

**Electronic Scientific Notebook
863E**

**Multiflo Plug Flow Modeling-Integrated
Testing**

Project # 20.06002.01.212

Lynn Sabido

3/21/07

Notebook Number 863E

Project number 212

This project is continued from bound notebook 762, pages 41-92.

Initially the project was to be continued in a bound notebook (797) however, because this was shared with another ongoing project, it was decided that all further entries for the Multiflo modeling project be completed in an electronic notebook. The pages were copied and scanned from notebook 797 and pasted here. Page 22 is missing because the page correlates to the other project in notebook 797.

LS

2/9/07

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

changed the BC value in gm for IISJK. This greatly improved the VFA stability (distributed evenly across mesh). Now I've changed back the CRBC and FK values of all the minerals. I also set delmax back to 0. The keyword PLI files needs to be added to gm for the sensor locations. Coupled run working without heat. (the max con change = 1).

LS

2/12/07 - Meta only -

Begin spreadsheet documenting various steps of this project where first source, side temp allowed to get 150° center for heat.

Step 1

↳ Dry $S_g=1$, $QBC=0$, No side heaters - valve 25°, System $T=25^\circ$. What heat load gives 150° at center, quickest

- 58 S/s gives a temp of 151° in 11.2 hours
- the max temp on this run was 158°
- 60 S/s gives temp of 150 in 14.4, 62 S/s in 11.6

Step 2

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

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

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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 3/8 and side heater temp of 40. This gave 150° in 11 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-

→ $S_g = 1$ OBC = 5L/day = 6.93×10^{-5} kg/m³s over 3 cells in the middle of the range. Changed Delta Top BC (cell 2426) started with 56 3/8 and 40° side heaters. This completed in 23 min and gave an estimate that it would reach up to 168 degrees at a high and take it to 150 within 17 hours also 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	Set 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	55	40	168	1.93E-03	16.93	23
8	1	55	40	168	2.13E-03	18.64	23

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2/14/07

Part 4

↳ same as part 3, but infiltration will be stopped
 various times (1, 5, 10 days) to look for freeze flow.
 Times changed (target times) are spreadsheet that
 comes in excel form with this workbook. For some
 reason keep getting error message about assumed
 data. Notei may have been selected based on
 the steady state time from part 3 (2M to 2.33 yrs) so
 in part 4, 2 yrs was chosen for the cutoff.

§

2/15/07

Micro file fixed and running. Added a
 line to the top BC to specify C_{bc} 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 10
 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 see where can freezing effects of water be seen and
 after how long.

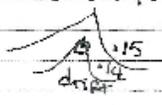
§

plot 107

↳ For we have run the same file stopping infiltration
 at 5, 10 hrs, and 25 hours not much happened.
 The files were rerun with the infiltration
 cutoff at 3 ~~days~~ 14, 30, and 200 days, once again
 the infiltration didn't change the S_L well
 enough to the DIRT to show any freezing effects.
 The file will be run with the cutoff at 10 yrs.

2/19/07

The cutoff 4 infiltration was set to 10yrs, second to be target time of 10yrs was added. Upon entering the file into deepplot the results of infiltration intersecting the drift wasn't clear. The file was run with 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 7.5 and 14yrs, and at 10yrs saturation the drift is 0.14 and 0.15 above and has created an inverted shape. At 20yrs the higher (0.15) has reached



Further below the drift than at 10yrs. By 20yrs 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 was 0.15 and in drift 0.09. My higher sat reached below the drift area, by 20yrs higher saturation back to position of 14yrs 0.02.

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

8 year cutoff was run with higher target times, the effects were the same.

2/20/07

Sur was run and graphed using Macro in Deepplot. By 8yrs (8yrs after cutoff) there is a small pocket above the drift that is \rightarrow perched.

INFLU OR SIGNAL (U)

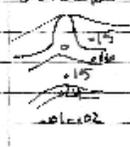
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2/20/07 more saturated (0.13) than the majority of the surrounding area (0.12). Near the area where infiltration occurred and a small area directly ^{to the} under the drift are yet even drier (0.09-0.1), the bottom of the ~~the~~ area 21(1-0.1), 21(1-1.2) are at a S_w of 0.1 to 0.2. By 10 yrs to 14 years a large and large dry spot (S_w 0.01-0.02) develops below the drift, 10/16 yrs and 14/16 yrs the



under area retreat, as the initial S_w creeps back upwards. And the original S_w in the experimental area creeps up beyond the drift by 30 years time.

With the two year run, the process is shown, but indicates the same processes. However the dry conditions do not reach the drift after 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.

8)

2/21/07

^{one drill} The two year run from 20-100" indicates that shortly after 30, as the dry out zone creeps back upwards and the two drilled points meet (under cables 24-26 and more drift) and create an upside down U shape dryout ^{at 30" depth} ~~at 100"~~. Within 100 yrs the infiltration ~~never~~ comes in contact with the drift if infiltration is cutoff with 1 year.

if the cutoff is at 2 years, between 30-100 yrs later about half the area is back to 0.01, but at 100 yrs the zone above (directly) is $S_w = 0.12$ → next page

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2/22/07 delineated Part 5.

#3 For cutoff at 2yr, continued infiltration at 30yrs there is no significance patterns (will run)
2, 50yr then it will run smaller time steps.
When the cut off was 1yr saturation levels (high) were 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 effects.

#4 2yr-cutoff

50yr - infiltration starts

#5 2yr cutoff ^{200 days}
50 yr on
60 yr cut

4.6 14 days off
30 days on
75 days off
150 days on
300 days off
1 yr on

when off means ²⁵⁻²⁵⁻⁶⁷ cut-off of infiltration, and on refers to re-start of infiltration

IS

2/28/07

Problem to of Part 5 was to come to a conclusion on the time when fingering flow would occur. After receiving these problems the another time was developed.

Be next pg.

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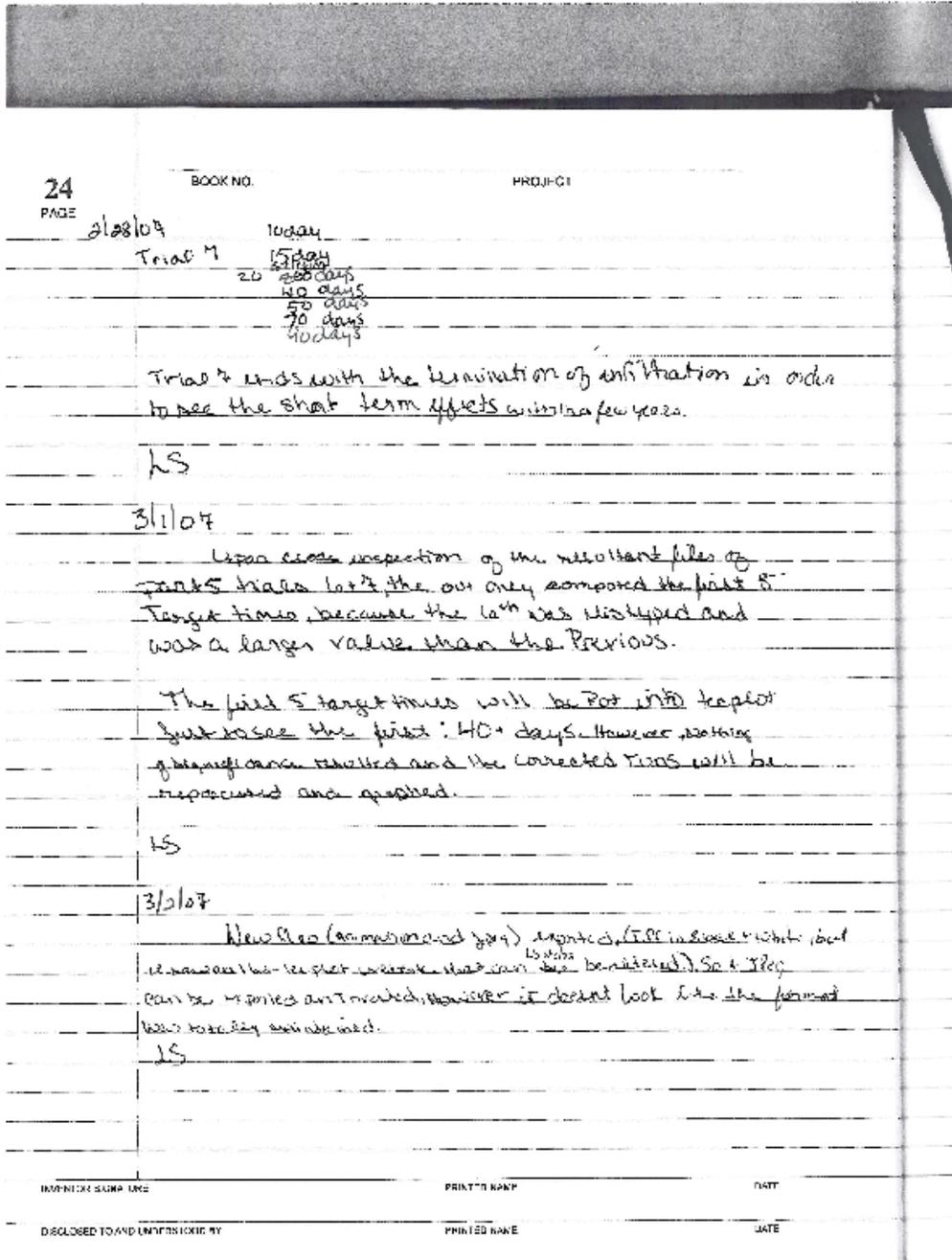
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BOOK NO.

PROJECT

2/28/07

Trial 7

today

- 15 days
- 20 days
- 25 days
- 40 days
- 50 days
- 70 days
- 100 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 cross inspection of the resultant files of parts 5 trials lot 7, the only one compared the first 5 target times, because the 6th was distorted and was a larger value than the previous.

The first 5 target times will be put into a plot just to see the first 40+ days. However, nothing significant results and the corrected times will be reproduced and plotted.

LS

3/2/07

New files (announcements) created, (if it is not right, but it is not the best, we can't see that in the ^{15 days} benefited). So it may can be revised and made, however it doesn't look like the format was totally suitable.

LS

End of entries from bound notebook 797

LS

3/21/07

Part 6 is very similar to part 5, however the heat load will be turned off when the center region reaches 150 degrees, which is at 1.25e-3 years or 11 hours. The file will be run with similar episodic flow patterns. Eventually the side heaters may also be turned off after 11 hours to see the desired affects.

LS

3/22/07

With some of the runs completed for part 6 the results should be graphed as contours for comparison, however Tecplot 10 was re-installed with Tecplot 7, however I'm having problems uploading the data. I tried to create a query and macro in excel to process the data, however even in excel there is a limit to the number of rows that can be graphed and due to the file format (FLD) it is hard to pull a reasonable query. I'm looking for an alternative program to use for the contour plots.

LS

3/23/07

All the runs for part 6 have completed, however visual conceptualization isn't possible, so adjustments can't be made. The results of parts 1-5 have been summarized within the original excel file "heat load tests".

LS

4/9/07

Tried using Sigmaplot to graph data, I just can't get the files into the correct format and then load all data for each time step.

I have begun looking up data to create the air layer around the heat source that is the drift. I took the specific heat capacity, thermal conductivity and kinematic viscosity for dry air to enter into the file source: http://www.engineeringtoolbox.com/dry-air-properties-d_973.html

I looked up the thermal conductivity for moist air from http://www.electronics-cooling.com/articles/2003/2003_november_techdata.php

The dry and wet air have the same thermo conductivity value of 0.026. I made porosity and permeability 0, and added the Conduction keyword. The heat load was at 56J/s and the side heaters are at 40 C. The file from step 2, no infiltration was used. The file ran in a few seconds.

LS

4/10/07

The temperature of the file didn't reach the desired temperature, it overshoot up to 800 degrees C. Will go back to step 1, no side heaters, just center heat to bring system to equilibrium and then use that as the initial file. The center was set at 50 J/s and the drift T was as high as 700C, however, above and to the right (.02m-two cells away) the temp only reached 90 degrees. SO the center temp was reduced to 40J/s, the center 581, sides 77C. At 30J/s (center 442 sides 64). At 10J/s (center 164- sides 38). This should be used as the initial conditions.

The heat source is set considerably low compared to that of the drift without the air pocket. Chandrika will give me her air thermo properties that she had used in the past, that are specific to this situation. Also she mentioned the PCKR needed to be updated with a different curve type.

LS

4/11/07

I'm thinking that the coreys curve will be used for the gas phase under PCKR. I removed the conduction keyword. At 10J/s (center 164- sides 38). The file was completely random and all results were off (temp-press-sl) and were not uniform. The Corey curve was added with a Critical (immobile) gas saturation of 0.1. The files when loaded into tecplot, were in different format and the individual variables had to be selected. This may be why the graphs are off (vertical lines of different values) probably incorrect columns for some parameters were read in.

LS

4/12/07

Chandrika gave me an old file that had all the properties of the air layer, the pckr, phik, and thermal properties all need to be changed. After these additions there are some input errors with in the thermal data that is preventing the file from being read in.

LS

4/16/07

All the air properties were removed and added one by one, due to various errors (debug, format); the Pckr section was added last. The initial conditions were reported in the actual file not the .int file. The heat load at 10w barely made a difference and at 56 w, the drift reached 101 degrees and at 60w the Temperature reached 107 degrees. At 85W, the temperature of the drift heated to 140 degrees after 2.93 days. With 100W, the temperature rose to 150 in one day and maxed out at 161. The initial condition file was updated and the file ran slightly faster. For part two (with the air surrounding the drift), the side heaters at 50-60 degrees C and the drift at 100W, predicted 150 degrees would be reached in 13.5-12 hours respectively and max temperature would be 185-195. I began part 3.

LS

4/17/07

For part 3 (with drift surrounded by an air layer) I used 100W and 50C for the side heaters. The temperature reached 150 within 14 hours and reached a maximum of 185, however it took 1 year to cool to temperatures below 150 degrees. The temperature steady state took about 3years and the liq saturation reached steady state in 2.9. The animation of part 3 with air shows that the drifts liquid saturation does not go above .01, but with out air the drift area SI increases. The plume over higher saturation above the drift is greater (larger extent) with the air layer included.

LS

5/15/07

Initially I thought the steady state file I originally used was wrong, due to the addition of the air layer surrounding the drift. However, it was correct and included are an excerpt from the recordruns spreadsheet.

Part 3 - Add .5L/day 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	100	50	185	1.56E-03	13.68	40
2	1	100	50	185	1.54E-03	13.49	24
3	1	100	70	204	1.29E-03	11.28	69

Temp
 **QB
 qbc C

LS

5/31/07

Due to problems accessing data on UNIX (can't map to Texas), and the uncertainty of the input file details parts 1-3 were rerun using a dos prompt and then graphing the data on a windows version of Tecplot 360. There were a few inconsistencies with the data. When the file was altered back to the original 100 yrs the heat source options were not changed. The heat source was in use for only the first 44 years.

LS

6/1

The input files were adjusted and additional comments were added to allow all users to identify the input parameters. Part 3 will need additional runs, because 100 W at the center isn't enough heat to bring the system up to 150 degrees. Although there is 1 error for all files, it's because the last time in the heat load is 100yrs the system termination time. The air balance files will be off, because the system has begun in a steady state. \

LS

6/4

Part 3 was rerun with a few different heat loads, but settled on 110W. All was regraphed in tecplot and either animations or screen prints produced for review. All three parts come into temperature and pressure steady state within the first day, however, just looking at exact numbers, it's a few years. (see recordruns spreadsheet). The last specified heat load time wasn't altered, but may be changed to 95yrs for part 4 episodic flow.

LS

8/22/07

The bench top experiment is currently underway. The dry system was heated up allowing the drift center to remain a constant 110 degrees, the side boundaries at 80C. Then water was infiltrated from the top and after a few days hasn't reached the drift. The goal is to predict when water will infiltrate the drift. The original iet1air file was modified to account for a constant temperature at the drift using the source keyword. The initial file was updated specifying 110 at the center and using options 2,1 meaning there is an air mass and the source can be specified as temperature in degrees C. The manual, which is old, states this option isn't supported. The program wasn't updated, because this option failed.

LS

8/28/07

The model of the experiment was cut in half, using the right half in the model. The upper boundary is specified 2 times one with a QBC of .5l/day and mixed air/water and the other specifies the mixed boundary without infiltration. The right side boundary is left as is and the left boundary specifies type 1 with a negative pressure and a temperature of 110. The remaining cells on the left boundary need not be specified, for they are assumed type 1. This prevents flow across the boundary. The initial file was run without flow. Then a new iet1.int file was created and infiltration was added, the cells viewed are the same as before, in the same locations of the bench top sensors.

LS

8/29/07

The file ran overnight and continually had to cut the time steps, making the process very slow and no where near completion. Initially I had altered the Limit and Auto keywords, but kept receiving errors. I changed the dsmx from .08 to .1 (limit keyword) and Fac1 to the default of .5 (Autostep keyword), and the newtnmx from 12 to 15. I then changed the infiltration cell to X=2 and Z=1, this decreased the run time, however, the file seems to still be getting caught up.

LS

8/30/07

The file is still getting bogged down even when changing the infiltration cell. The drift was increased in size as well as the infiltration area. This had similar results as before. The file was changed back to its original form and only the Fac1 and dsmx were altered. The run is still extremely slow and the time step is being cut continuously to reach convergence.

LS

8/31/07

The liquid saturation was graphed in the tecplot program to see look at what is going on when the program begins to get bogged down. Fix top boundary/tried without top boundary/Changed sg to .98 None of these worked. The constant high center temperature is preventing infiltration and the file Autostep for saturation is relatively high (dt of 3%, when the highest saturation is 17%). The DSMXE was changed from .03 to .01 and DTMPMXE from 3.0 to 2.0 (change in saturation and temperature respectively). The initial file was kept since the experiment was heated up and reached steady state while the center was stable at 110; this determined the pre-existing temperature gradient. However, due to the slow run, the center temp listed in the boundary condition was changed from 110 to 90, also the infiltration was returned to cell x=1, z=1. This run did finish within an hour, so the target times were adjusted to a finer scale. Two other runs with center temps of 110 and 80 were also run. The file with the constant drift temperature of 110, is considerably slow, it only reached 1.9 years within an hour. A file with the drift temperature of 80 will be run for comparison.

LS

9/4/07

The three files ran over the weekend with the 110 degree drift center taking the longest to complete (16.9hours) and the 90 and 80 degree drift temperature files taking about 20 minutes. None of which showed a increase of liquid saturation within the drift in a seven year period.

LS

9/11/07

I was told that “ It is more realistic to use Swir value of 0.1045. Also, at the end of the steady-state run, does the model predict that all the nodes will have a liq. Sat. of 0?”

I left the drift center at 110 and changed the initial gas saturation to 0.895 (liq sat .1045). Right now I’m trying to get the steady state to run so I can cut and paste the initial file. However, even for the steady state run, I’m experiencing slow run times (many cut times); I am trying to speed this up by modifying the steps and limits. So far, at the beginning of the steady state run the model has predicted a liq sat of 0 at the drift center and I imagine that will branch out.

Once the steady state run is complete, I will run it with the specified QBC. The transient run doesn’t have to specify any special keyword and if the balance file is still off after the run, I will ask Scott about it. I’m not entirely sure how to read/interpret the balance file, other than it lists what is out of balance.

I changed the Gas saturation to 0.9, DSM 0.5, and DTM back to 3.0. The file has run for six hours and has only reached 3.4 years. I will let it run overnight.

LS

9/13/07

The initial steady state file completed its run in 38 hours. Despite making limiting changes, I could not make the file run faster using the requested data. The QBC used for the initial transient run was $5.787e-4$ and the first attempt was running very slow. The autolimit steps for concentration and saturation were reduced. The file appears to be running faster and will be allowed to run overnight.

LS

9/17/07

The file took 12 hours to run, the requested Sl and Temperature contour plots were made. However the air balance doesn’t equal 1 and Chandrika requested that problem be addressed.

LS

9/21/07

After speaking with Scott, the initial steady state run should have the upper boundary defined in one BC block, but using type 1 and specifying the SGBC as 1, and the XABC needs to be added. It’s the mole fraction of air above the first cell. This is directly related to Relative humidity (in the lab about 30-40%) and must be calculated using the Fraction of air and the saturated vapor pressure. When the file incorporates infiltration,

the boundary condition for cell 1 is back to 5 (mixed air and water), and the rest of the upper boundary is defined as type 1 and specifying the SGBC as 1, and the XABC. I asked Scott P about the airbalance file not being unity, he said that not to worry about it, because it really shouldn't affect the run. It may be getting tripped up because the air mole fraction is relatively small, so dividing a small #/small # may indicate a larger error, but the air fraction that the file is dealing with is small, so the error shouldn't affect the results.

LS

9/26/07

I noticed after graphing the data from the transient run with the Upper boundary condition for cells 2-25 as type 1, the liquid saturation is off. Either way I think I need to re-run the steady state file (to get the initial conditions). I had let it run to 10 yrs just like how the transient run was set up, but this vastly alters the initial liquid saturation. The SI is set to .1045, but after letting it run for such a long length of time, the whole system dried out to 0.01. I believe that they ran the system without water for about a week. The main reason to perform the steady run is to create a proper initial file so the transient run is faster. This is what is probably slowing down the runs and why the resultant Liquid saturation is so off for the transient run. Also I was given a file that tracks the temperature of the sensor nodes and it appears they have set the side heaters to 80F, rather than 80C as we have it in our model.

LS

9/28/07

After Chandrika questioned the temperature of the side heaters, it was confirmed that they were set to 80C. The experiment was heated up without infiltration for what they think was 4-6 months. So I ran a steady state run using both the steady keyword, which automatically stops when steady state is reached, and then I ran a steady state -times of 1- a maximum of 6 months. I then used the information from the 6 month run to create the initial file and started a transient run.

LS

10/1/07

The transient run completed with in 6.75 hours. Upon looking at the data and making some plots in tecplot, I believe there is a major problem with the input file data. The liquid saturation data looks ok until at 2.5 years the whole system begins to dry out, even though infiltration is still occurring. By the end of the run the liquid saturation is minimal and below residual concentrations. There must be something wrong with how the infiltration is being considered, the temperature gradient hasn't changed much so I don't know why dry out is occurring.

LS

10/3/07

After viewing some of the files, I went back and recalculated the QBC with the correct area (m^2) to be $5.787E-4$ kg/m^2-s , I also set up two runs one with the initial file pulling

data from the steady state run using the steady state keyword and another using the “steady state” six month run, which never reaches steady state. The file using the steady state keyword takes about 8.1 years to reach steady state and by that time the $S_g=1$ (which is specified) and the mole fraction of air varies little (.9687). The transient run took a minute or two. However, the iet1air_sat.xyp file indicates all the chosen cells are 0 Liquid saturation for the duration of the run as do the FLD files. The run where the initial conditions were allowed to only calculate for 6 months was also used in a transient run and has taken a few hours so far.

LS

10/4/07

The file ran overnight and still had not completed, but was interrupted. It had made it to 6.5 years, however the saturations look much more reasonable in this run. This will be allowed to run tomorrow, but the existing files may be used for some graphing to see if further adjustments will be made.

LS

10/8/07

Looking at the results of the transient runs that used 1) steady state and 2) 6month initial runs. The file using the initial steady state run reported a 0 liquid saturation for the duration of the transient run (10yrs). The transient run with the 6 month initial file started with a higher liquid saturation, but the lower and possibly the upper boundary need to be modified.

LS

10/9/07

Some suggestions from Scott were to change the lower boundary to a type 1, but inserting a layer of air (same size as the rest of the cell blocks) to create a buffer. This should take care of the drainage problem at the bottom, because the mesh screen in the lab experiment (at the base of the sand) is effectively a capillary barrier and all the liquid in the bottom of the collection pans is most likely from water vapor hitting the Plexiglas walls and compensating. The upper boundary will be kept at type 1 and run with a gas saturation of 1 and a mole fraction as 0.9687, when the initial file is set up, the transient run will define the gas saturation as 1-residual saturation. This should hopefully take care of the drying out of the system from the bottom up.

LS

10/11/07

I began modifying the upper and lower boundaries. During the first 6months, allowing the upper boundary be a type one and defining the mole air fraction. For the lower boundary there were a few error messages, but essential a 121 row was added and defined as air.

LS

10/12/07

The initial six months were re-run several times with various combinations for the system temperature, drift temperature, and side heaters temperature to achieve the closest possible values as those recorded for the lab experiment, which is outlined in the document Pre-test temperatures. I used a system temperature of 25C(room temperature) and a side heater of 75, since the heater took some time to make it up to a temperature of 80C. The heater center was set at 100, even though it too gradually was raised over a several month period. Two transient runs were set up. One was run with the initial file for the first 6months with the temperature adjustments, the other with the current temperature settings.

LS

10/15/07

The runs were disrupted due to IT updates that ran over the weekend. While I don't expect there to be much differences between the two runs, the one using the initial file with temperature adjustments should be more accurate, however, the transient run using this initial file was slower than the regular initial conditions after 6months. Looking at the data seems more reasonable than the drying out problem as seen before. The saturation doesn't appear to change much or as expected. Future runs will be run on unix, specifically Katana once the multiflo program is adjusted for that platform. I did try to get the run up on coyote or texas using the multiflo.coyote and multiflo.texas files. However, there are many issues and I may not have all the proper permissions.

LS

10/16/07

While changing the lower boundary prevented dryout, there was also a buildup of liquid at the bottom. The file may have to be changed back to the original free drainage boundary. I will re-run these files on Coyote once we are able to access the proper program.

LS

10/17/07

In order to access multiflo.coyote a new unix account was created and the command syntax is `/home/spainter/multiflo/mflo2.0.1/multiflo.coyote iet1air`. The files also need to be converted to the unix format (`dos2unix` command). The six month (lower T) initial numbers were used to perform a transient run.

LS

10/18/07

The file was running incredibly slowly on coyote, so I was altering the limits to possibly make the file run faster. The bottom boundary was changed back to free drainage for the transient run only.

LS

10/19/07

Due to an error the file was re-started.

LS

10/30/07

The file that has been running currently on Coyote was rerun on a command prompt, while faster, the file was still being tripped up. A few modifications to the limits didn't help and a run was started using free drainage for the lower boundary but keeping the air layer (cell 121).

LS

10/31/07

Looking at the run from yesterday, the air layer couldn't allow free drainage and there was a build up of liquid at the bottom of the model. The run had also been run specifying the air fraction rather than liquid saturation. The file was modified to allow the first 6 months running with an air fraction of 0.982 and the air layer, cell 121, was eliminated. Once the initial run is complete the file will be set up with an upper boundary with a specific liquid Saturation instead of specifying the air fraction. The lower boundary will be elevated in temperature to see how this affects the results.

LS

11/1/07

The run was set up for 6 months with the bottom as type 6 free drainage, the top type 1. For the transient run the top was kept as type 1, but the upper was split into type 5 (Sg) and type 1 (Sg and air fraction specified). The lower right corner (x -23-25, cell 120) was changed repeatedly to higher temperatures (based on the initial output) to determine if that would progress the run. This didn't seem to increase the run, but by decreasing the limit parameters (.01 for change concentration allowed) the run finished in 2.4 hours.

LS

11/2/07

Once again the last run from yesterday (free drainage-no air layer) dried out from the bottom up, the porosity may be a problem, but for the times being runs with a lower boundary of type 1 were set up with different entries into the lower boundary pressure, saturation and air mole fraction.

LS

BCON 5

:

:itype iface i1 i2 j1 j2

5 TOP 1 1 1 1

:pbc, tbcf, sgbcf, xbcf

:qbc and timbc

:timbc qbc pbc tbc sgbc xabc emsivt

0.0 0 101325 25.00 0.895 0.0 0.0 :

:

/

:itype iface i1 i2 j1 j2

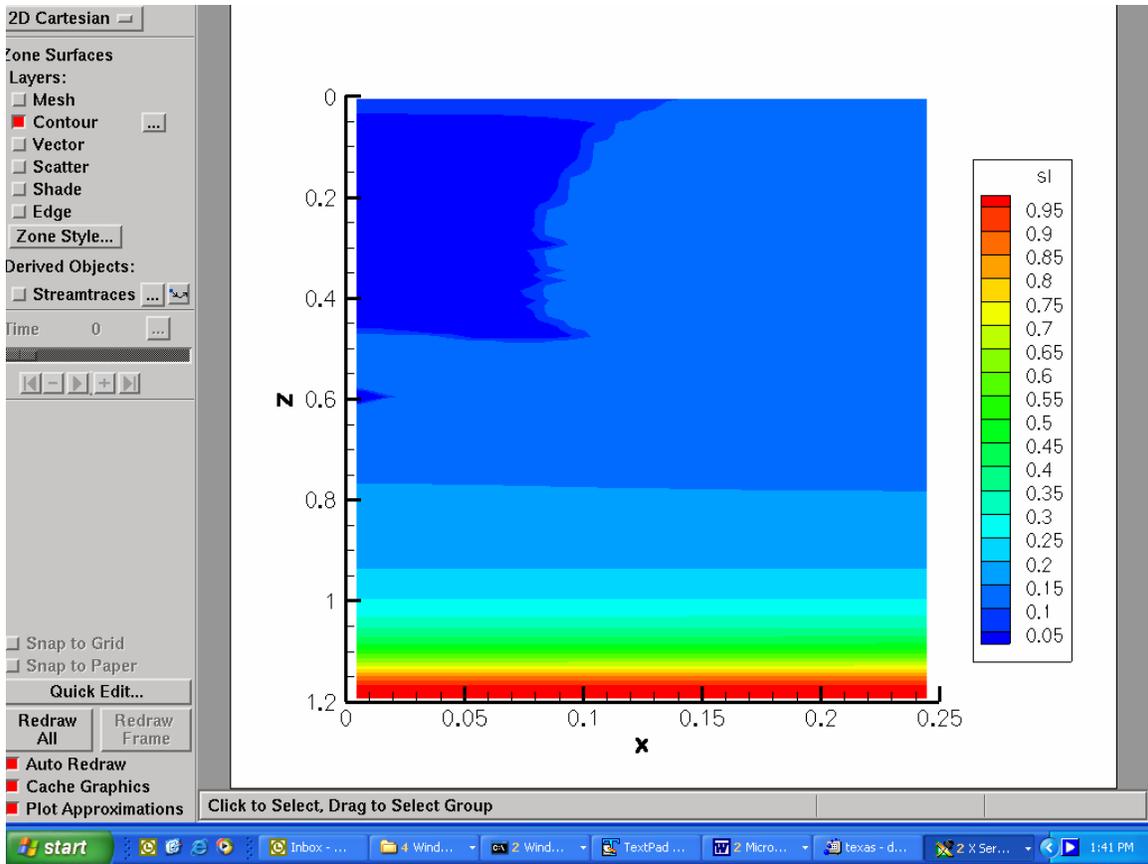
1 TOP 2 25 1 1

```

: pbc, tbcf, sgbcf, xabcf
: qbc and timbc
: timbc    qbc    pbc    tbc    sgbc    xabc    emsivt
  0.0      0      101325  25.00  0.895  0.982  0.0  :
:
/
: itype iface  i1  i2  j1  j2 Dirichlet (constant field variables) no flow but can have heat
transfer
  1  LEFT  1  1  60  60
: pbc, tbcf, sgbcf, xabcf
: qbc and timbc
: timbc    qbc    pbc    tbc    sgbc    xabc    emsivt
  0.0      0      -1    110.00  .0    0.0    0.0  :
:
/
: itype iface  i1  i2  j1  j2 Dirichlet (constant field variables) no flow but can have heat
transfer
  1  RIGHT 1  1  1  120
: pbc, tbcf, sgbcf, xabcf
: qbc and timbc
: timbc    qbc    pbc    tbc    sgbc    xabc    emsivt
  0.0      0      -1    80.00  .0    0.0    0.0  :
:
/
: itype iface  i1  i2  j1  j2  k1  k2
  1  BOTTOM  1  25  1  1  120  120 : no flow
: timbc qbc    pbc    tbc    sgbc    xabc    emsivt
  0  0  101372.1  25.00  .0  0  0  : qbc, sgbc is not required
:

```

Because the upper boundary was defined with an air fraction and liquid saturation, as time progressed the upper portion above the drift became more dry even with the infiltration of water. Below is an image at 10 years.



```

:
BCON 5
:
:itype iface i1 i2 j1 j2
  5 TOP 1 1 1 1
:pbs, tbcf, sgbcf, xabcf
:qbc and timbc
:timbc qbc pbc tbc sgbc xabc emsivt
  0.0 0 101325 25.00 0.895 0.0 0.0 :
:
/
:itype iface i1 i2 j1 j2
  1 TOP 2 25 1 1
:pbs, tbcf, sgbcf, xabcf
:qbc and timbc
:timbc qbc pbc tbc sgbc xabc emsivt
  0.0 0 101325 25.00 0.895 0.0 0.0 :
:
/
:itype iface i1 i2 j1 j2 Dirichlet (constant field variables) no flow but can have heat
transfer
  1 LEFT 1 1 60 60

```

```

: pbc, tbcf, sgbcf, xabcf
: qbc and timbc
: timbc    qbc    pbc    tbc    sgbc    xabc    emsivt
  0.0      0      -1    110.00 .0    0.0    0.0    :
:
/
: itype iface  i1 i2 j1 j2 Dirichlet (constant field variables) no flow but can have heat
transfer
  1 RIGHT 1 1 1 120
: pbc, tbcf, sgbcf, xabcf
: qbc and timbc
: timbc    qbc    pbc    tbc    sgbc    xabc    emsivt
  0.0      0      -1    80.00 .0    0.0    0.0    :
:
/
: itype iface  i1 i2 j1 j2 k1 k2
  1 BOTTOM 1 25 1 1 120 120 : no flow
: timbc qbc    pbc    tbc    sgbc    xabc    emsivt
  0 0 101372.1 25.00 .0 0 0 : qbc, sgbc is not required
LS

```

11/6/07

After reviewing the files for the previous run, there appears to be a pocket of dryness above the drift, but not immediately above it. The QBC rate was incorrectly entered and has since been fixed. Also the run should work as is and was rechecked to evaluate the sand parameters. Initially, the swirl (residual moisture) was changed to .1045, however I have changed it to .045, as indicated in the input details spreadsheet given to me by Chandrika. There may be a parameter out of balance, possibly the sand permeability. Before changing/reducing permeability, so runs were set up with the new swirl value to check the results. There are three runs each run initially with the lower boundary as free drainage, drift center and side heaters set to 80 Centigrade, and for only 3 months (0.25yrs).

Run-initial 3months	Type upper boundary	Liquid sat of upper boundary	Fmol air upper boundary	Type of lower boundary
1-UB1SL	1	0.895	0	6-free drain
2-UB1mfa	1	1	0.989	6-free drain
3-UB5SL	5	0.895	0	6-free drain

Transient runs were then set up for each run and an initial condition file was updated from the 3 month run's output file. The transient runs for the first two used upper boundary type 1 with a liquid saturation of 0.895, and the last run specified the upper boundary as type 5-mixed for the first cell (QBC) as well as cells 2-25.

Initial results of temperature are comparable to those taken from the lab experiment before water was added.

	Time	V8	V4	V2	H2	H4	H8
lab temps	8/1/2007	51.7	77.2	82.1	85.8	80.1	75.8
run 1	2.50E-01	7.47E+01	7.73E+01	7.83E+01	7.84E+01	7.84E+01	7.94E+01

run 2	2.50E-01	7.51E+01	7.75E+01	7.83E+01	7.85E+01	7.84E+01	7.94E+01
run 3	2.50E-01	7.48E+01	7.74E+01	7.83E+01	7.84E+01	7.84E+01	7.94E+01
	Sat	V8	V4	V2	H2	H4	H8
run 1	2.50E-01	1.15E-01	1.16E-01	1.16E-01	1.15E-01	1.15E-01	1.14E-01
run 2	2.50E-01	1.07E-01	1.08E-01	1.09E-01	1.08E-01	1.07E-01	1.06E-01
run 3	2.50E-01	1.10E-01	1.11E-01	1.12E-01	1.10E-01	1.10E-01	1.09E-01

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11/7/07

The three transient files ran overnight, however they didn't progress much stating the run times were between 5.5 5.75 hours, when they had been started more than 12 hours previously. Runs 1 and 2 (1-UB1SL and 2-UB1mfa) ran to about 2.3 years within 5 hours 35-40minutes, and run 3 (3-UB5SL) ran until 4.5 years with in 5 hours 40minutes. Since changing the swirl parameter, the transient file doesn't appear to dry out from the bottom up, as it had previously, graphs were generated via tecplot. The first two runs could have a lower level dry out, but its isn't know at this point because the runs only reached 2.3 years, when past runs dry out occurred at 2.5 years. However run 3 shows little indication of severe dry out towards the bottom of the experiment. This is probably due to the fact the system starts out dryer (residual saturation is .045 not .1045) instead of wet and the bottom being exposed to air doesn't dry out the system, the infiltration amount isn't enough to preserve the saturation level when using a swirl of 0.1045.

The same three files have been moved to another computer to allow the runs to progress. A fourth run has been set up, like run 3 with the sand permeability decreased in magnitude. Because the runs are slow its hard to say if the permeability lowered by one two or three orders of magnitude will affect the run. This file run 4, UB5SL-lowperm, was also set up on another computer with the other three to run overnight, but decreasing the permeability only one order of magnitude. The auto step change in saturation and temperature were increased to .04 and 3 respectively, but this didn't speed up the run any, so the values were kept as the original.

LS

11/8/07

Another run 5, UB5SL-lowperm-13, was created two orders of magnitude lower than the original permeability. Runs 1 and 2 were stopped as so 3+4 could run to completion in a reasonable amount of time. Run 5 were set up on my computer, while the others were on Carol's old computer. Upon completion, the results of runs 3, 4, and 5 were graphed using tecplot. The two runs with the lowered permeability started out much dryer and didn't show a zone of higher saturation above the drift. Run 3, with the original permeability value did show a zone of increased saturation above the drift. Animations for temperature, pressure and liquid saturation were made, and I created an excel spreadsheet comparing the temperature data to what Todd had initially given us and a Time vs temperature plot (modification comparison.xls). The plot indicates temperature steady state between 7-10days. The saturation plot shows the system coming into equilibrium shortly and within 10 years no seepage into the drift.

LS

11/9/07

Runs 1 and 2 were restarted and are as of today still running. After 16 hours both files have reached 7.5 hours. The files were graphed until this point, while different from run 3; they do not show significant dry out at the bottom.

LS

2/6/08

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

LS

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