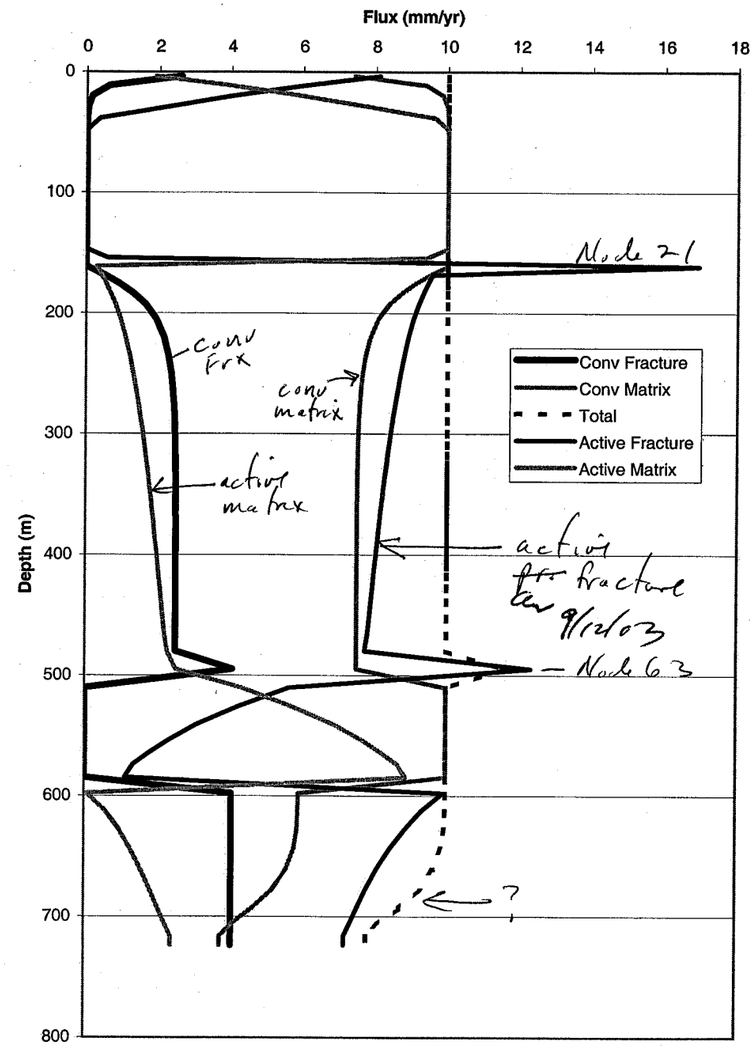
5/6/03 CW

periodic infiltration for the active fracture and conventional models.

As a test on the spreadsheet procedure for computing fluxes, ran steady-state simulations @ 10 mm/yr for both the active fracture and conventional models. The results extracted from the vertical flux output files simple_convVZ4.xyp and simple_activeVZ4.xyp are shown in the graph on page 37

In general the sum of the fracture and matrix fluxes total to 10 mm/y with two glitches at nodes 21 and 63. The first is transition from PTn to TSw Node 63 is transition from TSw to Ch.



9/12/03

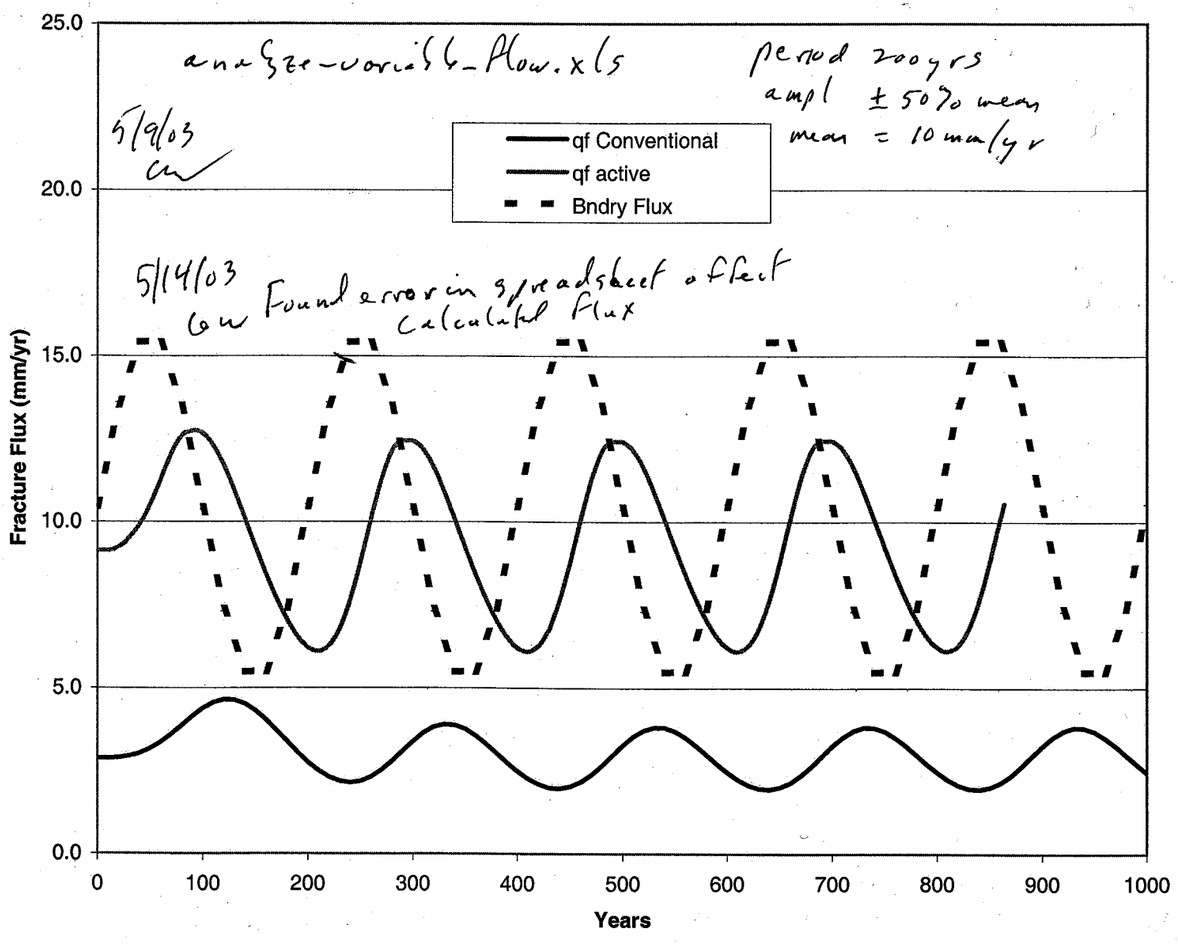
5/6/03 CW

simple_vert_sat

5/9/03 G. Walter

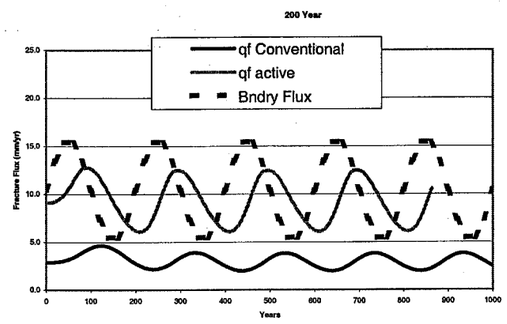
Resume work on UZ variable infiltration
The ~~various~~ various post-processing
~~stor~~ speadsheet procedures seem to
be working. The results for a period of
200 yrs and amplitude of ±50% ~~mm~~ of mean
are shown below.

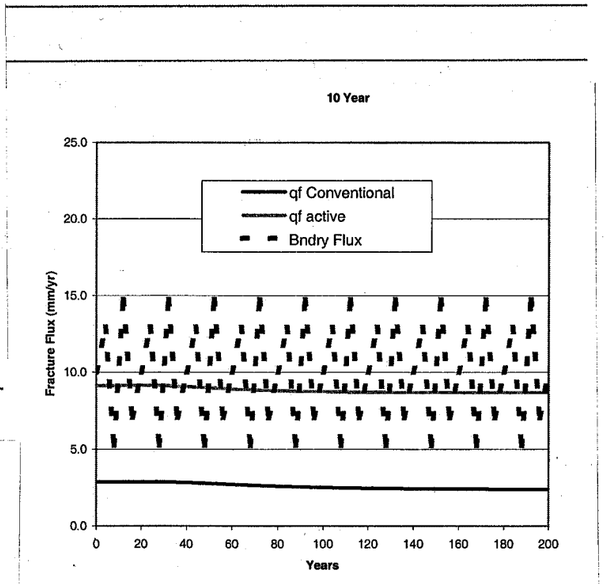
GW 9/12/03
GW 9/12/03
GW 10/27/03

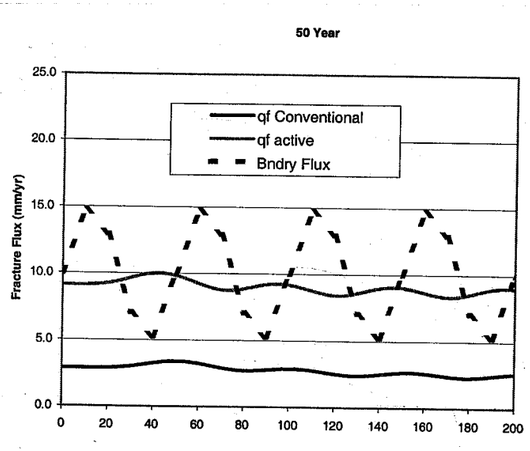


5/9/03 GW

Set-up simulations for oscillation periods of 1 year, 10 yr, 50 yr for both active fracture and conventional fracture models. The 1yr simulation displayed almost no variation in the fracture flux at node 30. A variation of a few 1 mm/yr is observed when the period is increased to 50 yrs. The results for 10, 50, and 200 year periods are shown below.







5/12/03 C. Walter

In reviewing the simple active fracture simulations I notice that the computed matrix saturations in the PTn were somewhat lower than those reported by Liu et al. in the calibrated parameters model (30-40% compared to 50%). To test the sensitivity of the model, created a new input file "simple-active-lookPTn.dat" in which I lowered the matrix permeability of the PTn from 9.9×10^{-13} to 9.9×10^{-14} m^2 ~~the~~ GW 5/14/03
That change only increased the PTn saturations ~~from~~ GW 5/14/03 by about 8% (30% to 38%) after 10^4 yrs simulations. Ran simulations with PTn at 9.9×10^{-15} m^2. That increased PTn saturations to about 41%

5/13/03 C. Walter

Further analysis of the simulation results above indicated to that reducing the permeability of the matrix simply results in an increase in fracture flow.

5/13/03 CW

Note on previous work:
Wu et al tr (2000) evaluated transient effect of 1 week pulses of infiltration occurring once every 50 years for a net average infiltration rate of 5 mm/yr ref. Wu, Y-S, W. Zhang, Leihua Pan, J. Hinds, and G. Bodvarsson. Capillary Barriers in Unsaturated Fractured ~~Roc~~ Rocks of Yucca Mountain, Nevada. LBNL-46876

To follow-up on PTn behavior, will ~~start~~ GW 5/23/03 runs transient simulation with 50 year period with PTn k_{matrix} reduced 1 order of magnitude. Input file is "simple_active_50yr_lowk.dat" and initial values in aclowk.ini generated from "simple_active_lowkPTn.dat"
Reduction in matrix k had no effect with effect on results and eventually further attenuated response.

5/14/03 G. Walter

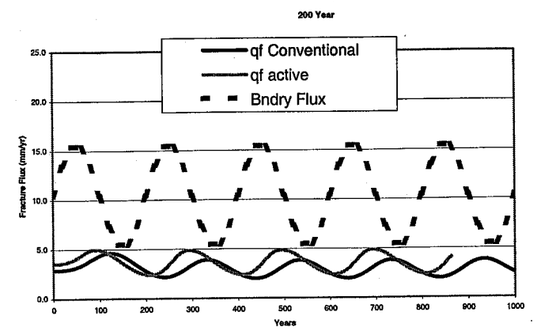
Found an error in spreadsheet called "analyze variable flow.xls" that affected calculations of vertical fracture fluxes. Corrected the spreadsheet and revised summary graphs are shown on page 43.
Created a new spreadsheet called "200yr vertical time variations" to process fracture fluxes at various nodes

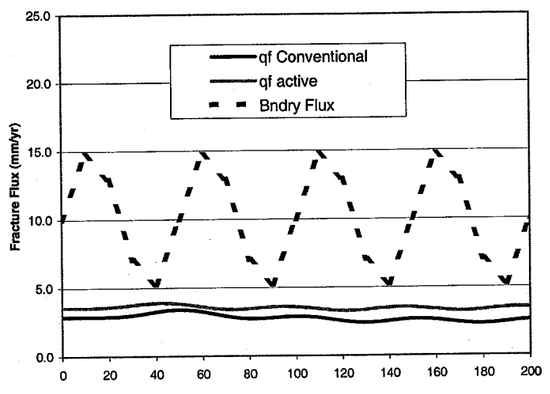
Still had an inconsistence between flux computed from saturations and fluxes reported by multiflo. Checked spreadsheet used to prepare property tables for active fracture model and found error in calculations of relative frax. permeabilities recalculated and rerunning models.
→ I am completely redoing all the input files.

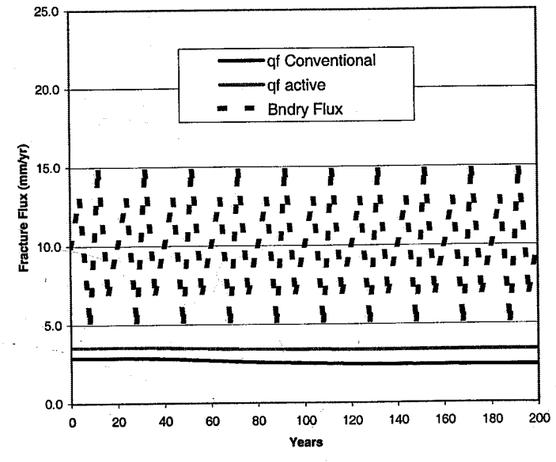
Reran simple-active.dat to generate new init file for transient simulations. Redo transient sims tomorrow

5/14/03 Gw

Revised Graphs





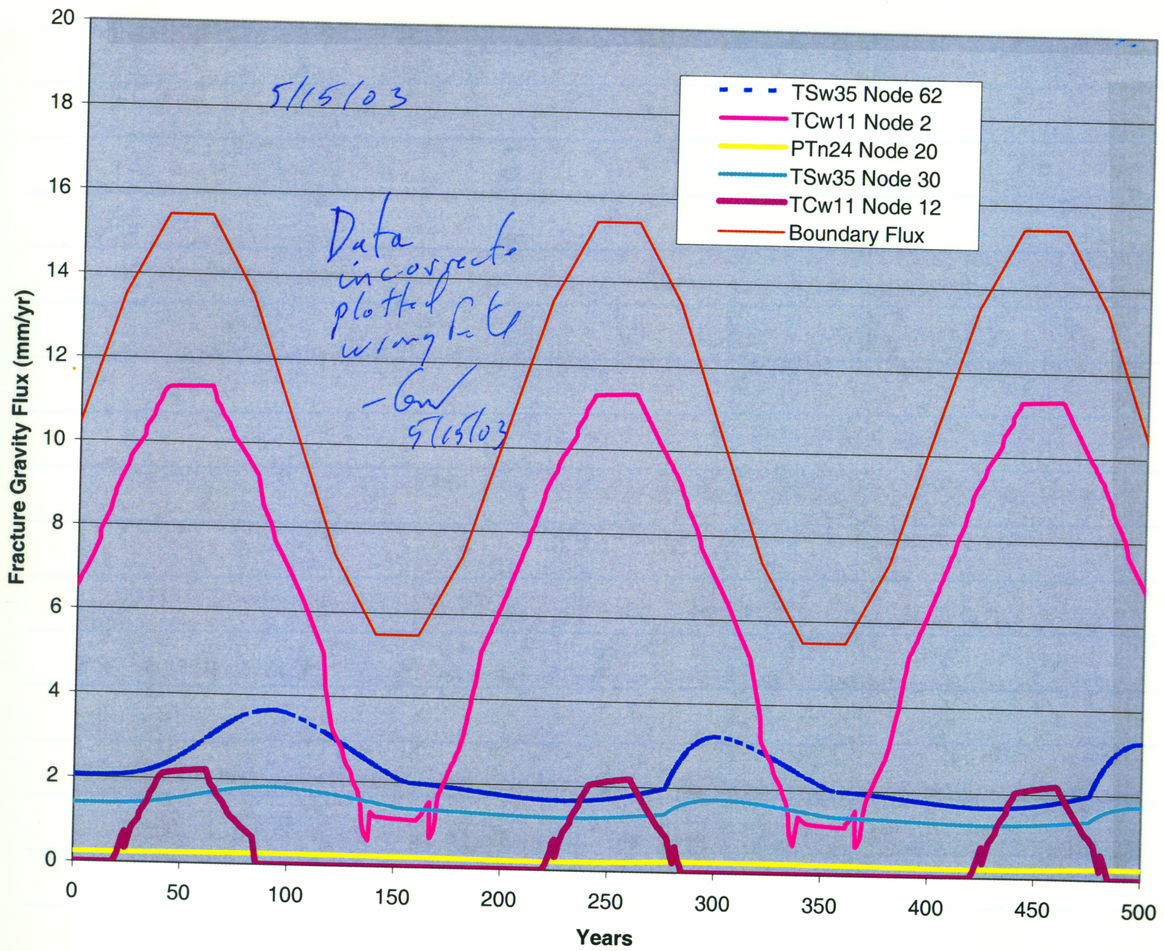


5/15/03 C. Walker

To facilitate processing, put the PCKR input from simple_active.dat into file "active.pck", copied old input files to *.sav and then modified all transient input files to read active.pck. Rerun 200 period simulation and results are shown on p 45 in terms of gravity component of fracture flux.
Something is still wrong with calculation of fluxes from saturation v. time file. They don't agree with fluxes produced by multiflo in *vz.xyp files. The cause of the problem is that mstra uses linear interpolation to compute rel. permeability from saturation + then to compute flux.
The spreadsheet was using the exact analytical relationship between rel. perm. + saturation.
At the low saturations in the fractures, the difference between the two methods ~~is~~ was significant.

To solve this inconsistency, I ~~wrote~~ wrote (5/15/03) a fortran program called "time-flux.f" to calculate the fracture flux from the time v. saturation output by linear interpolation. The resulting flux time history

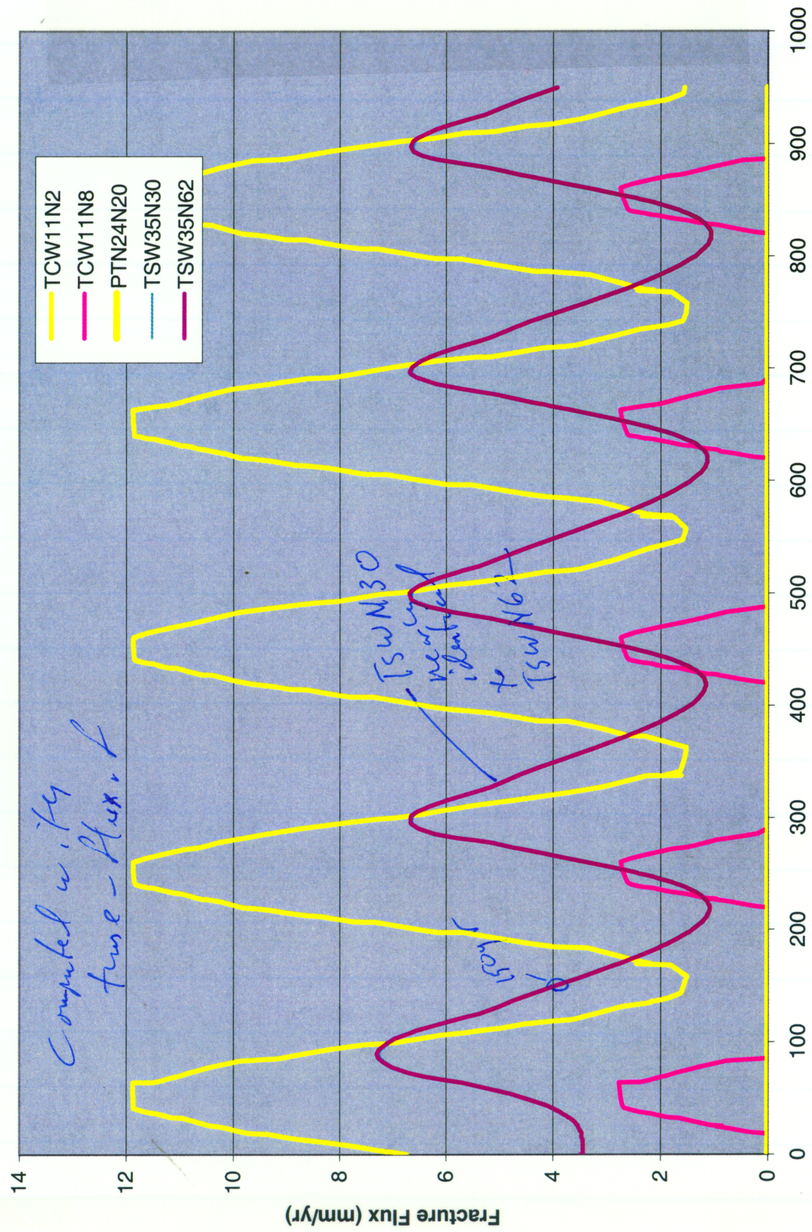
5/15/03 Gw



200 yr vertical time variation

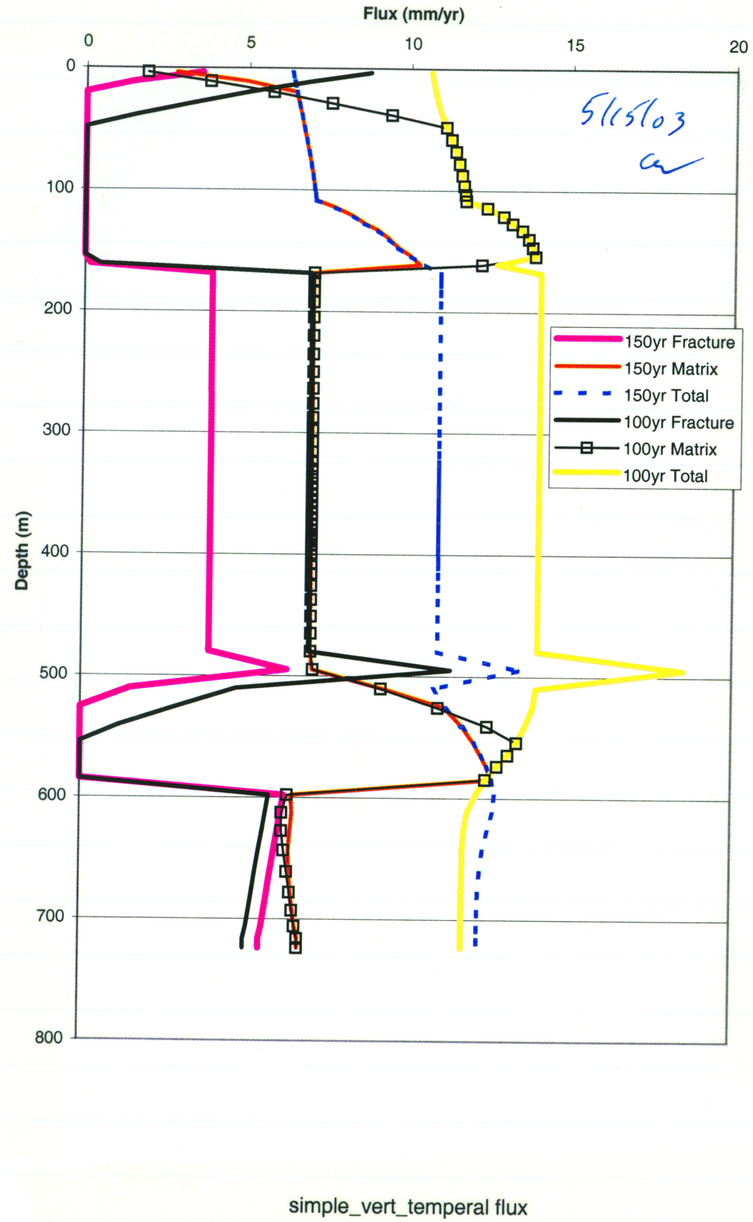
for a 200 year cycle is shown in the graph on page 46

5/15/03 CW



5/16/03 CW

To corresponding vertical total flux profiles for 100 and 150 yrs based on "simple_active_fracs_VBX.xyp are shown below

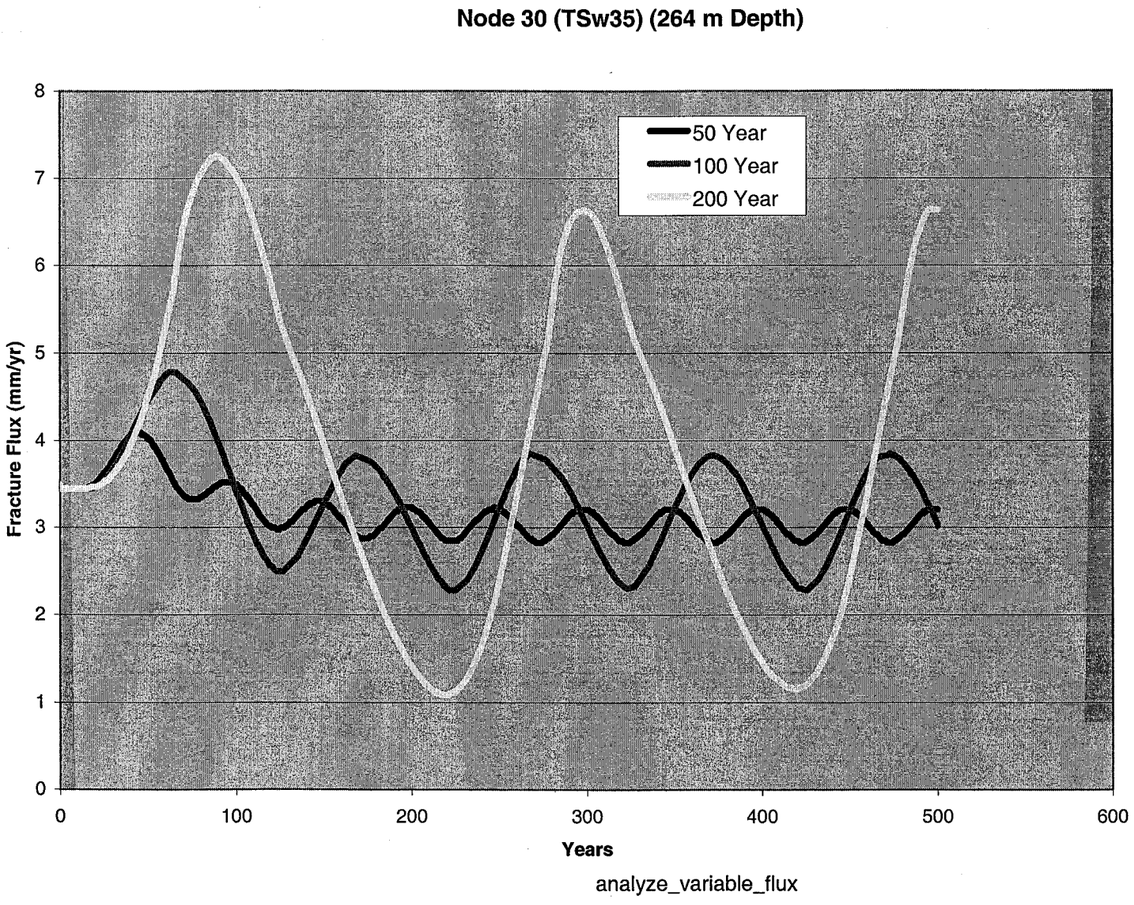


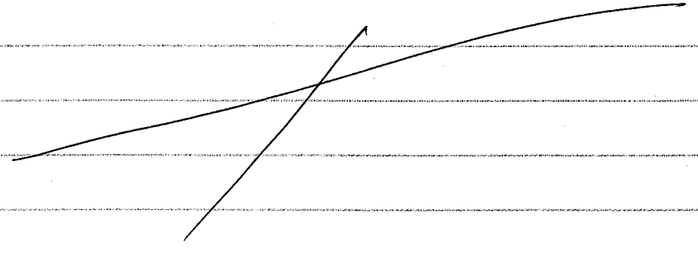
5/16/03 G. Walter

5/16/03 G. W - 16

5/16/03 C. Walker

The response at node 30 to various periods of infiltration variation is shown below.





6/2/03 C. Walker

In expectation of simulating a ~~long~~ 5/16/03 long period of hypothetical infiltrations, I asked Scott Painter to recompile a version of metra that would accept up to 1000 boundary conditions times. He created an executable in /home/spackle/spainter/bin/bigmetra2. I tested the new executable by running the input file VALdidat from .../spainter/multiflo/mflo1.5.2/AcceptanceTests/AcceptanceTest1. The results from bigmetra2 are in /home/spackle/gwalker/multiflomodels/acceptance_bigmetra2. The results using mflo1.5.2 are in a subdirectory called using_mflo1.5.2. A comparisons of the results is in D:/MULTIFLO/ldtransmdl/acceptance_test/comparison.xls. This spreadsheet compares the computed pressures which were practically identical except for small differences in the time steps taken by the two executables. Both ~~ex~~ on 10/24/03 simulations were run on texas, but were compiled with different compilers. Scott thinks that is the difference. I am going ahead and using bigmetra2.

5/21/2003 C. Walker

Created a hypothetical infiltration history from the raw tree ring precipitations record of Hughes and Graumlich (D:/MULTIFLO/1d transient/Drought a Paleo Respective/ precipitations from tree rings, x(s). The infiltration record was generated using the formula

$$I(t) = A*(\overbrace{P(t) - \bar{P}}^{\Delta P}) + \bar{I}$$

where $I(t)$ is the annual infiltration of year t

A is a scaling factor

$P(t)$ is the precipitation for year t

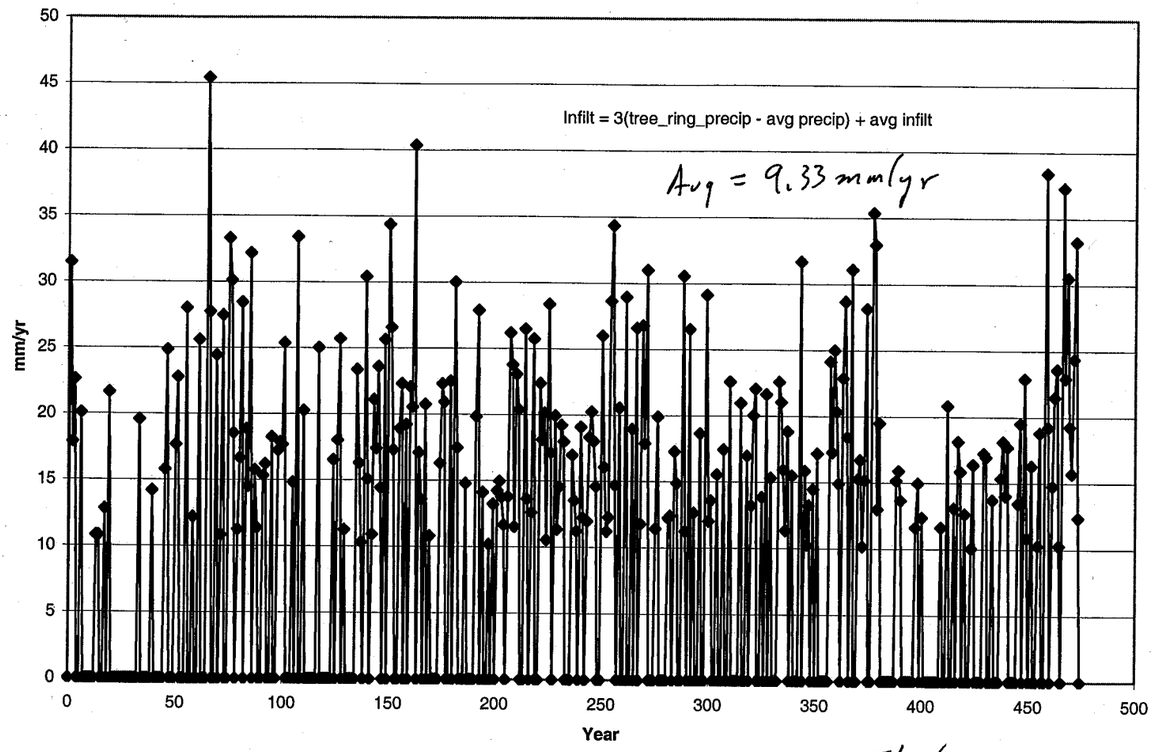
$\bar{P}$ is the averaged annual precipitation

$\bar{I}$ is the average infiltration

ΔP is the deviation from averaged

If $\Delta P < 0$, $I(t)$ was set to zero.

The resulting file (infiltration.txt) was then processed with a simple fortran program called "generate_scon_tree.f" (source in D:/MULTIFLO/1d transient/special programs) to create a boundary condition file for metra. The infiltration record generate is shown on page 53.

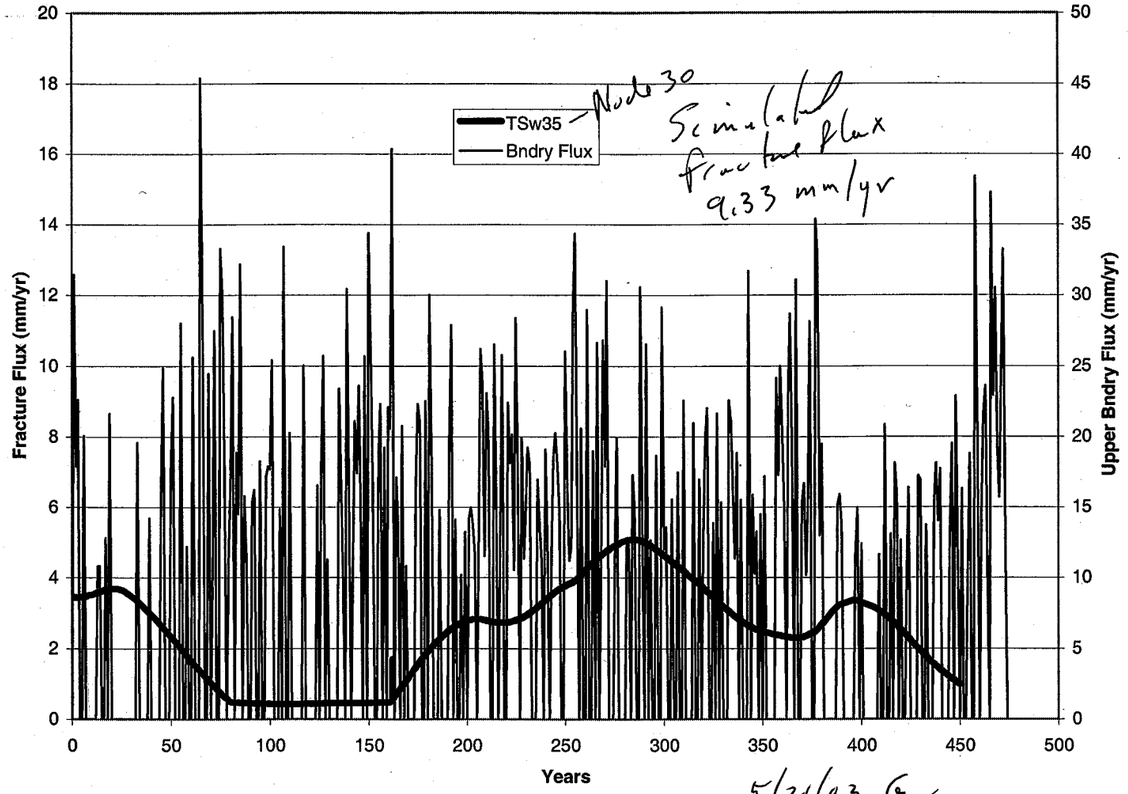


5/21/03 CW

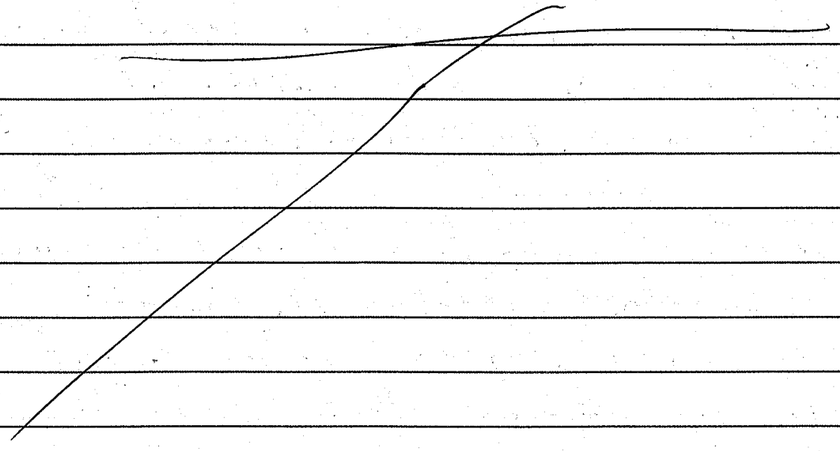
precipitation from tree ringscomputed infiltration

The infiltration history was then copied into the ~~fracture~~ file "simple_active_tree.def" in multi_flo_models/1d transient/simple on speck and simulated with bigmetra2 on texas. The fracture flux was computed from the simulated fracture saturations using the fortran program "time_flux.f". The resulting fracture flux is shown for Node 30 on page 54.

5/21/03

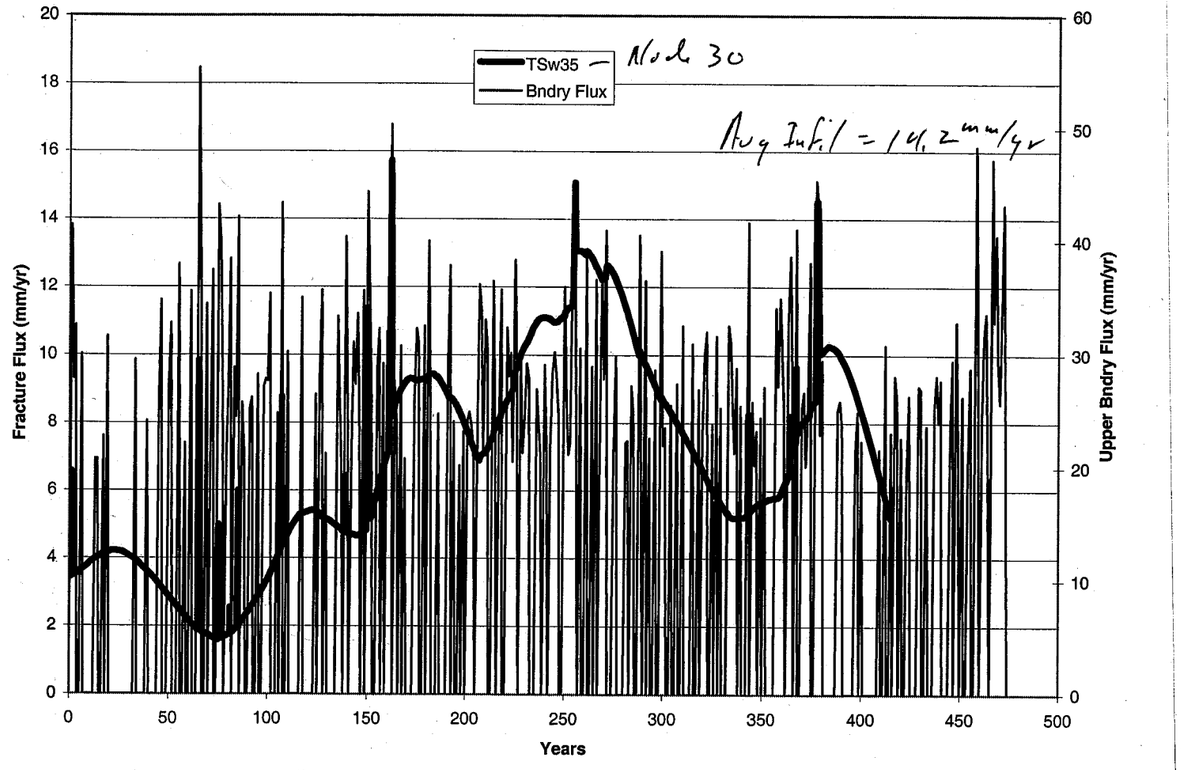


tree_flux Chart1



5/22/03

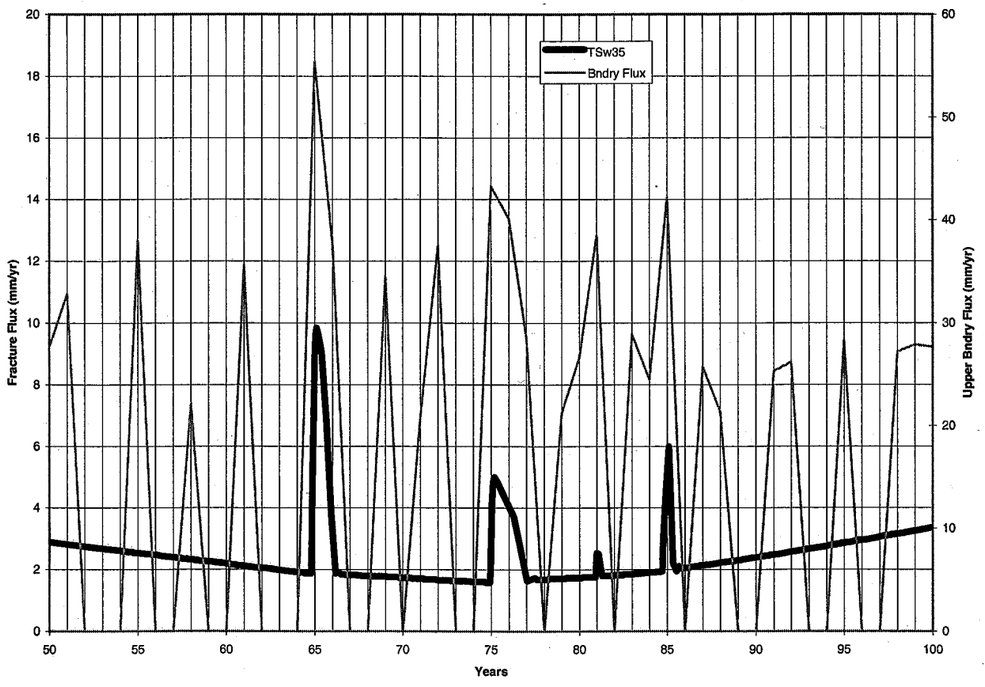
Ran another simulation with the average infiltration rate increased to 20 mm/yr. Using event filtering procedure described on page 52, the actual average infiltration rate imposed on the model was 14.2 mm/yr. The results are shown below.



tree_flux 20mmchart

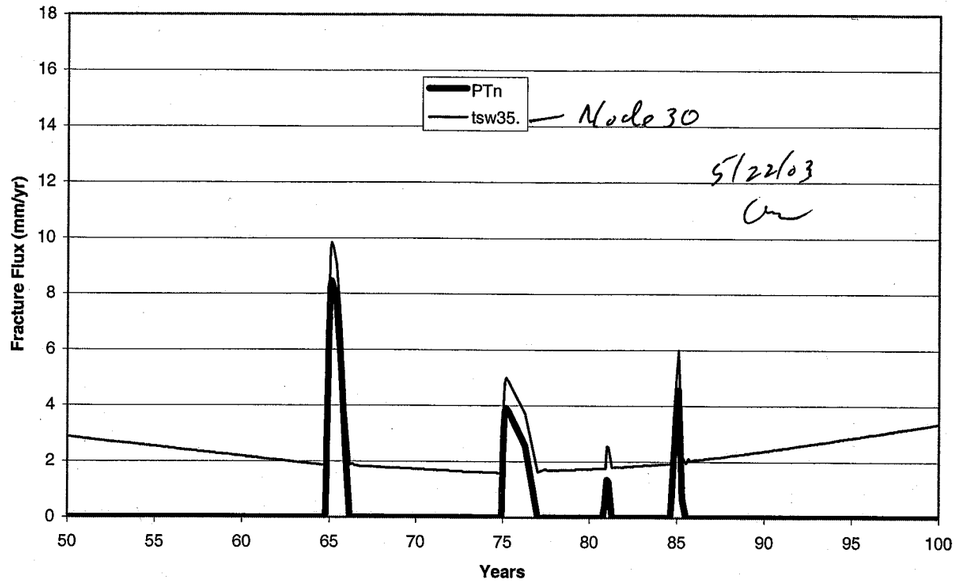
5/22/03

The results of the 20 mm/yr simulation shown on p. 55 display a number of sharp peaks in the fracture flux at node 30 (approximate repository horizon).



tree_flux 20mm_enlarge

The enlarge graph above indicates that these peaks coincide with peaks in the boundary flux. Need to see if this is a numerical effect or represents an actual hydraulic effect.



tree_flux PTn v TSw

~~Hear~~ 6/2/03

The figure above shows a comparison of the computed fracture flux in the PTn and that in the TSw. The peaks coincide indicating that the peaks may result from infiltration events that exceed the capacity of the PTn matrix to conduct them or to absorb the water flowing through the PTn fractures.

5/23/03 G. Walter

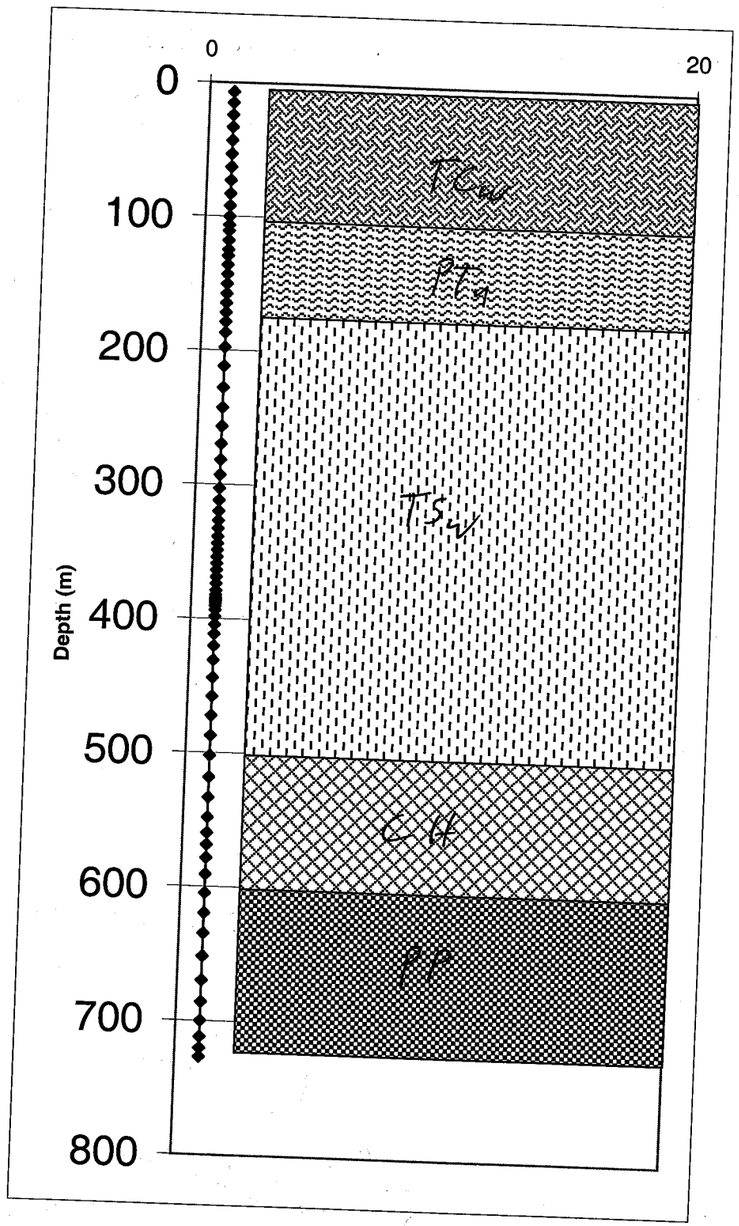
Summary of Metra input files in gwalter/multiflo_models/2d transient/simple

	Description
gwalter 7069 May 15 09:43 simple_active.dat	STEADY STATE ACTIVE FRACTURE 10 MM/YR
gwalter13448 May 16 09:36 simple_active_100yr.dat	100 YR PERIOD, 10MM/YR
gwalter13431 May 15 09:50 simple_active_10yr.dat	10 YR PERIOD, 10MM/YR
gwalter13433 May 15 09:50 simple_active_1yr.dat	1 YR PERIOD, 10MM/YR
gwalter13430 May 15 09:51 simple_active_50yr.dat	50 YR PERIOD, 10MM/YR
gwalter13448 May 15 11:06 simple_active_trans.dat	200 YR PERIOD, 10MM/YR
gwalter70264 May 21 15:57 simple_active_tree.dat	VARIABLE INFILTRATION BASED ON SCALED TREE-RING HISTORY, 9.3mm yr
gwalter70264 May 22 11:52 simple_active_tree20mm.dat	VARIABLE INFILTRATION BASED ON SCALED TREE-RING HISTORY 20mm/yr
gwalter14043 May 9 13:52 simple_conv.dat	STEADY STATE CONVENTIONAL FRX MODEL, 10MM/YR
gwalter20474 May 9 15:21 simple_conv_10yr.dat	10YR PERIOD,10MM/YR
gwalter20475 May 9 14:53 simple_conv_1yr.dat	1YR PERIOD, 10MM/YR
gwalter20473 May 9 15:49 simple_conv_50yr.dat	50YR PERIOD, 10MM/YR
gwalter20474 May 9 14:20 simple_conv_trans.dat	200 YR PERIOD, 10MM/YR

Lewis CGD 7/30/2007

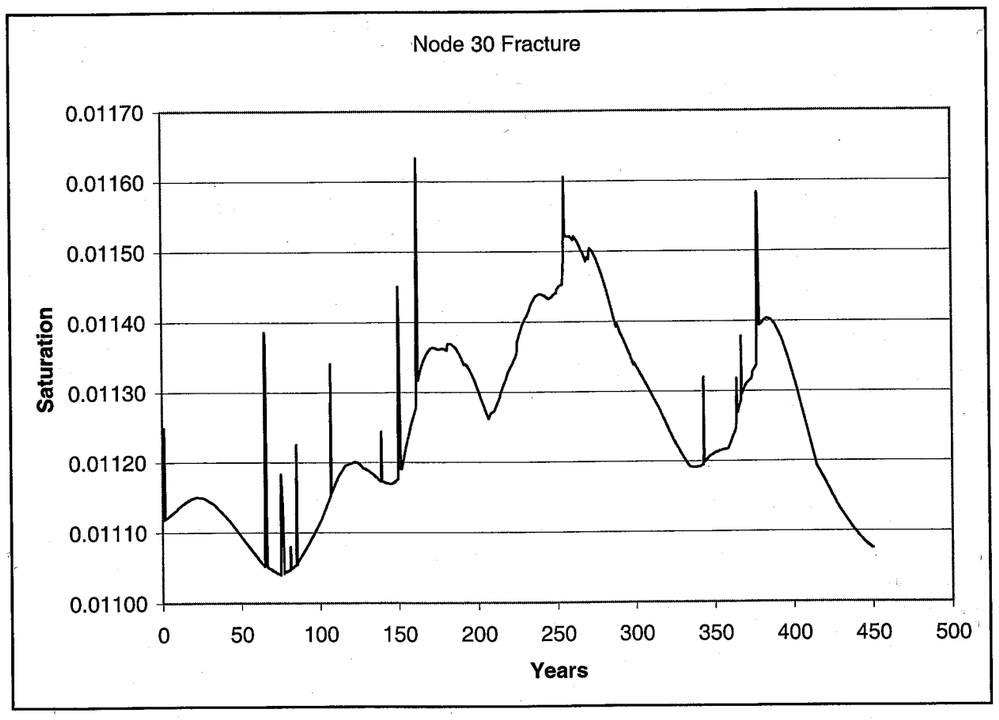
6/13/03 G. Walter

Vertical discretization in 1-D simple model



6/16/03

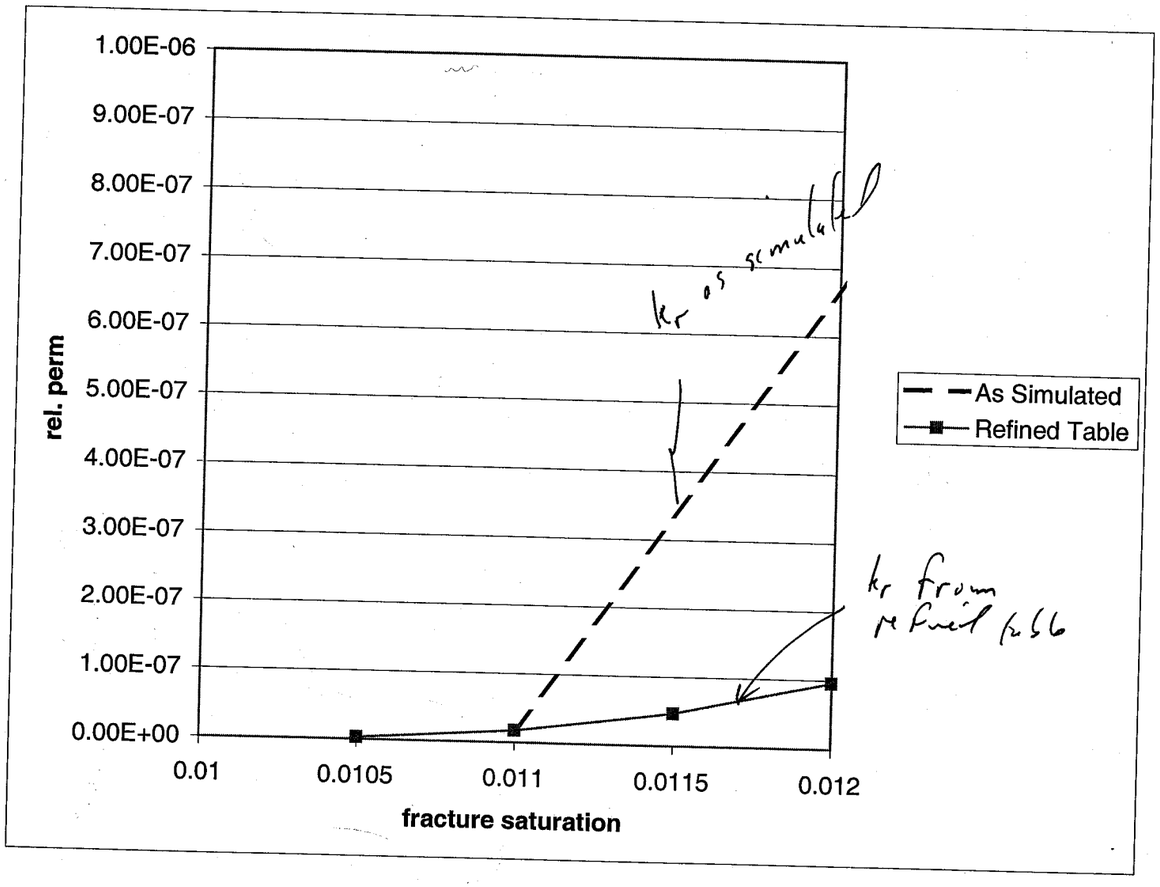
I am re-evaluating the transient modeling results with respect to the tabulation of permeability/saturation tables. Review of the simulated saturations indicated that the fracture saturations vary within a very small range. For example, the fracture saturation for node 30 in the TSw is shown below



simple_active_tree20mm_sat Chart 1 simple_active_tree20mm_sat Chart 1

6/16/03

The relative fracture permeability used in the preceding simulations was based on tables which were then used to estimate k vs saturation by linear interpolation. The figure below shows that at very low saturations, the table of



active fracture.xls Tsw35 Chart 1Tsw35 Chart 1

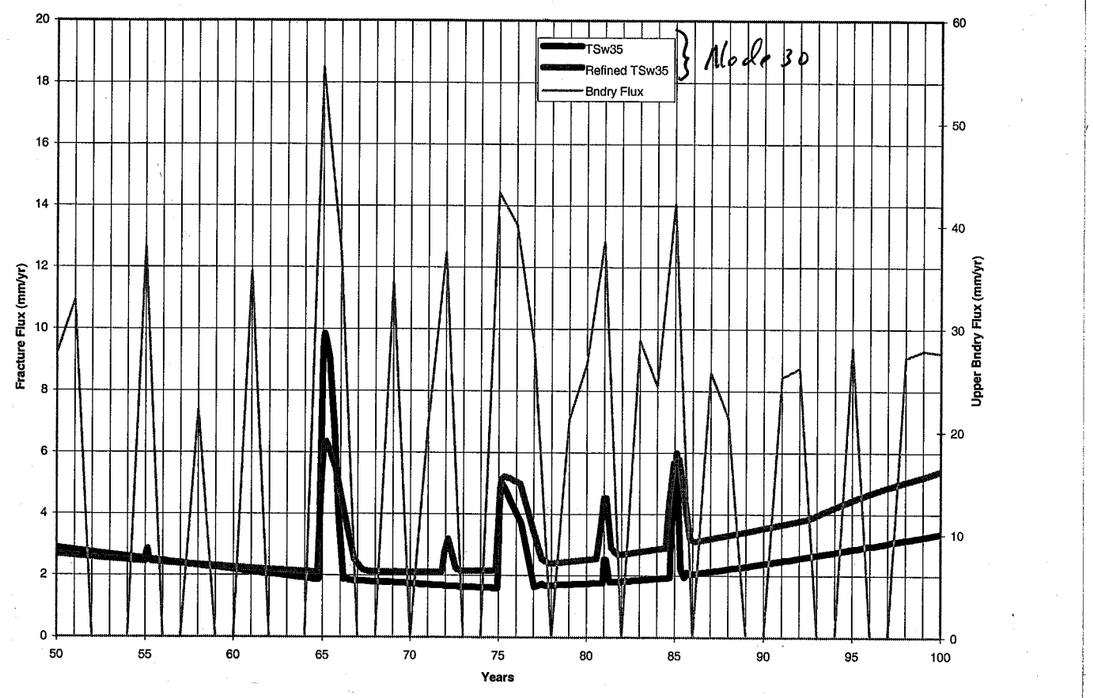
6/16/03

permeabilities was probably too coarse so that the permeability would have been over estimated with respect to that computed from the analytical expression given by the active fracture model. Inasmuch as no measurements of the actual fracture permeability at very low saturations have been made, this raises the philosophical questions as to validity of the actual fracture parameters at low saturation. Regardless, am going to rerun simulations using refined tables to see if there is a difference. Given the assumed linear relationship between q_z and k, there should be.

Created refined tables in "refined active fracture.xls" and "refined active fracture_matrix.xls" created new mstra input file called "refined_simple_active_tree20mm.dat"

6/17/03

Finished running "refined" simulations at nominal 20 mm/yr infiltration. A comparison of the results is shown below in terms of the simulated flux (fracture) at node 30 in the TSw



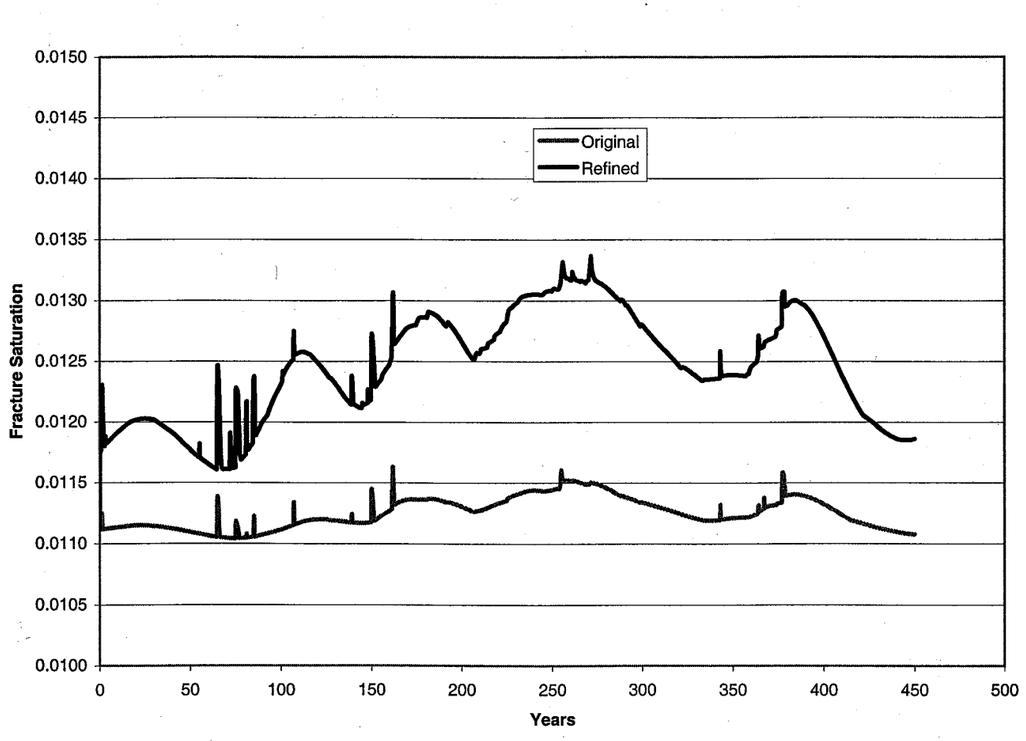
tree_flux 20mm_enlarge

The refined permeability tables reduce the magnitude of some of the higher peaks but don't eliminate the peaks. In fact,

6/17/03 CR

The refined simulations displays some new peaks and the magnitude of some of the smaller peaks is increased.

A comparison between the fracture saturation at node 30 between the original and refined permeability fields is shown below:



refined_active_tree20mm_sat Chart1

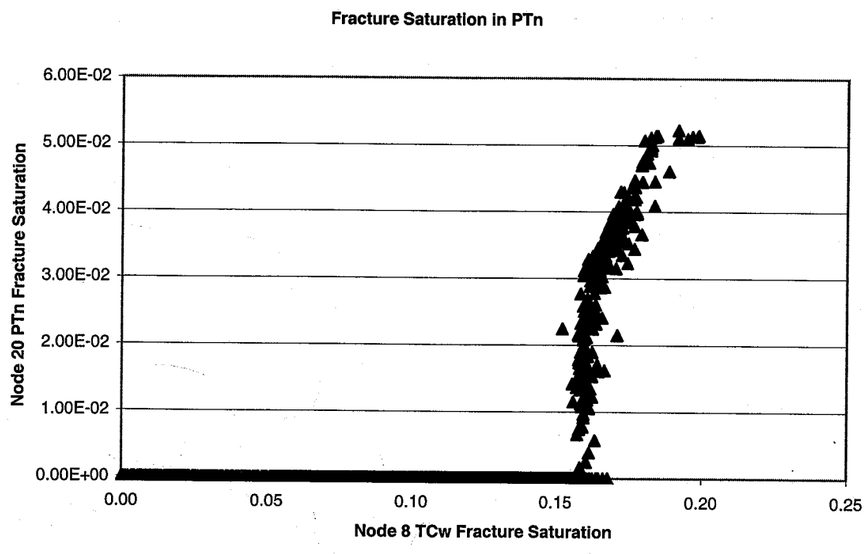
6/17/03 CR

The refined model results in higher saturation and sharper spikes than the original model because its effective permeability at a given saturation is lower.

To further summarize the simulation results, I have the following observations:

① The model indicate flow in TCw and node 8 fracture media most of the time

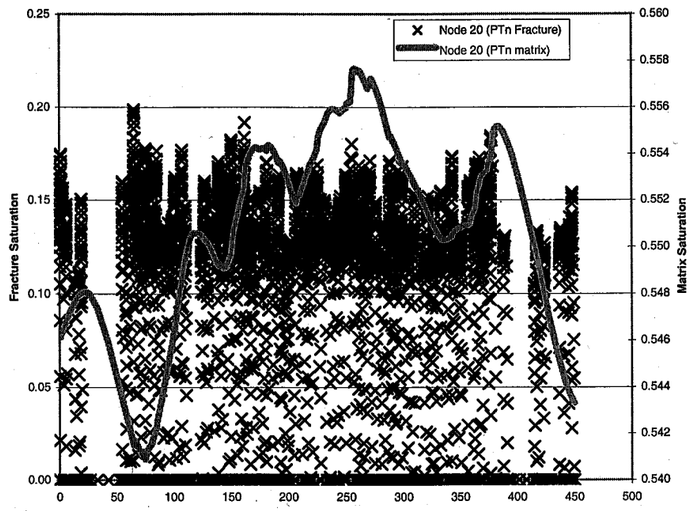
② Fracture flow in PTn at node 20 initiates at TCw fracture saturation of about 0.15 (see Sc(w))

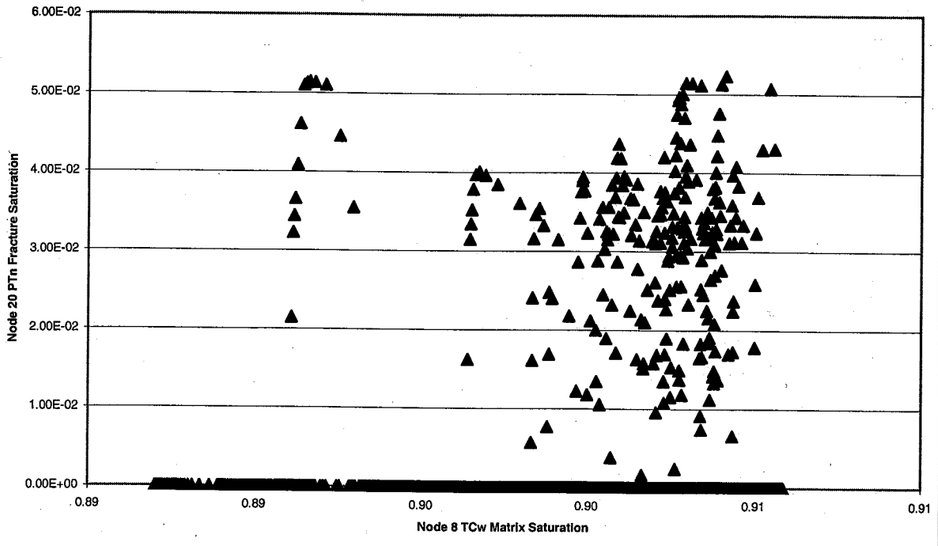


revised saturation analysis

6/17/03 Cnr

③ As illustrated by the two graphs below, there is no clear relationship between matrix saturation at Node 20 (PTn) and fracture saturation at Node 20



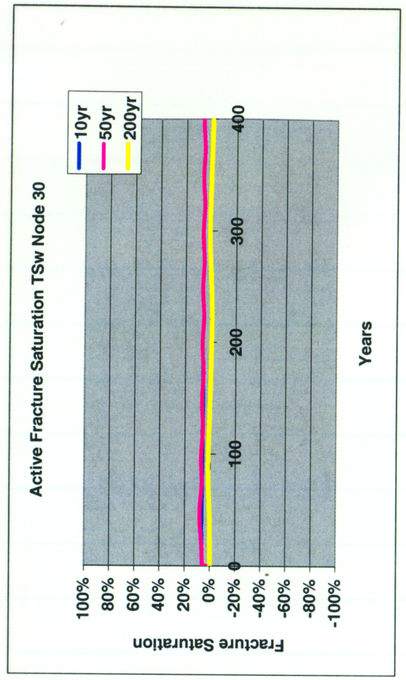


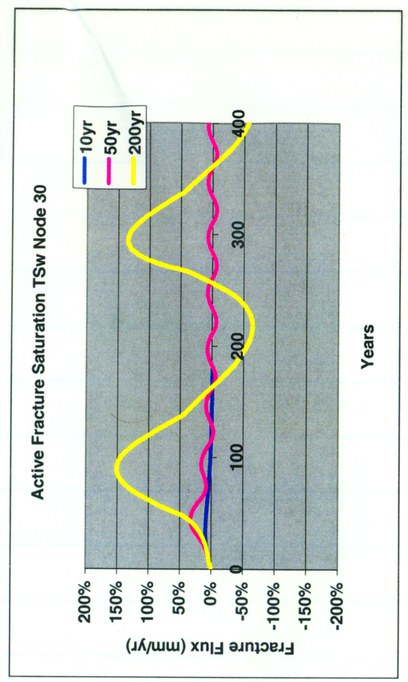
revised saturation analysis

6/18/03 Cnr

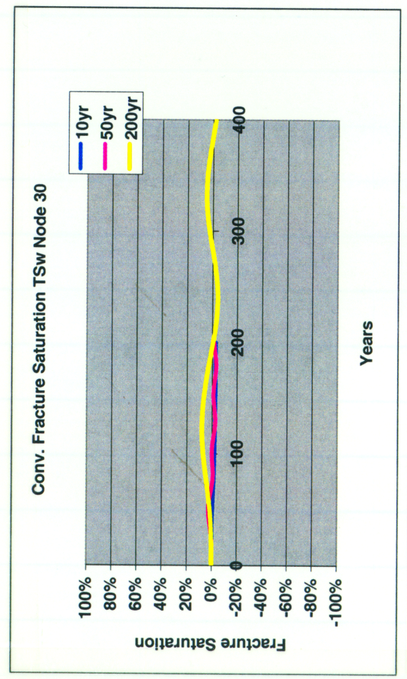
Redid the simulations with periodic boundary flux using the refined active fracture permeability tables. Results are in "temporal flux conv v active .xls" in D:multiflo\1dtransient\simple
The graphs on page 68 show results for Node 30.

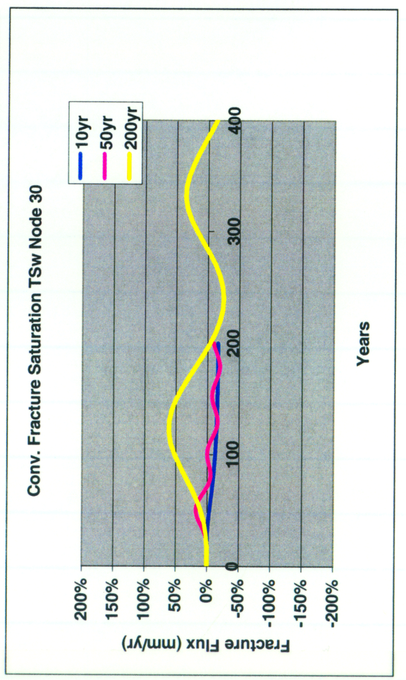
6/18/03 Cav





graphs





temporal flux conv v active

6/24/03

The previous simulations were performed with the active fracture permeability and fracture-matrix permeability computed using an Excel spreadsheet and then imported into an ascii .pcki file that was read by metra, i.e "activ.pcki". This provided to be an awkward and time consuming process that was prone to errors and omissions. In addition, Cav besides I had been computing the fracture → matrix permeability as a function based on the matrix relative permeability, see p. 32 but in reviewing Metra I see that the fracture → matrix flow is upstream weighted so should use fracture relative permeability as indicated below:

$$k_{rf\to m} = Se^{1+r} k_{rf}$$

To solve both of these Cav Glass problems I wrote a fortran program that generates the entire "pcki" table for Metra. A listing of this program is in D:\multiflo\1d transient\special_programs\generate_active_frac_table.f. I attempted to validate above program by computing TSw34 values and comparing them to values generated in Mathematic file Active-Fracture2.nb provided by Scott Painter. The comparision is shown for the fracture on p. 70 and for the fracture-matrix on p. 71

6/24/03 Cnr

Values for k_{rf}, P_c in fracture

```
: matrix TSw34-matrix
  1 Van-Gen      8.00000E-02    0.198300     4.01000E-06   0.150000 0.0  0
: fracture TSw34-matrix
    2 Table    0.010    0.608   0.100E-01   0.000E+00  0.0 0
 0.00000E+00  0.00000E+00  0.10000E+01  0.34776E+05
 0.10000E-01  0.00000E+00  0.10000E+01  0.34776E+05
 0.11000E-01  0.43873E-08  0.99999E+00  0.26709E+05
 0.12100E-01  0.31257E-07  0.99999E+00  0.20131E+05
 0.13310E-01  0.10423E-06  0.99999E+00  0.16922E+05
 0.14641E-01  0.25505E-06  0.99999E+00  0.14872E+05
 0.16105E-01  0.52722E-06  0.99999E+00  0.13390E+05
 0.17716E-01  0.98021E-06  0.99999E+00  0.12240E+05
 0.19487E-01  0.16950E-05  0.99999E+00  0.11306E+05
 0.21436E-01  0.27810E-05  0.99999E+00  0.10521E+05
 0.23579E-01  0.43856E-05  0.99999E+00  0.98460E+04
 0.25937E-01  0.67058E-05  0.99999E+00  0.92545E+04
 0.28531E-01  0.10005E-04  0.99999E+00  0.87287E+04
 0.31384E-01  0.14632E-04  0.99999E+00  0.82555E+04
 0.34523E-01  0.21050E-04  0.99998E+00  0.78256E+04
 0.37975E-01  0.29871E-04  0.99997E+00  0.74319E+04
 0.41772E-01  0.41901E-04  0.99996E+00  0.70687E+04
 0.45950E-01  0.58204E-04  0.99994E+00  0.67319E+04
 0.50545E-01  0.80175E-04  0.99992E+00  0.64177E+04
 0.55599E-01  0.10965E-03  0.99989E+00  0.61235E+04
 0.61159E-01  0.14902E-03  0.99985E+00  0.58469E+04
 0.67275E-01  0.20145E-03  0.99980E+00  0.55858E+04
 0.74003E-01  0.27106E-03  0.99973E+00  0.53387E+04
 0.81403E-01  0.36324E-03  0.99964E+00  0.51040E+04
 0.89543E-01  0.48508E-03  0.99951E+00  0.48807E+04
 0.98497E-01  0.64581E-03  0.99935E+00  0.46675E+04
 0.10835E+00  0.85757E-03  0.99914E+00  0.44637E+04
 0.11918E+00  0.11362E-02  0.99886E+00  0.42682E+04
 0.13110E+00  0.15026E-02  0.99850E+00  0.40805E+04
 0.14421E+00  0.19840E-02  0.99802E+00  0.38998E+04
 0.15863E+00  0.26163E-02  0.99738E+00  0.37254E+04
 0.17449E+00  0.34467E-02  0.99655E+00  0.35569E+04
 0.19194E+00  0.45374E-02  0.99546E+00  0.33935E+04
 0.21114E+00  0.59705E-02  0.99403E+00  0.32349E+04
 0.23225E+00  0.78549E-02  0.99215E+00  0.30805E+04
 0.25548E+00  0.10335E-01  0.98967E+00  0.29298E+04
 0.28102E+00  0.13603E-01  0.98640E+00  0.27822E+04
 0.30913E+00  0.17918E-01  0.98208E+00  0.26372E+04
 0.34004E+00  0.23627E-01  0.97637E+00  0.24943E+04
 0.37404E+00  0.31200E-01  0.96880E+00  0.23528E+04
 0.41145E+00  0.41281E-01  0.95872E+00  0.22119E+04
 0.45259E+00  0.54761E-01  0.94524E+00  0.20707E+04
 0.49785E+00  0.72884E-01  0.92712E+00  0.19282E+04
 0.54764E+00  0.97426E-01  0.90257E+00  0.17830E+04
 0.60240E+00  0.13098E+00  0.86902E+00  0.16329E+04
 0.66264E+00  0.17749E+00  0.82251E+00  0.14749E+04
 0.72891E+00  0.24320E+00  0.75680E+00  0.13042E+04
 0.80180E+00  0.33906E+00  0.66094E+00  0.11114E+04
 0.88198E+00  0.48761E+00  0.51239E+00  0.87386E+03
 0.97017E+00  0.76342E+00  0.23658E+00  0.49104E+03
 0.10000E+01  0.10000E+01  0.00000E+00  0.00000E+00
: fracture-matrixTSw34-matrix
    5 Table    0.010    0.608   0.516E-03   0.000E+00  0.0 0
```

$S_r = 0.01$
$m(1-m) = 0.608$
$\alpha = 5.16 \times 10^{-4}$
$\gamma = 0.41$

From Active Fracture 2.wb

S	k_{rf}	P_c
0.05	7.73×10^{-4}	6.45×10^{3}
0.19	4.4×10^{-3}	3.41×10^{3}
0.49	6.95×10^{-2}	1.95×10^{3}

Cnr 6/24/03

Values for k_{rf-m}

```
 0.00000E+00  0.00000E+00  0.10000E+01  0.25872E+06
 0.10000E-01  0.00000E+00  0.10000E+01  0.25872E+06
 0.11000E-01  0.97109E-16  0.99999E+00  0.16548E+06
 0.12100E-01  0.46535E-14  0.99999E+00  0.10256E+06
 0.13310E-01  0.49522E-13  0.99999E+00  0.76486E+05
 0.14641E-01  0.28731E-12  0.99999E+00  0.61508E+05
 0.16105E-01  0.11946E-11  0.99999E+00  0.51540E+05
 0.17716E-01  0.40358E-11  0.99999E+00  0.44317E+05
 0.19487E-01  0.11824E-10  0.99999E+00  0.38785E+05
 0.21436E-01  0.31236E-10  0.99999E+00  0.34382E+05
 0.23579E-01  0.76323E-10  0.99999E+00  0.30774E+05
 0.25937E-01  0.17549E-09  0.99999E+00  0.27753E+05
 0.28531E-01  0.38437E-09  0.99999E+00  0.25179E+05
 0.31384E-01  0.80941E-09  0.99999E+00  0.22955E+05
 0.34523E-01  0.16501E-08  0.99999E+00  0.21011E+05
 0.37975E-01  0.32735E-08  0.99999E+00  0.19296E+05
 0.41772E-01  0.63466E-08  0.99999E+00  0.17771E+05
 0.45950E-01  0.12067E-07  0.99999E+00  0.16406E+05
 0.50545E-01  0.22562E-07  0.99999E+00  0.15176E+05
 0.55599E-01  0.41577E-07  0.99999E+00  0.14063E+05
 0.61159E-01  0.75664E-07  0.99999E+00  0.13051E+05
 0.67275E-01  0.13619E-06  0.99999E+00  0.12127E+05
 0.74003E-01  0.24280E-06  0.99999E+00  0.11281E+05
 0.81403E-01  0.42923E-06  0.99999E+00  0.10503E+05
 0.89543E-01  0.75321E-06  0.99999E+00  0.97869E+04
 0.98497E-01  0.13132E-05  0.99999E+00  0.91254E+04
 0.10835E+00  0.22764E-05  0.99999E+00  0.85130E+04
 0.11918E+00  0.39261E-05  0.99999E+00  0.79448E+04
 0.13110E+00  0.67417E-05  0.99999E+00  0.74166E+04
 0.14421E+00  0.11532E-04  0.99999E+00  0.69247E+04
 0.15863E+00  0.19659E-04  0.99998E+00  0.64656E+04
 0.17449E+00  0.33417E-04  0.99997E+00  0.60364E+04
 0.19194E+00  0.56663E-04  0.99994E+00  0.56344E+04
 0.21114E+00  0.95887E-04  0.99990E+00  0.52571E+04
 0.23225E+00  0.16200E-03  0.99984E+00  0.49023E+04
 0.25548E+00  0.27336E-03  0.99973E+00  0.45678E+04
 0.28102E+00  0.46089E-03  0.99954E+00  0.42518E+04
 0.30913E+00  0.77682E-03  0.99922E+00  0.39524E+04
 0.34004E+00  0.13095E-02  0.99869E+00  0.36678E+04
 0.37404E+00  0.22089E-02  0.99779E+00  0.33961E+04
 0.41145E+00  0.37310E-02  0.99627E+00  0.31358E+04
 0.45259E+00  0.63152E-02  0.99368E+00  0.28848E+04
 0.49785E+00  0.10723E-01  0.98928E+00  0.26411E+04
 0.54764E+00  0.18286E-01  0.98171E+00  0.24023E+04
 0.60240E+00  0.31381E-01  0.96862E+00  0.21653E+04
 0.66264E+00  0.54338E-01  0.94566E+00  0.19261E+04
 0.72891E+00  0.95355E-01  0.90465E+00  0.16781E+04
 0.80180E+00  0.17095E+00  0.82905E+00  0.14097E+04
 0.88198E+00  0.31891E+00  0.68109E+00  0.10933E+04
 0.97017E+00  0.66562E+00  0.33438E+00  0.60634E+03
 0.10000E+01  0.10000E+01  0.00000E+00  0.00000E+00
```

Active Fracture 2.wb

S	k_{rf-m}
0.11	3.99×10^{-5}
~~0.31~~ 0.30913	3.46×10^{-3}

6/24/03

The values for k_{rf-m} do not agree because they were computed from the saturation in Active Fracture 2.wb

6/24/03 GW

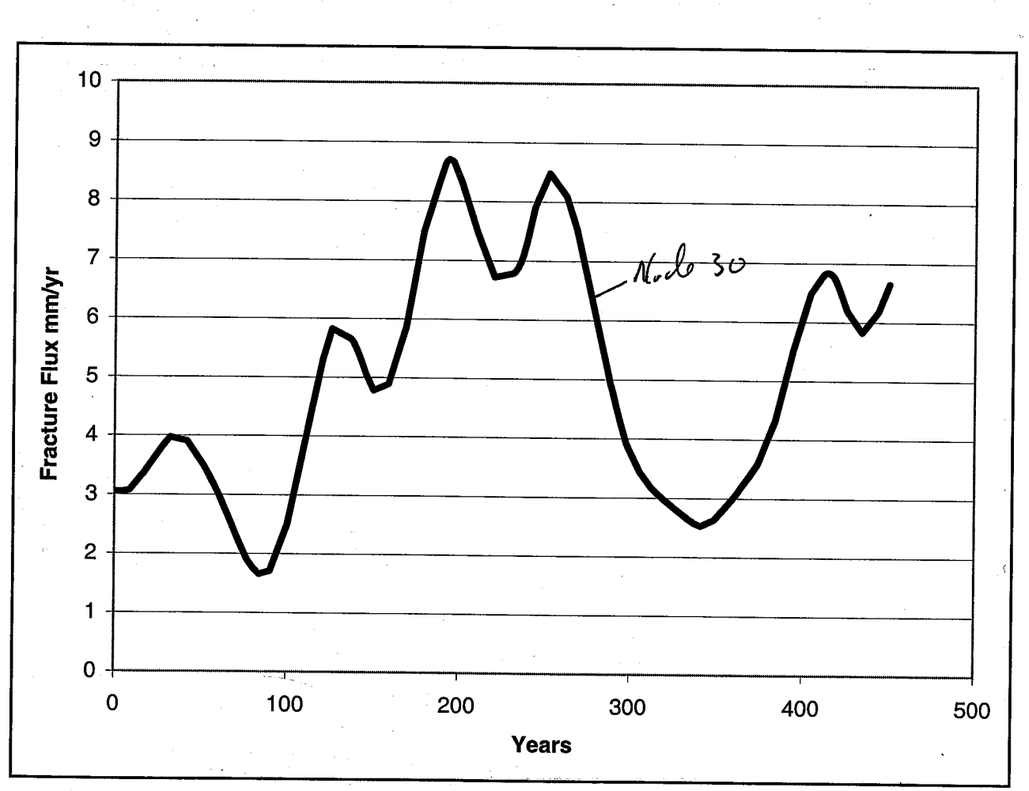
rather from Se, as described in Liu et al 1998 and ~~was~~ as was done in my program.
GW 6/24/03

I am satisfied that the program is working properly and will use it to resimulate some of the previous analyses. A listing of the program is provided in scientific notebook 580E starting on page 5.

GW 6/26/03

6/26/03 Gary Walter

I reran selected transient simulations using the updated fracture properties table in "refact.pck". For the simulation ~~pa~~ GW 6/26/03 based on the tree ring record with nominal infiltration rate of 20 mm/yr, (input file new_active_20mmy.dat), the simulated fracture flux at node 30 in TSw is shown below

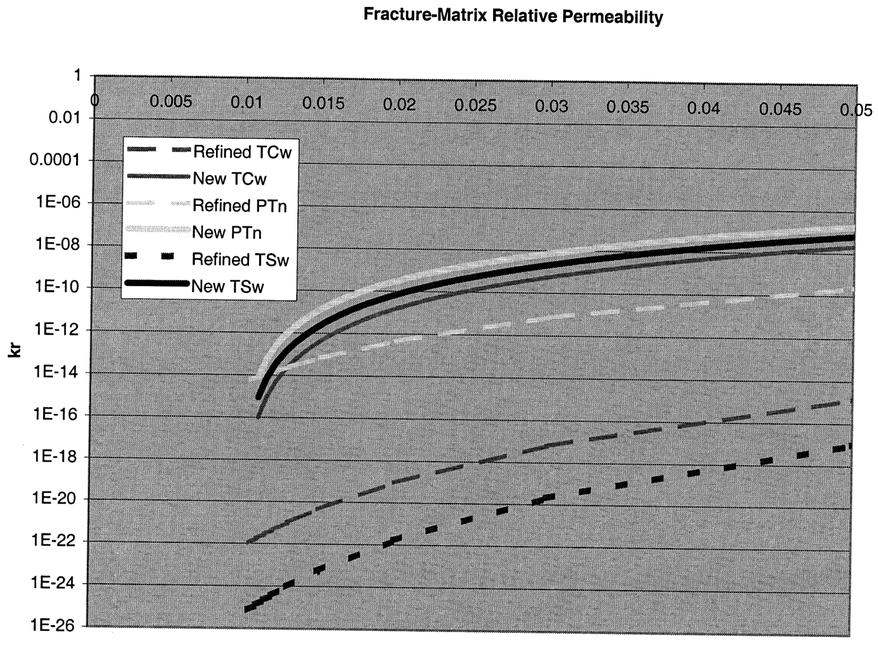


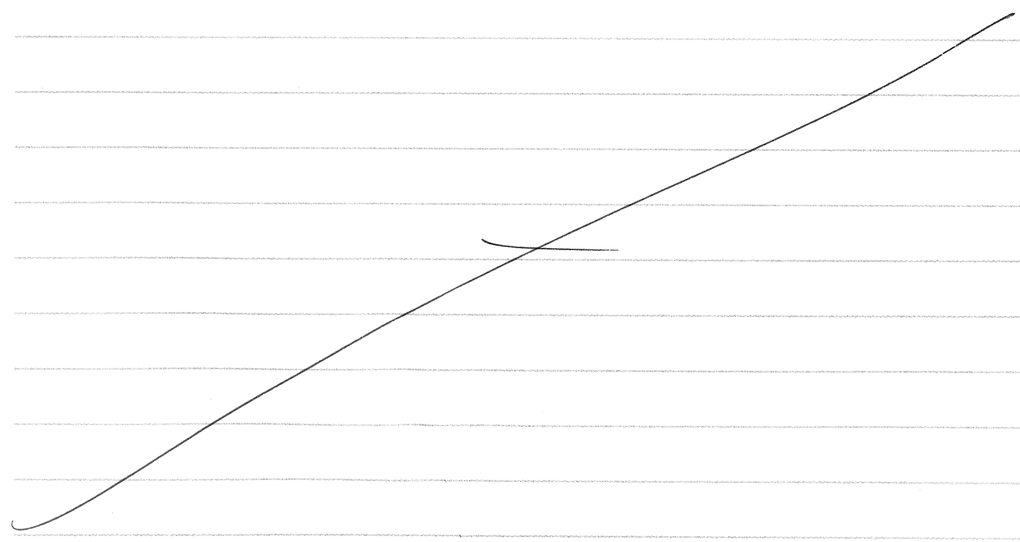
new_tree20mm Chart 1

6/26/03

Although this result illustrated on p 74 is broadly similar ~~the~~ 6/26/03 to that produced previously, such as illustrated on p 60 and p 64, there are two significant differences. First, the fractures in the TCw and PTn remained entirely dry throughout the simulations whereas in previous simulations they were wet. Second, the new simulated flux at node 30 does not display the sharp pulses as it did in previous simulations. Both of these effects are due to the fact that the revised matrix-fracture relative permeabilities are much higher than in previous simulations (see graph p 75) This allows the matrix to be much more effect in attenuating variations in the boundary flux. Nevertheless, variations in the flux with periods of 100 years or greater are still transmitted to the TSw fractures through the PTn matrix.

Note: fracture-matrix relative permeability was previously based on matrix permeability.



comparison fracture permeability

frac_matrix