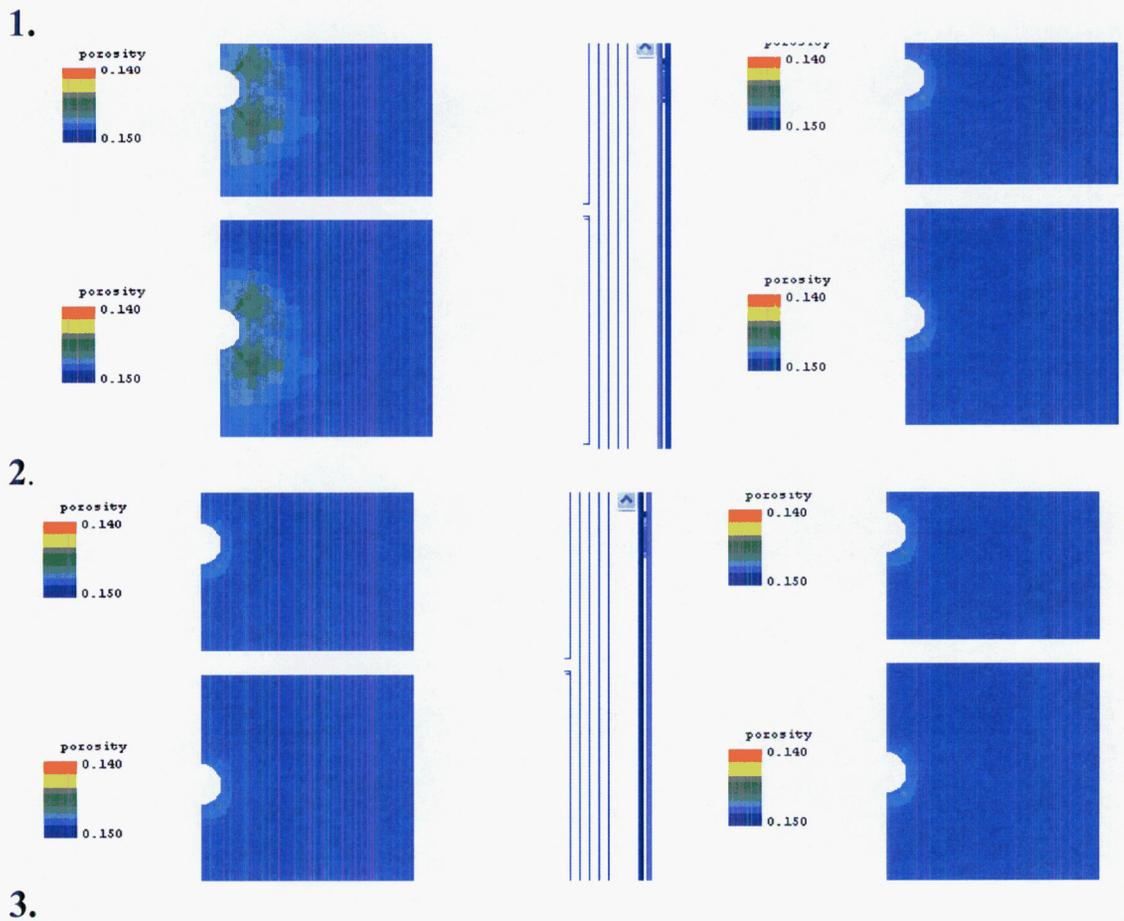
I have compared the cut near field run that used the simple chemistry with the original THC run (which again is on the right). I left them in a folder, which will accompany this notebook (Nearfield\2-D\MF-Dual\heat\1220chemoriginal\compare pics-same chem.).

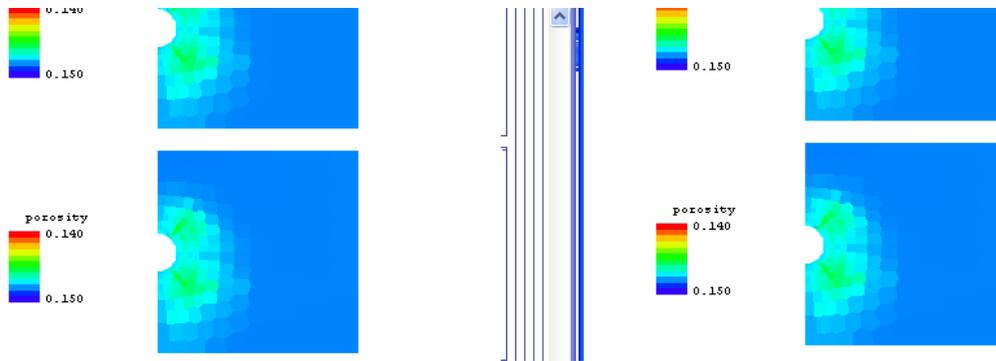
Once again the results were very compatible, however there may be multiple bitmap images of the same comparison (porosity 25-28 and porosity 25-28_2) to demonstrate that when re-graphing the same data in Mathematica, Two different results may be shown, this is dependant on which bracket was selected to initiate the re-graph. You may select to re-graph the whole file, or just the section your working on, and in this case for the animations there are two data input areas, one for the file, what series of files to pull data from and the graph command that selects what is to be graphed and from what range in the series to actually graph. If the same bracket is selected several times in a row, different results may appear.

Left near field simple chem.

Right Original THC run

Time step 25 and 26 repeated three times all have the same graph, data range. The first set shows that the change in porosity extends further for the Near field run, but when the third bracket is used to regraph, the second set shows the exact match to the THC run. In the third the graph is re-run in THC several times and sometimes it produces the results in figure 1, but it can produce the results in figure three which match those of the near field run when the whole spreadsheet was re-graphed.





I have been looking for an easier way to compare the numerical data, in addition to the Mathematica graphs. I'm not sure what forum would work best and be the most effective, FORTRAN, excel, but it needs to be able to pull data from 28 files and match the results to data pulled from both the near field and THC runs. This will be productive since once the near field run is averaged it needs to be compared to the 2-D dual continuum.

LS

1/4/08

I have been trying to set up the averaged properties file using the existing THC file, by altering each keyword one at a time. The Thermal keyword was altered to have two entries the averaged info for all the units and a separate set of properties for the drift. Most keywords were updated in this manner, however when omitting the pck file by adding the data directly to the metra file the phk file needed to be updated with the new curve and thermal data identification numbers. There have been error messages when running the files after these last changes were made. I will try to correct the errors or may keep the existing pck and phk files and just alter the pck curve data to the same for each of the listed curves, except that of the drift.

LS

1/8/08

I have replaced the files that I altered to make the average properties file. Instead I will first make the run a single continuum. There are a few items to change, block the DCM Parameters, change the grid keyword, delete the second set of boundary conditions in the metra file, and delete the 2nd set of aq species in the gem file.

LS

1/9/08

There were a few problems in converting the files to a single continuum. The first being within the gem file when deleting the second set of aqueous species, in the COMP section leave two periods (two separate rows) after the aqueous data section. Secondly, even though the manual states to enter the grid keyword as UNSTRUCTURED into the gem file only UNSTR can be entered to avoid an error message. The single continuum file is currently running. However, I would like to eliminate some of the external files that accompany the main gem and metra files. Cut down the Thermal keyword to only two

entries, the averaged values and the drift values, eliminate and exterior phk and pck files. However, many different error messages are occurring.

LS

1/10/08

There were many problems with eliminating files, so the remaining files had to be updated to reflect the values for the averaged run. The PHK file must remain because the block volume must be specified for each individual block, so the last few columns after the permeability have been deleted and the thermal and pck curve number have been changed to 1 for every entry except those of the drift. The Pck file had all the data curve 1-22 changed to that of the average, and 23 reflected the data for the drift. Also the boundary conditions in the gem file were changed to the top and bottom portion of the model since this is a vertical 2-D run.

A steady state run was executed and the resultant initial data was cut and paste to the .INT file and the files were then run again.

LS

1/11/08

There have been many changes in the phk file. All references to the thermal numbers and curve numbers were changed to 1, except the drift have a thermal number of 15 and a saturation curve number of 23.

```
1 1 1 1 1 0.2397 .1393 4.52E-13 4.52E-13 4.52E-13
429 429 1 23 15 0.5012 1e-05 0 0 0
```

The single continuum file is running, however when using the Mathematica script porosity is constant but the other parameters such as temp are comparable with the dual continuum. When originally altering the phk file the second column for porosity was deleted for the drift, upon modification this didn't fix the problem.

LS

1/15/08

The files were further updated. The pck file will no longer be used because the rock saturation properties were added directly to the metra file, it had been formatting in the past that caused the error.

PCKR

```
1 Van-Gen 0.14214 0.2898 1.788E-05 0.0 0 0 :
2 TABular 0.01 0 0 0 0 0
0.0 0 1 0.
1.0 1 0 0.
```

```
/
:
0
:
```

The PKH file has to remain due to the block volume. However since everything past the permeability in the x y z direction was deleted, the porosity is off. There are two columns at the end of the volume output file “porosity” and Por, I thought for a dual continuum the first was the current porosity and the “por” column was the original and for single continuum both fields report the same value. I’m not sure if I’m off, but I’m sure it has to do with the modification of phk file. I tried several modifications to the phk file such as changing the POR from .1393 to 1 and add porosity at the end, separate each line with a : character, add back two of the columns deleted PORM and PERM. None have worked, the drift porosity is right on, but the rock porosity calculates 1e-3 without change for the whole duration of the run.

```
1 1 1 1 1 0.2397 1 4.52E-13 4.52E-13 4.52E-13 .1393
2 2 1 1 1 0.5459 .1393 4.52E-13 4.52E-13 4.52E-13:
1 1 1 1 1 0.2397 .1393 4.52E-13 4.52E-13 4.52E-13 .1393 4.52E-13
```

LS

1/17/08

After going through the file, I realized the other day when I scrapped the files to start over not everything was updated for the average run. The mineral section in the gem file needs to be correctly updated. However the porosity will still be off because how Albite_low was calculated, concerning volume fraction. I calculated all the values to add up to one, but I believe in MF the volume fraction is $VF_{min}/VF_{whole\ rock}$. So the volume fraction should be $1 - porosity (.1393)$ which equals 0.8607.

LS

1/18/08

Once Albite was corrected and the mineral section correctly updated (modifying burkeites volume fraction) the file seems to become stuck around 55 years. I thought that it had something to do with the tolerance values, but this didn’t improve the run. Many attempts were made and the file was still stuck between time steps 9+10. It was suggested that maybe the activity coefficient calculation was causing the error, so the γ in the gem file was changed to 0, however the file also choked up in the same time frame. Metra was run alone and it was seen that there were cells that dried up completely; this is what may be causing the difficulty computing the chemistry in a dry cell. However, MF should ignore that and move on. Another thing to think about is the QBC in the metra boundary conditions file are the values used for the THC project and not necessarily the half liter per day planned on using for this project. Do to the unstructured grid each cells area isn’t apparent. For a trial run the value calculated for the 2-d structured run $5.7e-6$ was used, which is three orders of magnitude above the existing values. This run moved along much faster and made it further past time step 10, but eventually choked on step 22. Since this value isn’t confirmed the original qbc value was inserted. It was suggested that the files be run using method one, explicitly global (rather than a split operator). This file will be run over the weekend.

LS

1/21/08

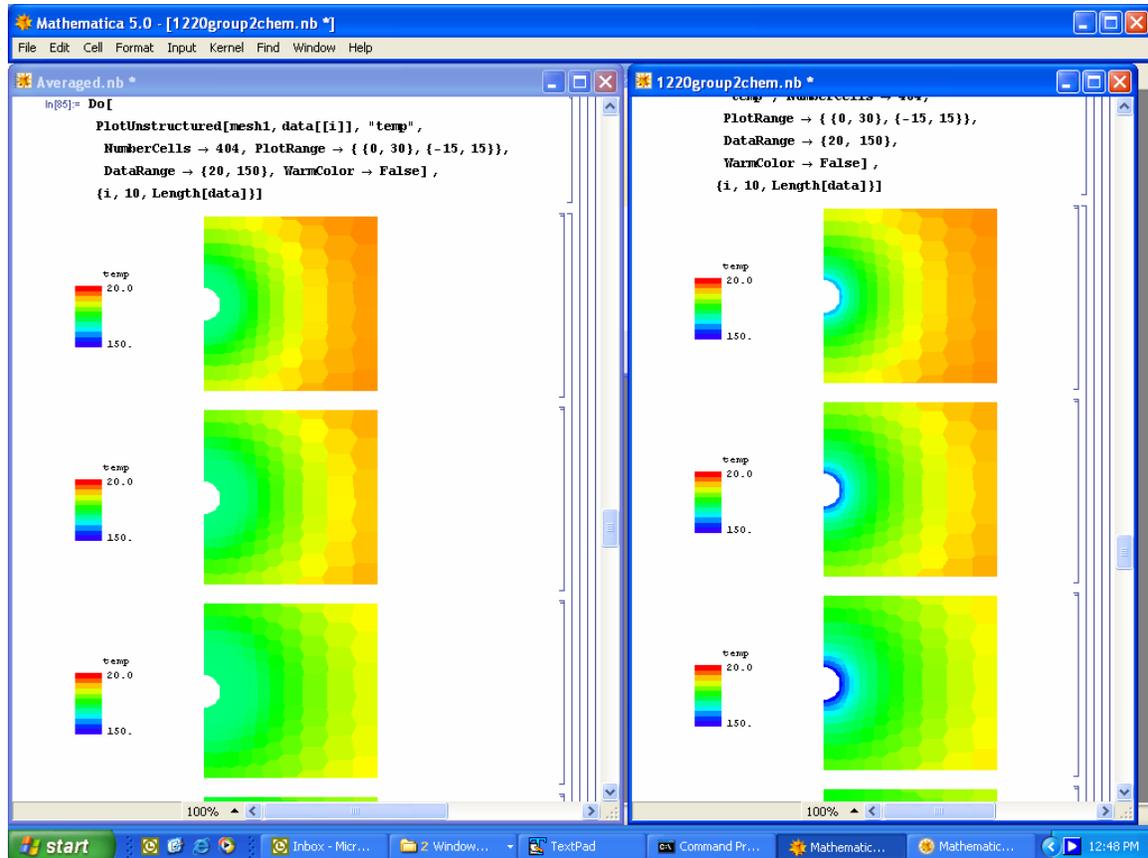
The file stopped on Saturday because it had exceeded the number of iterations. I really tried to verify the infiltration rate that was used in the original THC, however I searched elf and couldn't find anything. I thought it was a Browning et al, 2003 paper, but I was unable to find such a paper pertaining to MF and Yucca mountain. I would like to change the QBC value, but I have a block volume in m^3 and I did find a file that lists the estimated x y z distance and for blocks 399-404, the numbers do not correlate. I'm not sure how to calculate the proper number. I changed back to method 2 in order to debug the tripping problem. After altering the tolerances the file still seemed to be stuck but made it past time step 10. The method was changed to 1 (explicitly global) and allowed to run overnight.

```
: tol ttol tolneg tolmin tolstdste tolc
TOLR 1.d-5 1.e-1 0.001 1.e-3 1.e-12 1.e-12
LS
```

1/22/08

The file ran to completion. However, there are noticeable differences between the averaged run and the cut down THC run named 1220group2chem.

Temperature differences begin at time step 10, which is why the porosity and SI between the two is off.



There are differences within the gem file

Averaged run	1220group2chem run
Tortaq and Tortg = 0.6937	Tortaq and Tortg = 1

BCON Face 3+4 top and bottom	BCON face 1+2 left and right
Porosity = .1393	Porosity = .1486 difference of .0093
More secondary species	Fewer secondary species
Albite low included	No albite included

I set up two runs, one averaged run correcting the Tortaq and Tortg to be equal to 1, and a 1220group2chem run in which the Bcon faces were changed to 3+4, a few secondary species were added, burkeite was made to be .0001 volume fraction and Albite was added in its place using the information from the inputs spreadsheet. For now the units below the TSW were entered as arbitrary since they are outside the area of interest. In order to fix the porosity (closer to the given value) the albite volume fractions were reduced by .02. There is still a problem yet to be resolved and it's the conversion of Surface area from the toughreact problem 3 files to units used in Multiflo. The SA in TR is total surface area whereas in Multiflo its SA for that mineral. The SA is multiplied by volume fraction and also density to convert to 1/cm. However the values calculated are at least two orders of magnitude higher than what is seen in the MF files for the THC files. There must be something else to consider.

The averaged file in which the tortuosities were altered is also getting tripped up before time step 10.

LS

1/23/08

The averaged run with tortuosity of 1 failed, exceeded the number of iterations between time step 18 and 19. The modified 1220group2chem made it to step 18 before I cut the run. It was going slowly, but the temperature gradient wasn't any different. So I reran the run by only changing the method, tortuosity to 0.693, and bcon faces. The file still trips up at time step 10. The Averaged run was set up with a tortuosity of 1 and bcon faces of 1+2

The temperature gradient differs greatly between the averaged run and the modified THC run. There are probably several reasons, but when I ran the modified/cut version of the THC for comparison with the original, I left all the variables as entered. When comparing the modified THC with the averaged runs there are a few Major factors that need to be worked out.

Tortuosity 1 or .693

Boundary condition face selection in gem 1+2 or 3+4

Mineral selection (THC doesn't include albite) add it to modified THC

Porosity difference between the two, do I adjust the mod THC to reflect .1393

Surface area calculation from tough to MF is off two orders of magnitude, I believe.

Infiltration rate what value should be used (changing or constant). How to calculate it for the dual continuum.

LS

1/24/08

A few more runs resulted in no improvement making the temperature gradient a closer match between the two files. The THC model is based on an older revision (EBS rev2) and some of the numbers are significantly off from the values used to perform the averaged model in the EBS physical and chemical revision 6 (ie the averaged numbers do not reflect the average of the actual THC values). It was suggested that either the THC file be updated with the individual values extracted from the Toughreact example problem or the current THC values are averaged and replace the TR calculated average values. I would rather average the existing THC values and use them to replace the values previously calculated. This would eliminate several problems and concerns (ie the conversion of Surface area from TR to MF). A new spreadsheet will be created and data from the THC file will be extracted to calculate the average values based on the same unit weighing method. Upon asking how to average the phk values, it was decided to leave the run as a dual continuum and average the separate fracture and matrix values.
LS

1/28/08

A Spreadsheet named THC_Average_Dual was created and updated to calculate the average values for the fracture and matrix separately the four units of interest. The metra boundary condition file was updated with temperature and pressure values from the initial file to replace the existing values that represent the new top boundary (Cells 399-404). All the parameters values for units TSW 6 and 7 are reported together or have the same values in throughout the various input files except for those in the MNIR section of the gem file. When the files updated only the TSW6 info was considered an updated. All files were updated without error except when updating the mineral section of the gem file. The error report states

```
Factorization bandwidth exceeded: increase(d) band
current bandwidth: 108 needed = 120

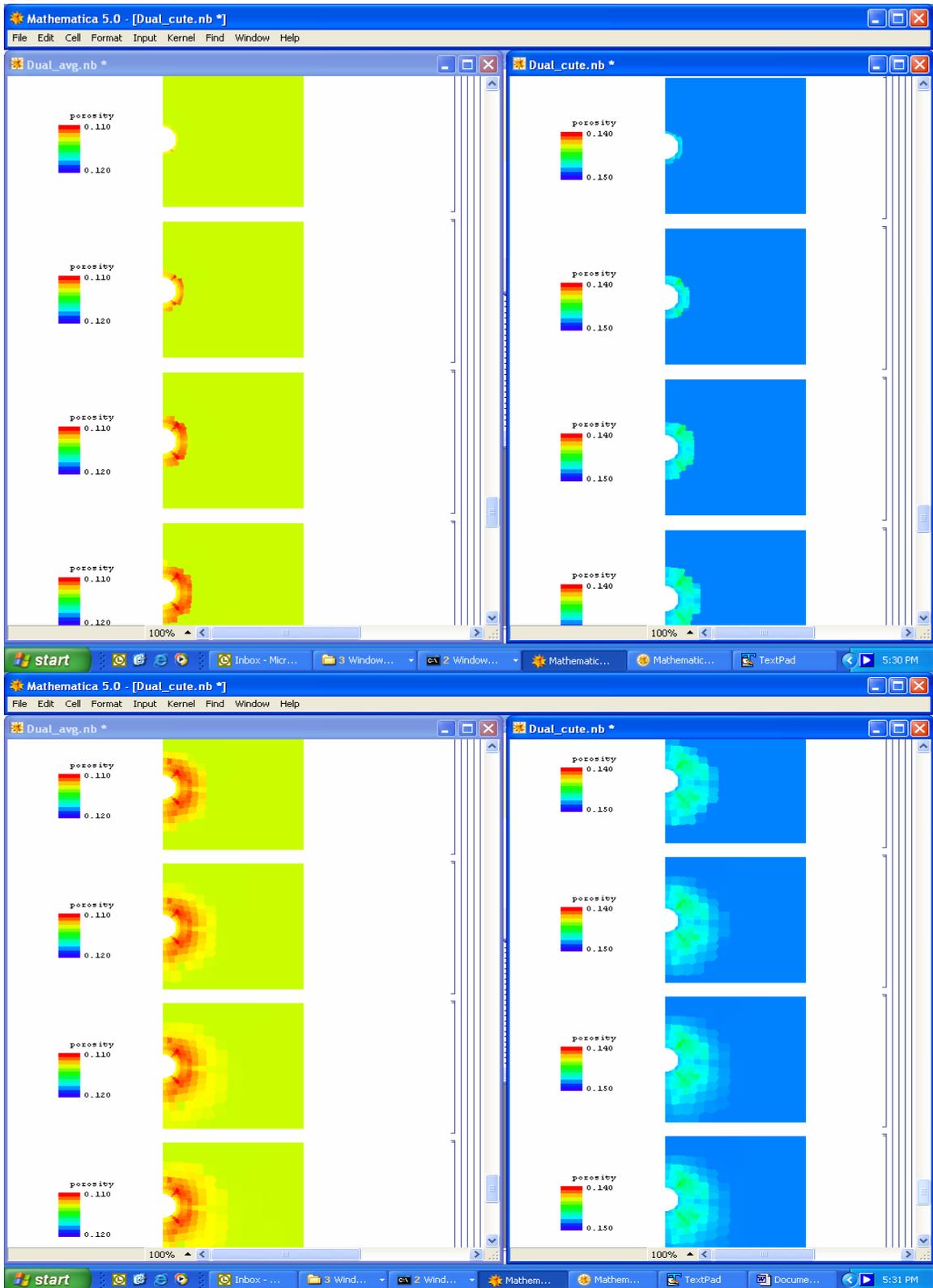
Symbolic Factorization Level: 2
Resulting Maximum Bandwidth: 120
--> Initialize GEM
--> read input file: icode = 3
**Warning: rel tol < 1.e-8: reset tol = 1.e-6
field used for the variable > internally specified
field used = 11 specified = 10 on the following- reduce field
381 404 1 0.19067 1.09803E-01 1.336E-03 4.1195E-04 !tsw33

reading error in frfmt.f
D:\Nearfield\2-D\MF-Dual-Averaged\THC_Dual_avg_group2chem>multiflo multi fi2
```

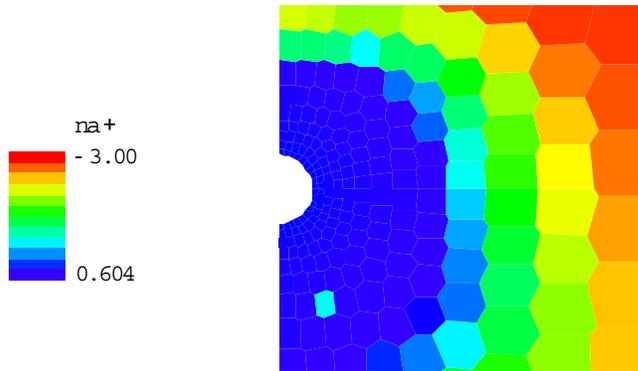
It probably is a simple error or tab error. The matrix SA used 11 digits to specify the value instead of ten.

$1 - \text{porosity}(.1372) = .8628$ however the total VF based on averages worked out in the spreadsheet equal 0.8872 so the actual VF minus VF based on avg porosity is $0.8872 - .8628 = .02442$ so the burkeite VF of .3967 minus .02442 equals 0.3723. I may alter the Burkeite volume fraction in order to have the porosity work out to .1372 rather than the .1127 as it is now. A separate run was started with a burkeite volume fraction of 0.3723.
LS

1/29/08



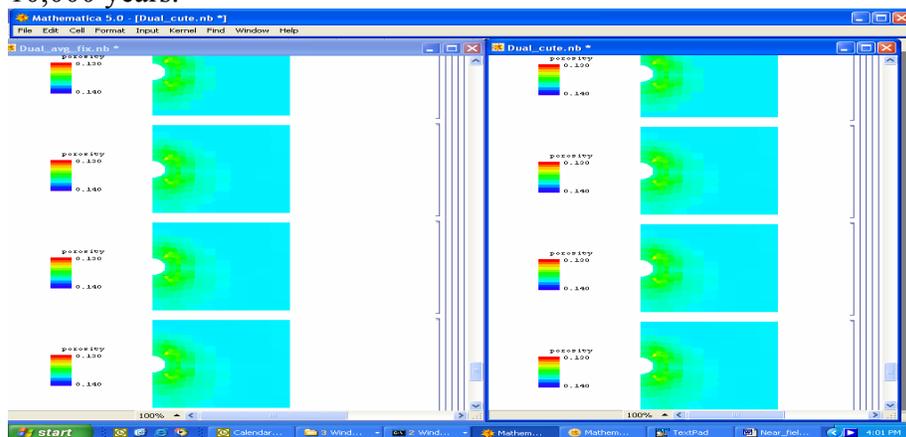
Even though the cut and average dual runs started off with different porosities, they both have similar evolutions. The average run has only gotten to time step 20 overnight, but it does reflect similar results to the cut run. There is one exception; a small area below the drift is somehow out of step with the other cells. I assume when the changes to create the average run were done, somehow an error occurred that made this area (in light blue within the dark blue area) off. This abnormality shows up in the liquid saturation, mineral, and other graphs.



There was an error in the phk file; a curve number for unit tsw35 was inadvertently altered. The fixed porosity average file is being re-run; the initial average file may be re-run for comparison.

As the fixed porosity average file is running, I made some comparisons using Mathematica. The temperature gradient and liquid saturation so far (first 150 years) agrees with the original cut down THC file. The files start off with different porosities, but they both have similar evolutions (just as seen in the above side by side comparison). The aqueous and mineral concentrations also show agreement between the cut THC and averaged Dual continuum runs.

Porosity with the same scale (left averaged, right cut THC) time steps 17-20 4,500-10,000 years.



The average run is taking a long time since it reached step 19, it appears to be due to re-dissolution of gypsum
LS

1/30/08

The file completed without any error, however looking closely at the Cl aq concentrations of the two runs shows the same trends but the concentrations (at certain areas) are much higher in the averaged file. Most other aqueous and mineral evolution for both looks the same. The temp, sl, and porosity show good agreement. Comparison of those three were put into an excel spreadsheet along with some other results that show slight variation.

LS

2/5/08

The output files for both runs were compared to pinpoint the time and cause of the deviation of Cl- results between the two. I'm not sure what is causing this deviation so an ambient run was conducted for the average properties file (with fixed porosity). These runs didn't seem to indicate a problem.

LS

2/12/08

Near Field Summary Report

Lynn Sabido

The following files have been burned to disk and also remain on computer in room 242. This is a summary explaining where this project was left off. The project left off with comparing a dual continuum with averaged THC properties with the original THC file. The file and their output are in the following folders:

D:\Nearfield\2-D\MF-Dual-Averaged\THC_Dual_avg_group2chem\fix_porosity

D:\Nearfield\2-D\MF-Dual-Averaged\THC_Dual_Cut_group2chem

The explanation of the past files is explained below including the point where the project left off.

File Location

D:\Nearfield

Within this folder are two subfolders 1-D and 2-D. There are two files one containing the tables from the TSPA report the average values were based on and a spreadsheet containing data and calculations for the averaged properties, which was also based on the TSPA report. The 1-D folder has the older files that treated the problem as a 1-D plug flow run. There are two files one containing the tables from the TSPA report the average values were based on and a spreadsheet containing data and calculations for the averaged properties, which was also based on the TSPA report. The folder also contains two subfolders one for Toughreact and Multiflo. The TR file is based on example problem 3 (YM_calcite) and the Multiflo files were constructed from a structured grid and only an averaged single continuum run was created. The project was changed to a 2-D simulation and the focus shifted to just Multiflo runs, one as a dual continuum and one as a single averaged continuum.

File Location

D:\Nearfield\2-D\MF-Dual

Initially the original THC run (minus the top layers above TSW33) was to be compared to the THC run as a single continuum using the average properties from the input spreadsheet that was prepared using the TSPA data. Initially the upper layers were to be made in active by selecting Burkeite as the only rock unit. It was then decided to cut the file down and eliminate the unnecessary top layers. These runs are in D:\Nearfield\2-D\MF-Dual\Runs_past\ambient, however the initial THC run had the total mineral volume fraction greater than the rock porosity. The burkeite volume fraction in some cases was above 1 or even above the porosity. The folder marked D:\Nearfield\2-D\MF-Dual\Runs_past\Averaged contains a first failed attempt at cutting the top layers off the THC run. These files were discarded.

File location

D:\Nearfield\2-D\MF-Dual\heat

This file contains four folders, one with the original THC results, one with failed attempts at correctly making the top layers inactive or cutting the file down. The other two folders contain a successful running dual THC files that had the top units eliminated. One has the original THC chemistry; one has the Group 2 chemistry discussed in the TSPA paper. (1220chemoriginal and 1220group2chem). The unsuccessful runs were lumped into the folder D:\Nearfield\2-D\MF-Dual\heat\otherruns\. This included the corrected run where the burkeite volume fraction was set equal to 1-porosity; all attempts to make the above layers inactive didn't seem to work. This folder also contains some attempts at cutting the file down.

File Location

D:\Nearfield\2-D\MF-Dual\Averaged2

Once the cutting of the top units was successful, the gem (with group two chemistry) and metra files were made into a single averaged continuum using the values from the input spreadsheet created. Trying to compare the results of this single continuum averaged run with the original THC file (once cut down), was difficult to make any sort of conclusions because the average properties calculated in the spreadsheet, were not based on the same set of the properties found in the original Dual THC file (which I believe the rock, mineral and other properties were taken from an older revision of the DOE engineered barrier report). It was decided to take the THC properties and average them for a more accurate comparison.

File location

D:\Nearfield\2-D\MF-Dual-Averaged

There are three folders and three spreadsheets. The spreadsheets THC Averaged_single and THC Averaged_Dual contain the average properties of the original THC file. The spreadsheet marked single has averaged the fracture and matrix properties together, however when trying to average the rock saturation characteristic properties (PCKR file), which just doing a straightforward averaging process wouldn't correctly calculate the van genuchten values. It was then decided to average all the matrix and fracture properties separately and keep the file as a dual continuum. This averaged dual continuum file would then be compared with the original THC dual file. The average value calculations for the dual continuum are in a separate spreadsheet and the folder labeled THC_Dual_avg_group2chem contains the runs. Within this folder is another folder marked Fix_porosity in which the burkeite volume fraction was adjusted to achieve the same matrix porosity (porosity calculated as $1 - \text{the sum of the averaged minerals volume fraction} = 0.1128$) as that calculated in the averaged dual spreadsheet (0.1372) which was an averaged value based on the data in the phik file. The other two subfolders in the MF-Dual_averaged folder contain the results of the heated and ambient run of the cut down THC file (THC_Dual_Cut_group2chem) and a folder for an averaged single continuum using the THC values (THC_Single_avg_group2chem), but these files in this folder have not completely updated because for the time being this idea was put aside.

The comparison of the Dual THC and averaged show good agreement, however looking closely at the Cl aq concentrations of the two runs shows the same trends but the concentrations (at certain areas) are much higher in the averaged file. Most other aqueous and mineral evolution for both looks the same. The temp, sl, and porosity show good agreement. Comparison of those three were put into an excel spreadsheet (named aq_cl_compare) along with some other results that show slight variation. The output files for both runs were compared to pinpoint the time and cause of the deviation of Cl- results between the two. I'm not sure what is causing this deviation so an ambient run was conducted for the average properties file (with fixed porosity). These runs didn't seem to indicate a problem.

LS

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