

**Scientific Notebook # 797**

**Using TOUGH REACT to Simulate Flow and It's  
Corresponding Interactions in 2&3-Dimensions**

797

BOOK NO.

PROJECT

1

PAGE

6/7/06

Title -

Using toughreact to simulate flow and its corresponding interactions in 2+3-Dimensions. The systems will include simple Qtz and Tuff as the main components to more complex systems such as the rock layers above the proposed Yucca Mountain disposal site.

Performed by

Lynn Sabido

Objective:

To model pore water chemistry and its affects to the surrounding area of concern (processes include; precipitation, dissolution, porosity and aqueous concentration changes, corrosion etc. The systems will vary from all Qtz or tuff to the complex rock ~~system~~<sup>systems</sup> system that encompasses the Yucca Mtn site. Specifically the effects of Ca-Cl rich waters play in the potential for corrosion.

Training

To become familiar with Toughreact; to accurately ~~simulate~~<sup>simulate</sup> simulate the aqueous environment in order to predict the chemical, aqueous processes that may occur.

Approach -

To create through various input files <sup>systems</sup> that describe the proposed chemical and physical system near and in the drift at the proposed Nuclear waste site at Yucca Mountain. First starting with 2D runs using only Qtz or Tuff as the surrounding rock, run using four input waters; Pure, Neutral, Ca-Cl rich, and alkaline. Eventually model the units that lie above the proposed drift and leading to the migration of these new chemistries to observe precipitation, porosity and ~~aqueous~~<sup>aqueous</sup> chemistry changes. Specifically looking for corrosive chemistries that could reach the drift.

Status

Currently under TOP-18 Compliance

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Location:

Program - A simulation program for non-isothermal multiphase reactive description geochemical transport in Variably Saturated Geologic Media. It consists of ten equations of state modules, however the current version is distributed with only six of them. Toughreact is a program written in Fortran 77 and runs on the DOS prompt. A PC with Windows XP was used.

Input Files

The input files will be created by altering existing files in order to resemble the chemistry and surrounding rock units found around and above the potential drift. Various water chemistries will be used as initial input; they include, pore, alkaline, neutral, and Ca-Cl rich waters. Specifically toughreact example problem #4 (Water-test) will be used and slightly modified. This existing problem is already set up for the Yucca Mountain site, however a few minor changes need to be made, like allowing <sup>to 200</sup> ~~precip~~ water infiltration and possible changes to time step/output times.

There is a possibility that borehole samples that plot high on the Piper diagram, indicating high Ca+Mg plus high Sulfate+Cl<sup>-</sup> concentrations, will be used as starting pore water compositions. This initial water chemistry, that has the potential to be corrosive, would be run through the rock units that lie above the potential drift. After the model predicts water-rock interactions, the resulting water chemistry will be evaporated to see if corrosive waters form.

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6/2/06 Toughheart example problem #4. Incorporating recharge into problem to see the effects, if any.

a. Chemical.inp change the # of initial boundary conditions to 1 pure water influx plus current water composition.

Add to Gener file (p term) Source H<sub>2</sub>O coming in as rain water

Created 2 extra output files flow.out and runlog.out  
\* just really missing from the original folder I was given

§ The user defined output files are blank.

6/3/06 Copy and pasting, line Gener files indicated in Hexg watr, from the Qz+toff files given to me (From a training class). Then change grid # to one present in current file. Program would run for a bit, then freeze up the entire computer.

6/6/06

Name the SLINOS (Sink/Source) your own name?

Change Flow to similarly found in file given to me by Chandrika.  $1 \text{ kg/Day} \cdot \frac{1 \text{ day}}{86400 \text{ sec}} = 1.1574 \times 10^{-5} \text{ kg/sec}$

enthalpy H<sub>2</sub>O in J/kg from internet use  $7561 \text{ e}^5$

§ Used grid cell Mo 031; <sup>Program is 6/6</sup> Stalls 60+ before 1 yr is complete. However, the file is set up to run for 2.75 yrs. Tried various rates (infiltration) still it locks up or quits.

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15/6/20  
~~6/7/06~~  
 6/7/06

6/6 - made graph of XZ coordinates for problem #4 §

took graph to see what gridcells reside at the top of the grid.

they are as follows one of each Fracture F and Matrix M

~~700~~ § 6-7-06

700, 695, 690, 684, 713, 712, 657, 571, 631, 632  
 603, 609, 614, 619.

heron problem M with m 700 as beginning grid block stating that the next B blocks (total 14) would also allow the same infiltration rate across the top of the Grid. Not sure if you need to specify the next 27 blocks because <sup>§ 6-7-06</sup> because each grid block is broken into Fracture / Matrix # block.

File ran to completion - even created a save file, where it had not before.

§ - Compare files

6/6/06 used original chemical inp, without changing any of the boundary conditions, like I had done before. also changed Printout frequency in Solot, inp file to 10. This Created error

Back to original print out frequency  
 1) changed infiltration to one grid F700 / M700  
 - Same Error message -

Recopied original data back into folder, no changes can not get seen to completion.

6/8/06 Will have to calculate ratio of Surface Area of Fracture to Surface Area of Matrix in order to calculate how much infiltration should be specified for the Fractures and Matrix, (these #'s will eventually be divided by 14 because there are 14 Matrix + 14 Fracture grid blocks that make <sup>28</sup> the upper boundary

6/9/06 With all other windows closed (because previously runs all failed on Frye computer), I added infiltration at the top most cell. No more error messages, however it did not compute beyond time=0

Changed Greiner file back to having infiltration all in one cell. Computer didn't lock up, however didn't complete run

6/12/06

To figure the difference in surface Area (SA) between the Fracture and Matrix grids along the top of problem #4's grid block (28 in total) in order to correctly divide the amount of infiltration, I made an excel spreadsheet. I marked down the SA of the area between each grid cell (to the left and to the right) and the SA between the cells in the top row with the cells that lie below. It appears that the ratio of SA between the Matrix and Fracture cells are the same.

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6/13/67 ran the original files once more - really need to add virtual memory.

Working on the SA problem. Page 166 of the tough react manual, ix 3 mentions Reactive Surface areas manual on Fractures <sup>8/6/13/66</sup> walls were calculated from the fracture - matrix interface area/volume ratio, the fracture porosity, and the <sup>4/13/66 derived</sup> mineral volume fractures.

I actually took a look at volume/area. The volume coming from the ELEMENT keyword in the mesh file and I tried it with 3 different area values - the area to the left of the grid cell, area to the right of the grid cell (area between cells), and area between grid cell and the one below. I then added up the ratios for all the matrix + then all the fractures, I then took the <sup>8/6/13/66</sup> ~~Matrix~~ matrix ratio and divided it by the total ratio - I got the same results for all three area volumes - 99.34% of the SA ratio belonged to the Matrix, 0.66% belonged to the fractures.

So the matrix infiltration =  $1.57 \times 10^{-5} \text{ kg/sec} \cdot 0.9934 / 14 = 1.114 \times 10^{-6}$   
Fracture infiltration =  $1.57 \times 10^{-5} \text{ kg/sec} \cdot 0.0066 / 14 = 7.401 \times 10^{-9}$

gg Enter in the above data, using previous enthalpy to update the GENER file.

2806  
gg

6/14/06 Virtual memory was added to my computer today. the file ran, and got further (in Flow file) than it had before. However, when I try to repeat run either the program quits with a Domain/SEG error or acts as if has completed, but the files have not run to the end.

I calculated the infiltration rate per cell incorrectly. I used the volume of each cell to calculate the volume fraction  $\frac{Vol_{f700}}{Vol_{f700} + Vol_{m700}}$  for each cell.  $\frac{SA_{mf700}}{SA_{total}}$  which was then multiplied

by the infiltration rate of  $1.57e^{-5}$  kg/sec See Table

#	across top	row1	x	y	volume	Vol Fraction	SA Below	sa fraction	sa frac*vol frac	frac*infiltration	
1	f 700		-8.150E+01	8.419E+01	2.981	0.00660125	16.25	0.105103	0.000694	1.08929E-06	
1	m 700		-8.150E+01	8.419E+01	448.600	0.99339875	16.25	0.105103	0.104409	1.63923E-06	
2	f 695		-6.600E+01	8.419E+01	2.522	0.00659999	13.75	0.088933	0.000587	9.21526E-06	
2	m 695		-6.600E+01	8.419E+01	379.600	0.99340001	13.75	0.088933	0.088346	1.38704E-06	
3	f 690		-5.400E+01	8.419E+01	1.903	0.00660069	10.37	0.067072	0.000443	6.95073E-06	
3	m 690		-5.400E+01	8.419E+01	286.400	0.99339931	10.37	0.067072	0.066629	1.04608E-06	
4	f 684		-4.525E+01	8.419E+01	1.490	0.00659905	8.125	0.052552	0.000347	5.44461E-06	
4	m 684		-4.525E+01	8.419E+01	224.300	0.99340095	8.125	0.052552	0.052205	8.19615E-07	
5	f 713		-3.775E+01	8.419E+01	2.119	0.00660086	8.125	0.052552	0.000347	5.4461E-06	
5	m 713		-3.775E+01	8.419E+01	318.900	0.99339914	8.125	0.052552	0.052205	8.19614E-07	
6	f 712		-2.200E+01	8.419E+01	2.977	0.00660122	9.685	0.062641	0.000414	6.49211E-06	
6	m 712		-2.200E+01	8.419E+01	448.000	0.99339878	9.685	0.062641	0.062228	9.76979E-07	
7	f 657		-5.000E+00	8.419E+01	2.466	0.00659948	11	0.071147	0.00047	7.37164E-06	
7	m 657		-5.000E+00	8.419E+01	371.200	0.99340052	11	0.071147	0.070677	1.10963E-06	
8	f 571		5.000E+00	8.419E+01	2.466	0.00659948	11	0.071147	0.00047	7.37164E-06	
8	m 571		5.000E+00	8.419E+01	371.200	0.99340052	11	0.071147	0.070677	1.10963E-06	
9	f 631		2.200E+01	8.419E+01	2.977	0.00660122	9.685	0.062641	0.000414	6.49211E-06	
9	m 631		2.200E+01	8.419E+01	448.000	0.99339878	9.685	0.062641	0.062228	9.76979E-07	
10	f 632		3.775E+01	8.419E+01	2.119	0.00660086	8.125	0.052552	0.000347	5.4461E-06	
10	m 632		3.775E+01	8.419E+01	318.900	0.99339914	8.125	0.052552	0.052205	8.19614E-07	
11	f 603		4.525E+01	8.419E+01	1.490	0.00659905	8.125	0.052552	0.000347	5.44461E-06	
11	m 603		4.525E+01	8.419E+01	224.300	0.99340095	8.125	0.052552	0.052205	8.19615E-07	
12	f 609		5.400E+01	8.419E+01	1.903	0.00660069	10.37	0.067072	0.000443	6.95073E-06	
12	m 609		5.400E+01	8.419E+01	286.400	0.99339931	10.37	0.067072	0.066629	1.04608E-06	
13	f 614		6.600E+01	8.419E+01	2.522	0.00659999	13.75	0.088933	0.000587	9.21526E-06	
13	m 614		6.600E+01	8.419E+01	379.600	0.99340001	13.75	0.088933	0.088346	1.38704E-06	
14	f 619		8.150E+01	8.419E+01	2.981	0.00660125	16.25	0.105103	0.000694	1.08929E-06	
14	m 619		8.150E+01	8.419E+01	448.600	0.99339875	16.25	0.105103	0.104409	1.63923E-06	
total							154.61				

AS

-2006-  
6/16

I've tried to make various changes and swapping unaltered files to make problem work. Also I tried to alter the Genes file to include infiltration, it would only allow a few cells to be added before an error occurred.

88

6/17 Copied files and sent to my home computer. Used Genes file with all 28 cells across the top indicating infiltration, the file ran "normally" to the same point the example file had - with a param of 99 instead of 9999.

88

6/18 Ran the file for 4 cells, 2 to the <sup>right</sup> left of the drift and 2 below. The results of the cells that allowed infiltration varied little from the ones without.

88

7/4/06

I ran 4 more cells 875/545/866/341 that are closer to the drift, more apparent differences are noted. I also ran the initial 4 cells (6/18/06) - in a param of 9999 for the max timestep. Results have not yet been put in spreadsheet form.

88

7/24

Transfer files for above tests to work computer files in folder D:\Toughreact/p4-06

7/28

~~15 8/1/06~~  
Tried running all ambient runs at 25 and 90 degrees for the 4 water types (Quartz) Neutral, Pore, Ca-Cl, and alkaline. I changed all proper parameters (abc) and started the runs, computer freezing up. LS

~~7/31/06 -  
Continue to run updated Quartz Ambient files,  
had to manually turn off computers a few  
times because it was going through a  
physical dump. Most files completed successfully.  
LS~~

~~8/1/06 Finished running last of the Quartz ambient files  
successfully with few problems (errors and shutdowns)  
LS~~

~~8/4/06~~

~~Copied the files Jim Myers used to create the  
Ambient quartz run in toughreact and copied  
them onto my computer (D: toughreact/quartz)  
& modified the chemistry to create the various  
water compositions mentioned (7/28/06). However,  
because  $\text{CO}_3^{2-}$  isn't a primary species, it couldn't be  
added to the initial composition, so it had to  
be recalculated as  $\text{HCO}_3^-$  and added to the existing  
concentration of that species. A few minor changes  
to the chemical files and the runs were  
completed and ready for comparison.  
JS~~

~~8/2/06~~ 8/5/06

8/5/06

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8/2/06

Saved data into spreadsheet form for the weekly run data (see 7/4/06).

LS

8/3/06

Took a column to the right of the drift to verify temperature and Saturation (liquid) changes. Altered Flow and  $S_{0.0k}$  files to reflect the cells we want to look at. The temperature files reflect not much change.

LS

8/7/06

Used a Column closer to the drift, changed only the cells to report in the output files. However for some reason I keep getting an error message "M6202: Math"

LS

8/8/06

I created another folder and retyped the information for the cells I am interested in, hoping that there was a typing error. However, this is not the case and the file runs but it is not much help. I also copied the executable file in case the one I was using was corrupt. I reran the problem <sup>8/8/06</sup> files on Myers Computer. Worked

LS

8/9/06

I also ran the two columns of interest on Jim Myers computer, but I changed the time step with the Param keyword to 9999. Both files completed with out problems, however, there really is very little temp variance. (24-26°)

LS

8/10/06

Since neither of the previous columns show much temperature variation, I chose a third column (even closer to the drift and ran it (Timestep 9999) on 5 Myers computer. I also ran another column in the input, would show a temperature variance.

8

8/29/06

Try to make the columns I picked run to completion - by altering a time parameter in the Param keyword. My computer keeps crashing - so file can't run through.

88

8/30/06

Looking to see what needs to be changed in order to alter the input files to include various water types such as alkaline, Ca-Cl, and Neutral. The flow file can stay same as long as the rock types don't change. The only thing in the Solute file that needs to change are the cells of interest. Only the chemical file needs to be altered. That is if the files rock types remain the same.

8/31/06

Cannot get run to complete through to specified time (longer than 10yrs), must be some time parameter that correlates to the selected cells of interest.

Can change first time parameters as a first Error however each run takes a few hours. Checked the manual again, no luck.

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9/5/06 changed the param keyword to have the simulation begin at time = 0 and end at 100 yrs. Once these changes were made the file actually quit even earlier (less time) than it had before. I also tried changing the times with the TIME keyword, the results were not any better because the file was getting cut off in the same time position.

§§

9/6/06

I reworked the Flow file, however the problem will not run to completion and its not because it has come to equilibrium. Having computer shutdown problems, so I can't tell if changes made allow the problem to run to completion.

§§

9/11/06

Set up 2 of the columns (3+4) to run on a separate computer. The run will take the remainder of the day

§§

9/12/06

The 4<sup>th</sup> column (which is closest part of the drift) was still running when I came in, I had to manually abort the run. It hadn't even reached a year and the files were too big to be run with, rather opened with notepad or wordpad. I set up column 3 and also ran it on his Harrell's old computer.

§§

§§

9/13/06

it appears as problem 3 ran to completion, but the run didn't go far. I changed the ~~pr~~<sup>LS 9/15/06</sup> First writing control variable from 20 to 60 ~~and~~<sup>LS 9/15/06</sup> in the solve file and the ncypr from 99 to 999 in the param keyword of the flowinp file. I ran the file on the same computer.

§§

9/14/06

The run looked to complete without error, however upon opening the times.dat and Gasjobs files it appeared the the run did not complete to the desired time. I switched some of the print options in the solve.inp, to allow the program to reduce the printing in order to decrease the file sizes

§§

9/15/06

The file ran overnight and I manually cancelled it. It had barely reached one year (the file set up for 100 years) I changed the print parameters to 60, then reran the problem.

§§

9/18/06

File is still running, I transfer copies of the files to my computer to look at the time and flow files. I stopped the ~~run to change solve.inp file and restarted it~~ §§ 9/18/06  
§§ I decided to let the file run to see how far it could get and if it would complete.

§§

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9/19/06 The file is still running, and its completed up to 8 years.  
LS

9/22/06

I changed the print frequency, the relative tolerance of aqueous concentrations, and MCFRH (keyword Param in the following file) and let it run.  
SS

9/25/06

A list of file needs to be compiled of initial conditions where the initial file cuts off (or non-convergence) at about 8 yrs. This file can be feed into a new set of input parameters to allow the run to pick up where it cuts off at the 8 yr mark.  
SS

10/05/06

The file was rerun and the times were changed to end the run at 8 years, in hopes to collect the proper data to pick up the run where it left off.  
SS

10/30/06

Had to end run due to network issues, the file didn't converge and had not reached the 8yr cutoff.  
LS

12/22/06

In an effort to help the houghreact runs, I re-started problem HBy running the file without →  
LS

12/22/06 cont

The infiltration in order to see where dryout occurred various cells were checked and only those very close (outside) dry out completely.

JS

12/16/06

The file was then extended to run past the specified 2.75 hrs, slowly. Unfitation will then be specified

LS

2/12/07

Page 160 will start the continuation of the Integrated test. Starting with the new layout that corresponds to the bench top experiment.

Former notebook # 762 project 20.06002.01.212

Continued on page 22

→ This project copied and made into Electronic notebook 863E LS 3/19/07

3/19/07  
made side note:

~~JS~~  
2-8-07

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and

Moved to Notebook 863E 3/22/07 LS

2/9/07

Integrated tests continued from notebook 76Z  
This is the new design that corresponds to the bench top experiment.

changed the BC values in gem con I I S S K K  
this greatly improved the VF OR + Porosity (distributed evenly across mesh). Now I changed back the CBC and PK values of all the minerals. I also set delmax back to 1.0. The keyword PLT files needs to be added to gem for the sensor locations.

Coupled run working without heat (the max con change = 1)

LS

3/22/07  
2/12/07 - Meta only -

Began spreadsheet documenting various steps of this project, where heat source, side temp I asked to get 150° center fastest.

step 1

- ↳ Dry  $S_g = 1$ , CBC = 0, NO side heaters - value 25°, System  $T = 25^\circ$ . What heat load gives 150° at center quickest
- 58 J/s gives a temp of 151° in <sup>LS 2/12</sup> total 2 hours
- the max temp on this run was 158°
- 60 J/s gives temp of 150 in 14.4, 62 J/s in 11.6

Step 2

↳ Dry  $S_g = 1$ , CBC = 0, System temp 25, What temp and heat load give 150° center in shortest amount of time?

Started run with 58 J/s, but needs to decrease in order for side walls to be above 25°. I asked Chandraiken the max temperature that's accepted, she indicated that keeping the temp around 150 max would be ideal, however I'm having a hard time finding the right combination that keeps the max T in the 150's range.

Moved to Notebook 863 E at 3/22/07 LS

2/13/04

I ran another lot of tests and decided that I can't stay in the 150's range and under 20 hrs. I assume that the actual bench top test will require a higher heat than predicted. So I chose 56 J/s and side heater temp of 40. This gave 150° in 17 hours with a max temp of 168. If a max temperature of 170-180 are acceptable the run may complete in 13-16 hrs.

Step 3-

→  $S_g = 1 \text{ OBC} \cdot 5L/\text{day} = 1.93e^{-5} \text{ Kg/m}^2\text{s}$  over 3 cells in the middle of the range. Changed Meta Top BC (cell 2426) started with 56 J/s and 40° side heaters. This completed in 23 min and gave an estimate that it would reach up to 168 degrees as a high and take it to 150 within 17 hours. I'm trying other combinations to see if the process can be speed up.  
SS

2/14/07 Results From part 3

Part 3 - Add .5L Heat load needed to reach 150 center in shortest time. Using Center and side heaters

start	Sat gas	Heat Load	side Temp	center T-high	Time yrs	Hours	run time Min
1	1	56	50	207	2.33E-06	0.02	stopped
2	1	57	50	207	2.28E-06	0.02	stopped
3	1	57	80	203	2.31E-06	0.02	stopped
4	1	57	60	189	1.27E-03	11.11	30
5	1	55	50	175	1.81E-03	15.86	26 min
6	1	55	45	170	1.95E-03	17.08	25 min
7	1	56	40	168	1.93E-03	16.93	23
8	1	55	40	166	2.13E-03	18.64	23

RESEARCH SIGNATURE

*in order*  
*SS*

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Cont Next Page

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2/14/07

Moved to Workbook 863E 3/22/07 SS

Part 4

↳ same as part 3, but infiltration will be stopped  
various times (1, 5, 10 days) to look for finger flow.  
Times changed (target times) see spreadsheet that  
comes in disk form with this workbook. For some  
reason keep getting error message about recurrent  
data. Note: Max time was selected based on  
the steady state time from part 3 (2.14 to 2.33 yrs) so  
in part 4, 3 yrs was chosen for the cutoff.

SS

SS

3/22/07

2/15/07

Meta file fixed and running. Added a  
line to the top BC to specify QBC decreased to  
0 at specific times. After each time step a series  
of graphs will be made with keplot to show the  
effects of cutting off the infiltration for each of the 16  
time steps a graph of Temperature, pressure, liquid saturation,  
and relative humidity. These will be used to proceed to  
the next time cutoff for infiltration. The point being is  
to know where can fingering effects of water be seen and  
after how long.

SS

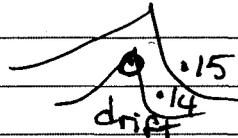
2/16/07

So far we have run the same file stopping infiltration  
at 5, 10 hrs, and 25 hours not much happened.  
The files were re-run with the infiltration  
cutoff at 3, 14, 30, and 200 days, once again  
the infiltration didn't change the  $S_w$  close  
enough to the DIFT to show any fingering effects.  
The file will be run with the cutoff at 10 hrs.

Moved to Notebook 863E 3/22/04

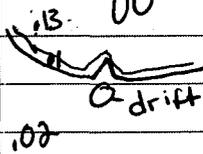
2/19/07

The cutoff infiltration was set to 10yrs, so a extra target time of 100yrs was added. Upon entering the file into feplot the results of infiltration intersecting the drift wasn't clear. The file was run w/ a cutoff of 5yrs and 10yrs and the original 15 target times. With the cutoff of 10yrs the infiltration water reaches the drift somewhere between .75 and 1yrs, and at 10yrs  $S_e$  around the drift is 0.14 and 0.15 above and has created an inverted shape. At 20yrs the higher <sup>(at 20yrs)</sup> (0.15) has reached



Further below the drift than at 10yrs. By 30yrs the saturation at the drift was 0.02. The time steps will be adjusted accordingly

Cutoff 5yrs - just at drift in 1yrs, at 10yrs drift area



at 15 and in drift .09-.11, higher sat reached below the drift area, by 20yrs higher saturation back to position of 1yr.

May need to decrease cutoff to see effects of the heated drift more carefully. Also changing target times more more to small increments close to 1 and before and after 10yrs.

5 year cutoff was rerun with higher target times, the effects were the same.

88

2/20/07

Sur was run and graphed using Macro in feplot. By 8yrs <sup>(at 20yrs)</sup> (30yrs after cutoff) there is a small pocket above the drift that is → next pg.

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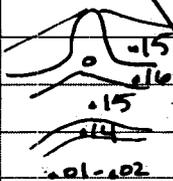
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3/22/04

Moved to notebook 863E 3/22/07 SS

2/20/07 more saturated (0.13) than the majority of the surrounding area (0.12). Near the area where infiltration occurred and a small area directly <sup>25 2/20/07</sup> beneath under the drift are yet even dryer (0.09-0.1), the bottom of the sub area X(1-50), Z(1.1-1.2) are at a  $S_u$  of .01 to .02. By 10 yrs  $\rightarrow$  to 14 years a larger and larger dry spot ( $S_u$  0.01-.02) develops below the drift, by 16 yrs and by 18 years the



wet areas retreat as the initial  $S_u$  creeps back upwards. And the original  $S_u$  for the experimental area creeps up beyond the drift by 30 years time.

With the two year run, the process is slower, but indicates the same processes. However the dry conditions do not reach the drift before 30 yrs. The one year run indicates that within 30 yrs the saturated layer has yet to reach the drift, so the time (targets) will be changed to see the process.

SS

SS

2/21/07

3-22-07

The <sup>one station</sup> two year run from 30-100' indicates that shortly after 30 yrs the dry out zone creeps back upwards and the two driest points meet (under cells 24-26 and above drift) and create an upside down U shape dryout <sup>55</sup> <sub>120</sub> <sup>11</sup> <sub>0.01</sub>. Within 100 yrs the

infiltration never comes in contact with the drift if infiltration is cut off with 1 year.

If the cut off is at 2 years, between 30-100 years takes about half the area is back to .01, but at 100 yrs the zone above (directly) is  $S_{sat} = 0.12 \rightarrow$  next page

SS



2/21/07  
~~2/21/07~~ Problem H tough react-continued  
2-2207

Starting over I bumped up the target time to 10 yrs, the file was taking too long to process so I controlled C and began to slowly decrease the file target time. After several runs I began to increase the target time from 2.75 yrs, even then having problems with the file processing.

LS

2-2207  
LS 2/22/07  
2/25/07

Looking at the files some <sup>LS 2-2207</sup> tolerances may need to be altered along with some time steps. Once the file gets to 2.75 years (2.79), the problem w/ time step and 1K4C begin.

LS

2/23/07

Changed Param Line 2 (Length time step to negative) with no luck. Also change the maximum time step change, which appears to be too high. This caused an error. I believe the book and file (Both manual) do not exactly correlate.

LS

LS  
2/23/07

Moved to Notebook 863E 3/22/07

2/27/07

clerked Part 5.

#3 For cutoff at 2yr, continued infiltration at 30yrs there is no significant patterns. I will run 2 50yr then I will run smaller time steps. When the cutoff was 1yr saturation levels (high) never reached the drift. This should be a preferred time frame. Also times of cutoff and continued infiltration will be conducted for times below 1yr, which may be more ideal for fingering affects.

#4 2yr-cutoff  
50yr - Infiltration start.

#5 2yr cutoff <sup>IS</sup>  
50yr on <sub>2/27/07</sub>  
60yr cut.

#6 14 days off 3-  
30 days on 2-27-07  
75 days off  
150 days on  
200 days off  
1yr on

where off means <sup>IS 2/27/07</sup> cut-off of infiltration, and on refers to re-start of infiltration

IS

2/28/07

Problem 6 of Part 5 was redone to concentrate on the times where fingering flow would occur. After reviewing these problems 4-6. another trial was developed.

IS Next pg.

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2/28/07

today

Moved to Notebook 863E 3/22/07 JS

Trial 7

15 day  
20 ~~200~~ days  
40 days  
50 days  
70 days  
90 days

Trial 7 ends with the termination of infiltration in order to see the short term effects within a few years.

LS

3/1/07

Upon close inspection of the resultant files of part 5 trials 6<sup>th</sup> & 7<sup>th</sup>, the out only composed the first 5 Target times, because the 6<sup>th</sup> was mistyped and was a larger value than the previous.

The first 5 target times will be put into keplot just to see the first 40+ days. However, nothing of significance resulted and the corrected runs will be reproduced and graphed.

LS

JS  
3-22-07

3/2/07

New Res (animation and jpeg) exported. (Tiff in black + white but I saw on the keplot website that can be altered.) So a jpeg can be created an inserted. However it doesn't look like the format was totally maintained.

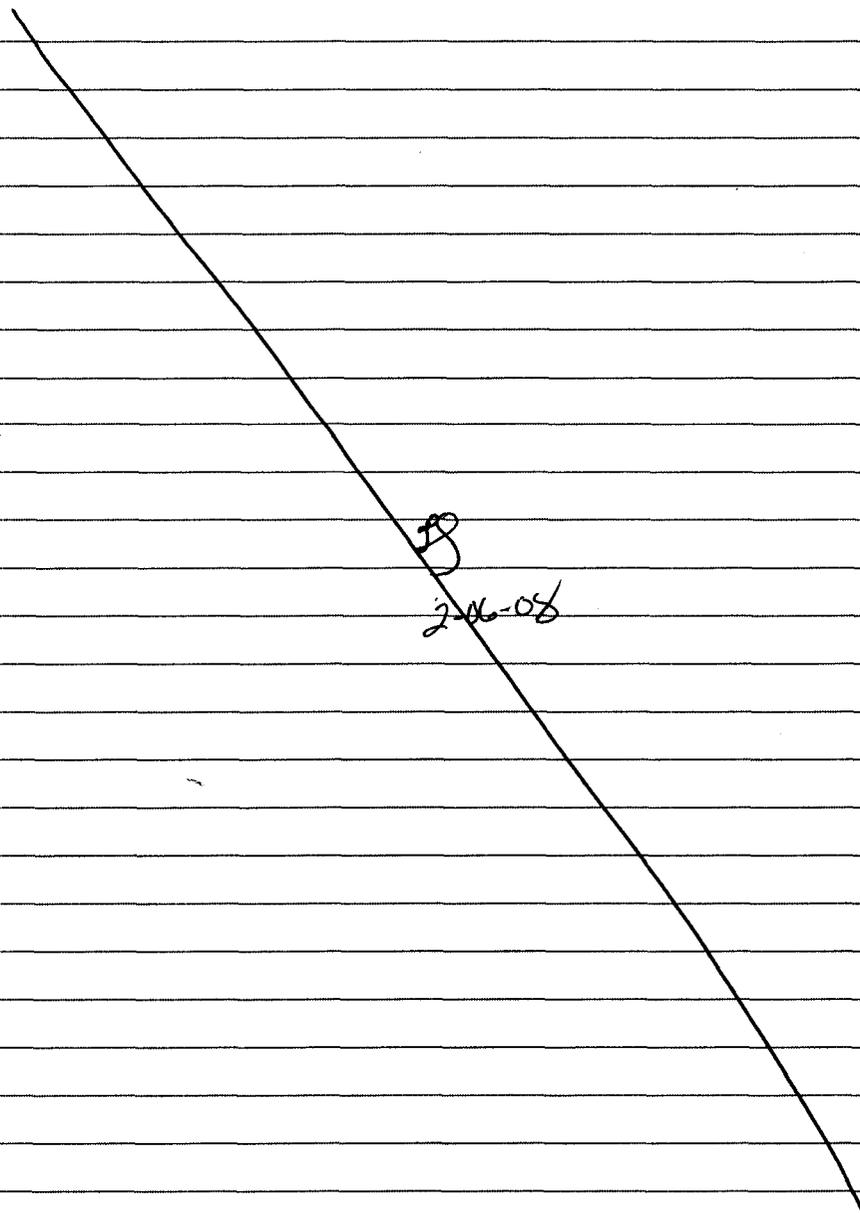
LS

2/6/08

Work on this project has ended; 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.

NO ENTRIES beyond this page.

LS



LS

2-06-08

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