CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

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Scientific Notebook of Gary R. Walter

Started April 1, 2003

Purpose:

This notebook will be used to record various observations that I make in reviewing DOE reports related to Yucca Mtn. Any specific calculations or experiments related to specific issues will be clearly noted.

5/2/03 GRW - Contents of this notebook was not used for any deliverables to NRC.

April 1, 2003

The UZ models were generally run 9/16/03 starting from an assumed steady-state moisture distribution. The 1-D calibrations were apparently performed using this same assumption (need to check). The UZ Flow Models + Submodels report clearly states, however, that the models required 10's of 1,000's of years to equilibrate. Is the assumption of steady state initial conditions any good and does it make any difference?

April 3, 2003 Gary Walter

Further review of basis for calibrating UZ model and assumptions regarding steady-state unsaturated flow.

Conceptual and Numerical ~~Model~~ Models for UZ Flow and Transport AMR references Wang and Narasimhan frequently wrt to calibration of UZ models. Review of ~~work~~ Wang and Narasimhan (1993) revealed their conclusions based on 1-D numerical models. On 9/12/03

① Unsaturated flow in Y-M dominated by matrix

② Matrix Ksat plays limit on infiltration rate. For TSw, Ksat is 1 mm/yr and at reported saturation of 0.8, max. infiltration rate is 0.1 mm/yr.

③ Variations in infiltration are averaged out in the PTn

④ p 353 Raymentions reviewer questions about assumptions of steady state moisture distribution wr on model calibration. They perform analysis by simulating moisture distribution in PTn and TSw in response to a fix volume of recharge occurring at periods up to 50 years. Their model showed nearly constant moisture content in PTn and TSw

April 3, 2003 Gw

for all periods

The calibration results in the Calibrated ~~Prop~~ Properties Model AMR (MDL-NBS-HS-000003) don't seem to be consistent with Wang + Narasimhans conclusions. The calibrated matrix permeabilities show little sensitivity to infiltration rate over the limits considered (0.8 mm/yr to 7.65 mm/yr) see Dilustro UZ Model Calibration/infiltration estimates.xls

April 8, 2003 G. Walter

Further evaluation of effects of transients on fracture/matrix flow and calibration of the Y-M model. The active fracture concept in TOUGH assumes hydraulic equilibrium between frx and matrix. The numerical experiments of ~~Wang~~ On 9/12/03 Wang + Narasimhan (1993) p. 345 would seem to support this wrt pressure. Need to look at sensitivity of saturation to pressure. According to Liu (1998) frx + matrix in equilibrium coupled thru fluid pressure I assume.

April 8, 2003 C. Walter

On rereading Lie about active frx, I now understand that frx and matrix are NOT assumed to be in equilibrium but what does this mean for steady state calculations?

April 10, 2003 C. Walter

To further investigate the steady state assumptions in calculation of the UZ models, consider a simple case of linear unsaturated water flow in a block of tuff bounded by two fractures illustrated below

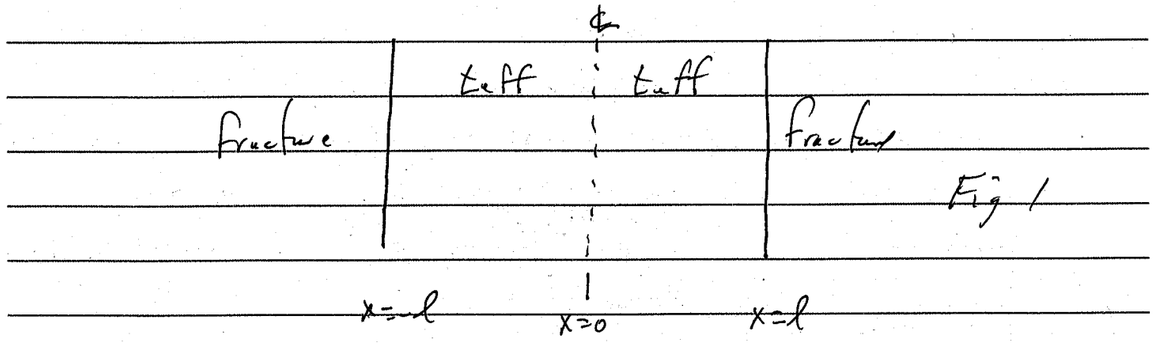


Fig 1

A first-order estimate of the time required for the moisture content in the tuff matrix to equilibrate can be made by assuming that the moisture content

April 10, 2003 CW

does not change significantly so that the matrix has a relatively constant hydraulic diffusivity. The hydraulic diffusivity is defined as (Hillel, D., 1982, Introduction to Soil Physics, Academic Press, San Diego.)

$$D(\theta) = \frac{K(\theta)}{(\partial\psi/\partial\theta)} = K(\theta)\cdot\partial\psi/\partial\theta \quad (1)$$

CW 5/23/03

where $D(\theta)$ is the diffusivity at wetness θ [L^2/t]
$K(\theta)$ is the hydraulic conductivity at θ [L/t]
ψ is matrix suction [L]
θ is the wetness [$-$]
The wetness (θ) is defined as ϕS
where ϕ is the porosity and S is the saturation.
The values of $D(\theta)$, $K(\theta)$ and $\partial\psi/\partial\theta$ can be computed using the Van Genuchten relationships

$$\psi(\theta) = \frac{1}{\alpha}\left[S^{1/m} - 1\right]^n \quad (2)$$

~~$K(\theta) = S^{1/2}\left[1-(1-S)\right]$~~ CW 5/23/03

$$K(\theta) = S^{1/2}\left[1-(1-S^{1/m})^m\right]^2 \quad (3)$$

(Van Genuchten, M. 1980, A closed-form equation for predicting the hydraulic conductivity of unsaturated soil. Soil Sci Soc. Am J. 44(5) 892-898)

Apr 10, 2003

Following these assumptions, the linear flow of water in the matrix can be described by the following PDE

$$\frac{\partial \theta}{\partial t} = D(\theta)\frac{\partial^2 \theta}{\partial x^2} \qquad (4)$$

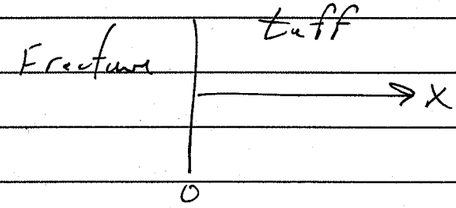
Referring back to Fig 1, assume that tuff is at an initial saturation of about 0.8 which is roughly in the range of saturations reported in Calibrated Properties Model (MDL-NBS-HS-000003 Rev 00) for the Topopah Spring welded units.

If the surface of the matrix is suddenly wetted, then the boundary and initial conditions are $t=0$

$$\theta(t) = 0.8\phi \quad \text{for } -l < x < l$$
$$\theta(-l) \text{ and } \theta(l) = 1.0\phi \quad \text{for } t > 0$$

Because the solution to (4) for these BC's is a bit tedious and I am only interested in an approximate estimate of the response time, consider the case of flow in a semi-infinite domain shown in Fig 2

April 10, 2003



In this case, we can set the initial and boundary conditions as

$$\theta_0 = \text{low saturation}$$
$$\theta(t=0) = \theta_0 \qquad x > 0$$
$$\theta(x=0) = \theta_1 \qquad t > 0$$

The solution to this problem in terms of the relative wetness defined as

$$\theta_R = \frac{\theta - \theta_0}{\theta_1 - \theta_0}$$

can be gotten from the equivalent heat flow problem in Carslaw and Jaeger (1959) Conduction of Heat in Solids

$$\theta_R = 1 - \text{erf}\left[\frac{x}{2\sqrt{Dt}}\right] \qquad (5)$$

April 10, 2003 CW

To perform the calculations, use the matrix properties for the Topopah Springs welded units given in Fedors et al (2002) Unsaturated Zone Flow at Yucca Mtn Nevada: Effects of Fracture ~~Het~~ Heterogeneity etc.

k intrinsic = 8.3×10^{-17} m^2
ϕ porosity = 0.09
α = 1.65×10^{-5} Pa^{-1}
m = 0.26
μ (water viscosity) = 10^{-3} Pa-s
g (gravity) = 9.8 ~~m~~ m/s^2 CW 9/11/03

The diffusivity is then

$$D(\theta) = \frac{k}{\mu} \partial\Psi/\partial\theta$$

These values were used in an Excel spreadsheet D:\USFEC\UZ Calibration\1-d_diffusivity.xls to compute values of $D(\theta)$. These calculations are on the sheet labeled "values". Eqn (5) was solved at a saturation of 0.8 for the relative wetness at various distances (x) from the fracture as a function of time.

April 10, 2003 CW

At a saturation of 0.8, the diffusivity is 6.2×10^{-8} m^2/s. CW 9/11/03 At a distance of 0.5m from the fracture, 80% relative saturation is reached after about 1yr. Thus, one would expect the saturation of the matrix to be in approximate local equilibrium with the water content of the fractures. One might also expect that the approach to equilibrium would actually be faster in a matrix ~~bou~~ block bounded by fractures as opposed to the 1-D ~~semi-infinite~~ CW 10/27/03 semi-infinite case used in the calculations. This seems to conflict with the statement in the UZ Flow Models AMR [MDL-NBS-HS-000006 R6000] p. 53 that "In general, it takes simulation times of thousands to millions of years for the system to equilibrate."

With respect to solute transport, CW 9/12/03 a similar analysis can be performed simply by replacing the hydraulic diffusivity in (5) with the effective molecular diffusion ~~coef~~ coefficient and interpreting the relative wetness as a relative concentration.

April 10 2003 GW

Assume a representative aqueous diffusion coefficient of $1 \times 10^{-5}\ cm^2/s = 1 \times 10^{-9}\ m^2/s = D_o$

The effective diffusion coefficient in the matrix is defined as

$$D_e = \tau D_o$$

The tortuosity, τ, can be estimated using Millington's ~~rep~~ relationship (in Hillel, 1982)

$$\tau = S^2 \cdot S\phi_T^{4/3}$$

where S is the saturation and ϕ_T is the total porosity. For $S = 0.8$ and $\phi_T = 0.09$, $\tau = 0.27$, so D_e is 2.7×10^{-10}.

~~The analysis part of the~~ GW 5/12/03
The "analysis" worksheet of the previously reference spreadsheet has a table showing the 80% response time as a function of D at a ~~pene~~ penetrating depth of 0.5 m. It indicates that for $D = 10^{-10}\ m^2/s$ the 80% response time is 600 yrs, so the diffusion response time would be a little less.

April 14, 2003 G. Walter

To continue the analysis of the steady-assumptions, am setting up a 1-D Multiflo simulation based on general UZ stratigraphy of YM. GW 5/12/03
For convenience, the model vertical ~~dist~~ discretization is taken from existing Multiflo validation file VAld.dat. Data files are stored in D:\Multiflo\1dtransient and on ~~Spot~~ GW 10/2/03 Solaris in home/gwalter/multiflo/1dtransient. The primary Multiflo ~~input~~ GW 10/31/03 input file is in 1dtransient.dat. Simulations will be run using executable in /spacetime/multiflo/mflo1.5.2 on Solaris.

Boundary Conditions

Upper Model Boundary is specified liquid mass flux (16 mm/yr to fracture) and ambient pressure and temperature. saturation, GW 5/12/03
Lower boundary is fixed ~~pressure~~ pressure and temperature. 100% liquid saturation.

Initial Conditions

Model will be run to achieve a steady state using initial values from VAld.int, then transient runs will be performed.

Apr 14/03 Gw

Material Properties

Material properties were assigned for a dual continuum medium based on the calibrated fracture and matrix properties from Table 13 in the Calibrated Properties Model [MDL-NBS-HS-000003 Rev 00]. The layers in VAId representing the repository were assigned the properties of tsw35. Although the correspondence between the layering in the Calibrated Properties Model and VAId. Model layers ~~38~~ ~~9~~ Gw 9/12/03 tsw38 and tsw39 were apparently not included in VAId or were lumped with other layers. This may be specific to the USW SD-12 borehole simulation. Will stay with descretization in VAId for now.

April 15, 2003 G. Walter

Continuing creating 1d transient input file. V-G parameters were assigned per Calibrated Properties Model report (CPM). Fracture porosity (fracture volume / bulk volume) (~~volf~~ sigmaf in DCM Parameters) was kept as in VAId. Gw 4/15/03

April 15/03 Gw

Gw 5/13/03 This is volf in input file

The calibrated fracture permeabilities from CPM were divided by sigmaf to get intrinsic fracture permeabilities. In general, the intrinsic permeabilities are a factor of 10 to 50 lower than those originally in VAId.

April 16, 2003 G. Walter

Finally debugged 1d transient input deck. Metra doesn't accept commas as field separator despite what manual says. Was able to run simulations out to about 750 years but Metra is having convergence problems. Reducing Δt_{max} to 1 yr helped but did not eliminate the problem.

Metra seems to be sensitive to output times. Am running some experiments to try to figure out behavior.

April 16, 03 — Chw

Output times	max Δt = 1 yr
1, 250, 500, 750 yrs	run successfully completed
1, 250, 750 yrs	begins cutting Δt after 587 days and continues with very small Δt, maxing out on newton iterations
1, 500, 750 yrs	same as above
250, 500, 750 yrs	same as above
repeat 1, 250, ~~75~~ 500 GW 9/12/03, 750 yrs	run successfully completed
1, 250, 600, 750 yrs	convergence problems, cut Δt @ 587 days
250, 500, 600, 750 yrs	same as above
1, 250, 500, 600, 750 yrs	run successfully completed
100, 250, 500, 600, 750 yrs	convergence problems
100, 250, 500, 750 yrs	"
10, 250, 500, 750 yrs	"
repeat 1, 250, 500, 750 yrs	successful
2, 250, 500, 750 yrs	convergence problems

April 17, 2003 — G. Walter

Tried to repeat yesterdays strange results with Multiflo and could not. Model has convergence problems after 587 days.

Since I ~~get get~~ GW 5/23/03 can't get the model to work with the parameters from the calibrated model report, I put the PCKR values from VAld back in the input file called 1dtranVAld.dat. I am going to look at sensitivity of model to infiltration rate and response time

~~Simt~~ Simulation GW 5/23/03	Infiltration Rate mm/yr	Infiltration Rate kg/s-m²	Comment
Sim 1	16	5.06×10^{-7}	same as VAld
Sim 2	31.5	1.00×10^{-6}	Result the same as SIM1?

April 18, 2003 C. Walter

There doesn't seem to be any difference in vertical distribution of saturation after 1000 yrs between SEM1 and SEM2. No difference after 10^4 years either. Actually, there is a very small increase in saturation, less than 1%, in the upper 10 model layers for the higher infiltration rate. After checking the mass balance output from multiflo and doing my own check of the envelope. It may be that whoever constructed the original VAId input file to did not properly assign upper boundary flux to fracture. User's manual says fracture flux is mass per unit area of FRACTURE in DCM model, not per unit bulk area.

Ran a test by dividing the ~~#~~ boundary flux of 5.06×10^{-7} kg/m^2-s specified in VAId.dat by ~~#~~ 9/1403 fracture volume fraction for layer 1 of 2.33×10^{-4}. This fixed the mass balance problem but simulation had convergence problems after 750 yrs.

Changed specified flux to 5 mm/yr, but

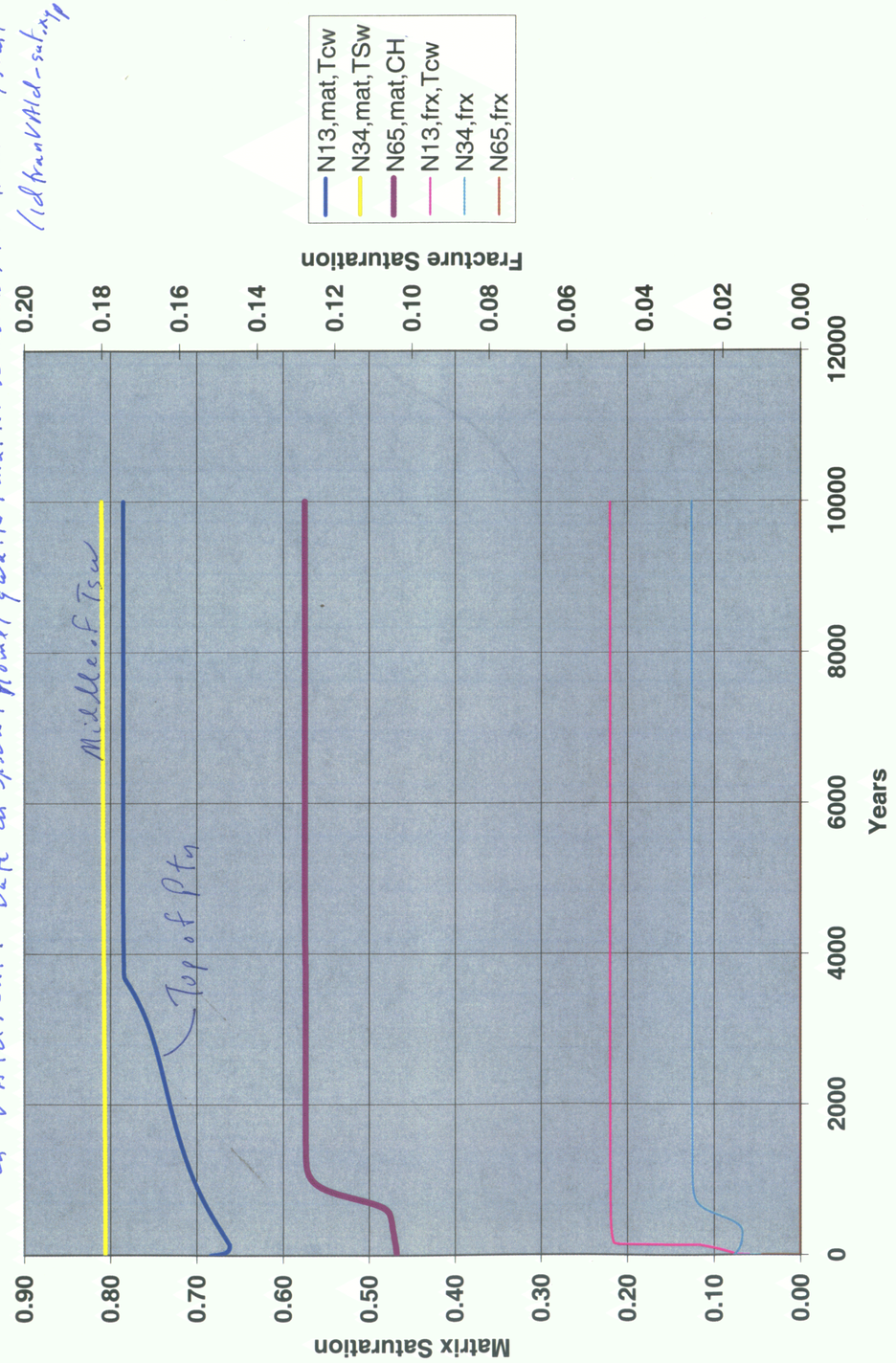
April 18, 2003 CW

had convergence after 1000 yrs.
Based on output, convergence problems occurring around layers 13 to 15, matrix characteristics 5, 7, 9 and fracture characteristics 6, 8, 10. In an effort to improve convergence I changed ~~Sw~~ 10/31/03 SWEXT for material 7 from -1×10^{-8} to 0.15.
That helped a little, so I went thru and changed SWEXT for all the materials with RPMM < 0.3 to positive numbers about equal to SWIRM + ~~0.05~~ 10/27/03 0.05. That didn't solve the problem.
Was able to get convergence at problem nodes by increasing RPMM. Am going to reset RPMM to original values at raising SWEXT. That didn't work. Was able to achieve convergence by changing RPMM for material 3 (Tcw12) from 0.2447 to 0.3447. Will experiment with intermediate values.

10/27/03 ~~RR~~ RPMM — Result

0.3 — non-convergence after 2000 yr
0.32 — " " "
0.34 — ran OK to 10000 yrs

Infiltration rate 5 mm/yr starting initial values in VAld.int. Data in Spoke/home/gwalter/multiflo-models/1d transient/sim1/1dtranVAld-sat.xyp



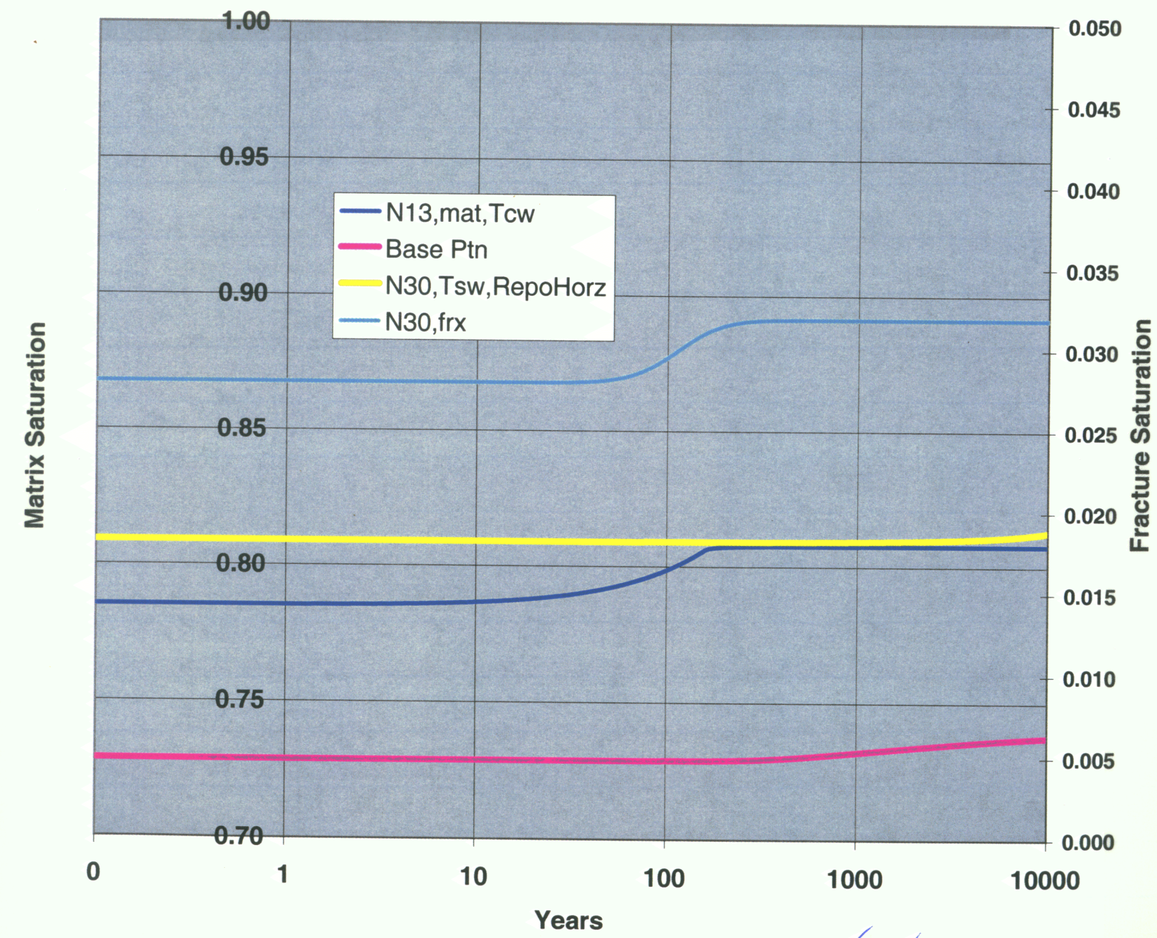
4/18/03 GW

sat_vs_time

d:\multiflo\1dtranient\sim1

April 21, 2003 G. Walter

Took the output from the simulation in directory sim1 and used it as input to multiflo ~~vr~~ for input file 1dtranVAld.dat in directory sim2, and doubled upper boundary flux. Computed saturation vs time is shown below



4/21/03 GW

d:\multiflo\1dtranient\sim2

sat_vs_time

4/21/03 CW

These results indicate that

1. Matrix saturations are not very sensitive to infiltration rates

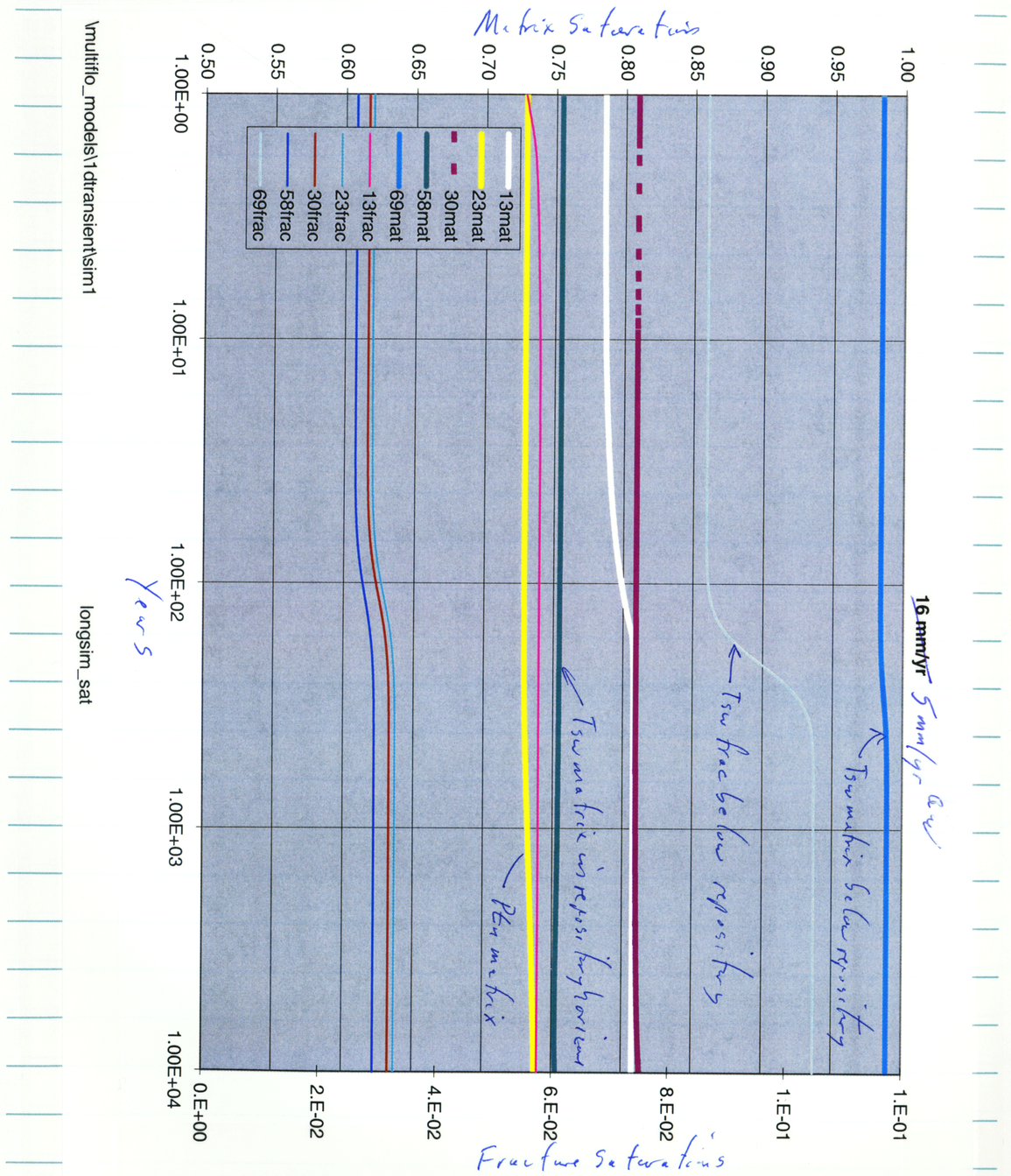
2. The Ptn matrix requilibrates to a change in infiltration rate within a few hundred ~~he~~ CW 10/31/03 years whereas the Tsw takes much long.

To further address the response of the Tsw, need to run much longer simulation.

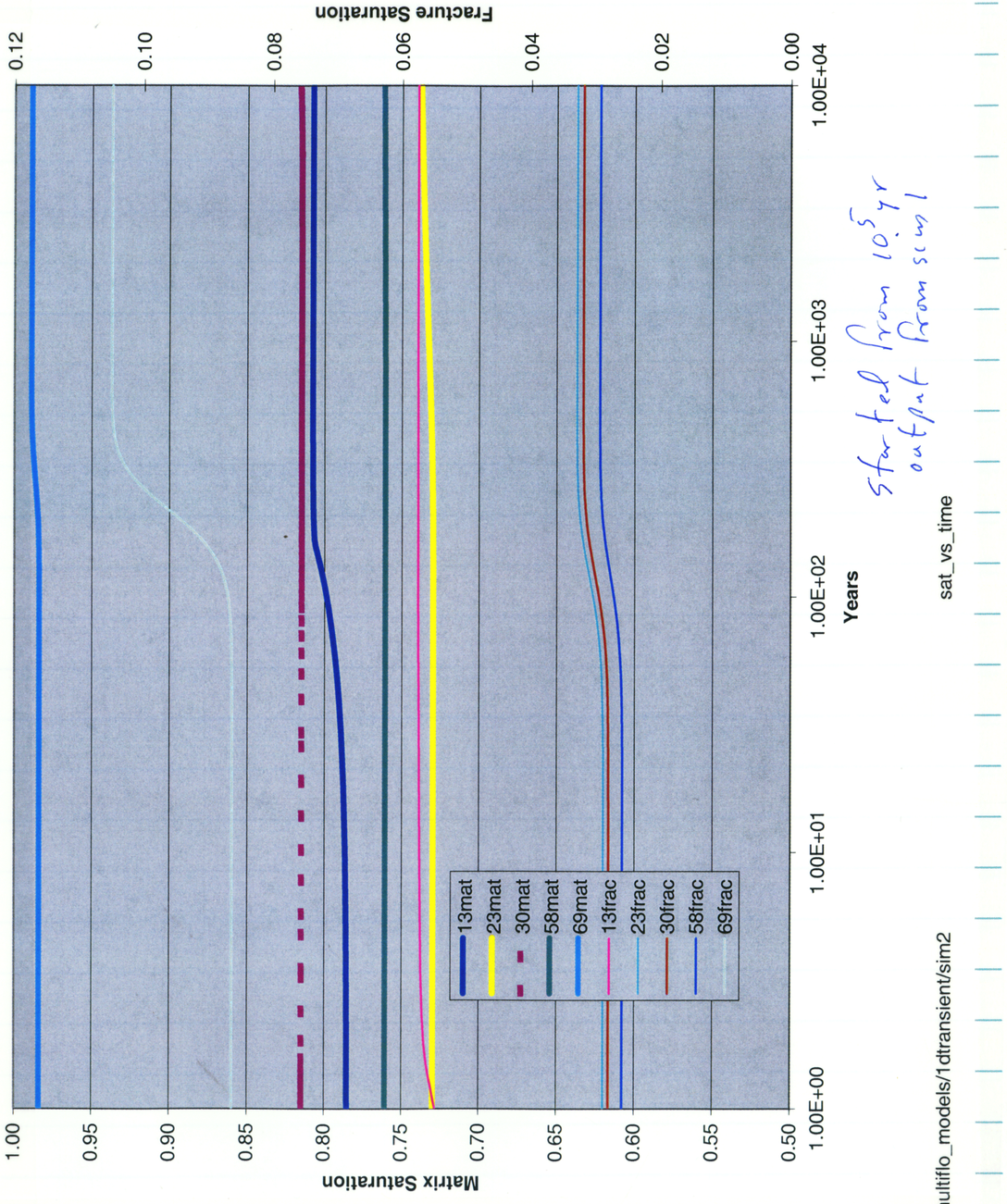
April 22, 2003 C. Walter

Reran base simulation in sim1 directory for 10^5 yrs (longsim1.dat). Graph on p21 shows saturation vs time. Fractures seem to equilibrate on a fast scale of a few hundred years. Matrix responds over 1000's of years and response is very subdued. Will rerun sim2 with 10^5 yr output from sim1. The result for the first 10^4 years is shown on the graph on page 22

4/22/03 CW



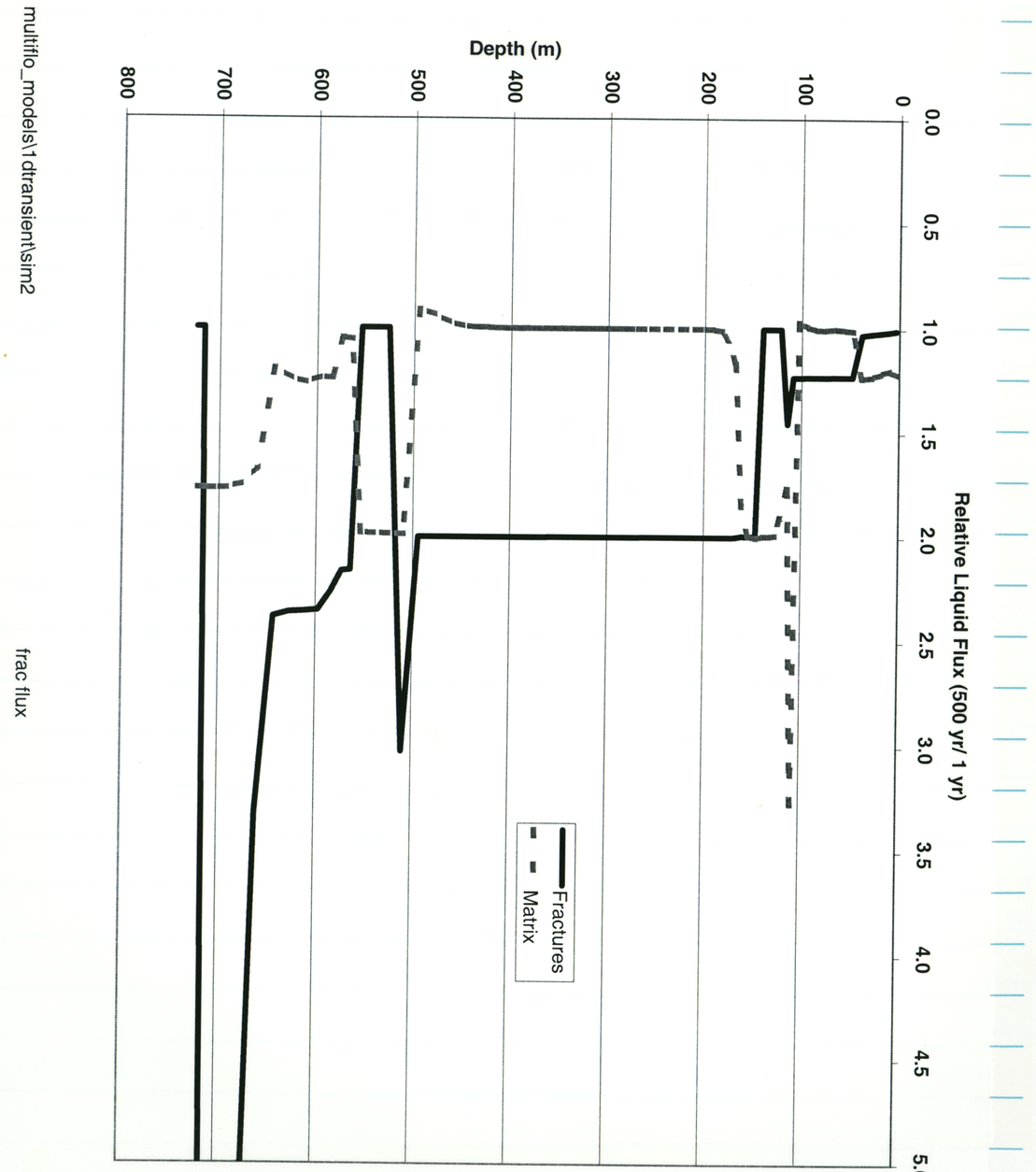
4/22/03 CR



Started from 10^5 yr output from sim 1

4/22/03 CR

The computed vertical distribution of fracture and matrix vertical flow is shown on the graph on page 23 at 500 yrs



4/22/03 GW

Conclusions:

1. GW 10/31/03 Matrix saturation is not sensitive to infiltration
2. Fracture and matrix fluxes equilibrate with infiltration fractures on a time scale of a few hundred years
3. These simulations seem to show less sensitivity of matrix saturation than those in the Calibrated Properties Model report which used the active fracture concept GW 9/12/03

New Work: Look at time varying upper boundary flux affect GW 10/31/03 on fracture fluxes.

Note: Spreadsheet calculations performed using MS Excel 2000
May 21, 2003 GW

Setup spreadsheet in variable_infilt called variable_flux to compute time variable of fracture flux from computed fracture saturation.

Assumption: Frac flow is primarily GW 10/31/03 driven by gravity

Thus

$$q_f = k \frac{k_{rel}}{\mu} \varrho g$$

4/22/03 GW

where q_f is fracture flux (within fracture)

k is intrinsic permeability
k_{rel} is relative permeability
μ is dynamic viscosity 1×10^{-3} Pa-s
ϱ is fluid density 998 kg/m^3
g is gravity 9.8 m/s^2

Compute k_{rel} from Van-Genuchten relationships.

April 24, 2003 G. Wolfe

The plan now is to:

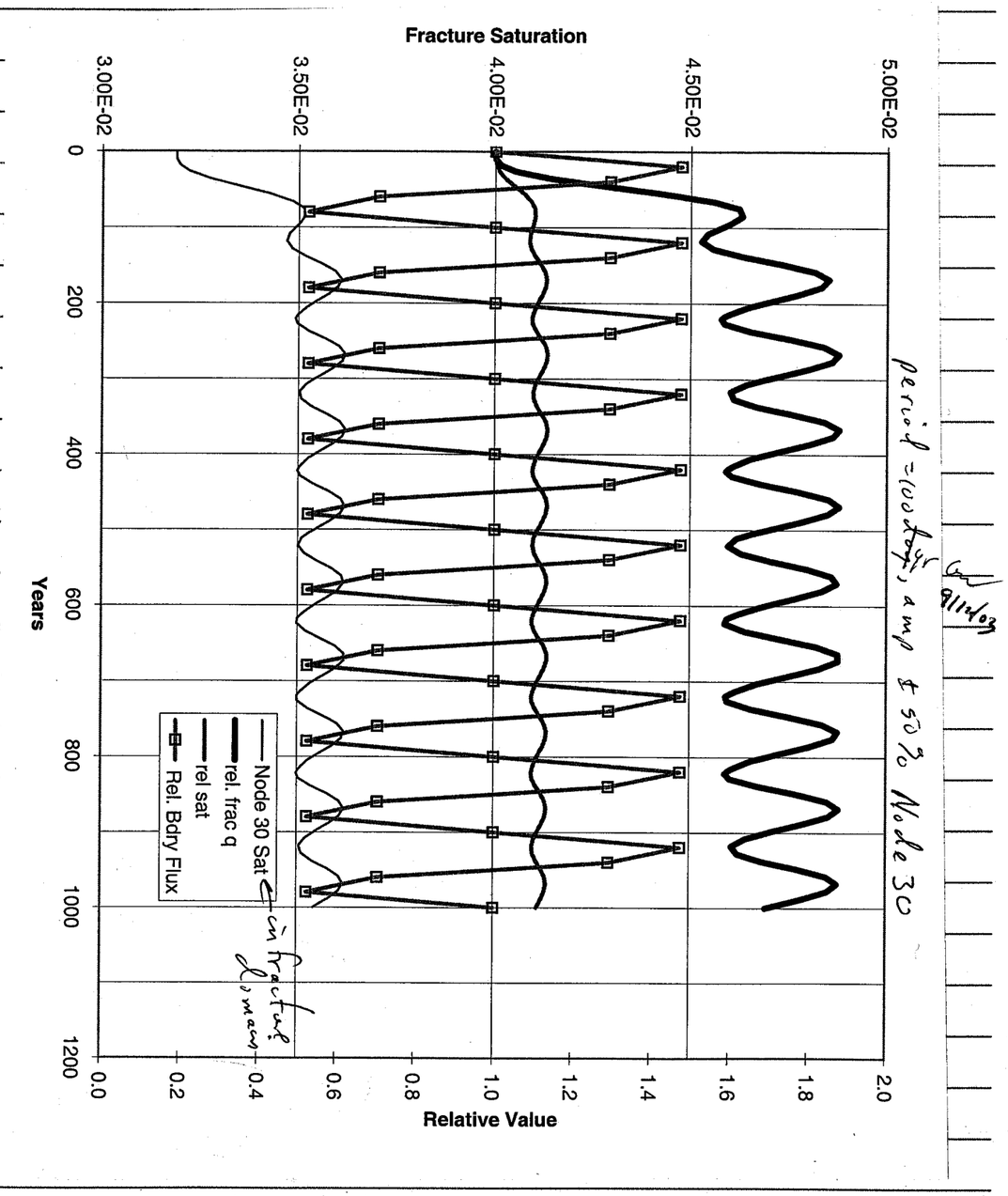
1. Look at UZ response to GW 9/12/03 hypothetical variation in infiltration imposed at upper boundary
2. See how "active fracture" concept affects response
3. Simulate response to a hypothetical infiltration history based approximately on paleo precip.

4/24/03

First, generate cyclic infiltration time histories. To do this, I wrote a fortran program called generate_bcond.f to compute a sinusoidally varying boundary flux and write it in PLT format need by multiflo. Source code in /multiflo_models/1d_transient/variable-infield/generate_bcond.f.

Simulation 1: Simulated a sinusoidal variation in upper boundary flux to fracture: period = 100 yrs
amplitude = +/- 50% of mean
mean = 2.35×10^{-3} kg/m^2-s
data file bcond100.txt
Mflo input file varia66.dat
cut+paste appropriate BCON data
saved saturation data in period-100-4yr-sat.txt
The results in terms of saturation in the fracture and fracture gravitational seepage velocity are shown in the graph on page 27. Matrix saturation was constant at 0.82. The results of a similar simulation for a period of 200yrs (bcond200.txt) is

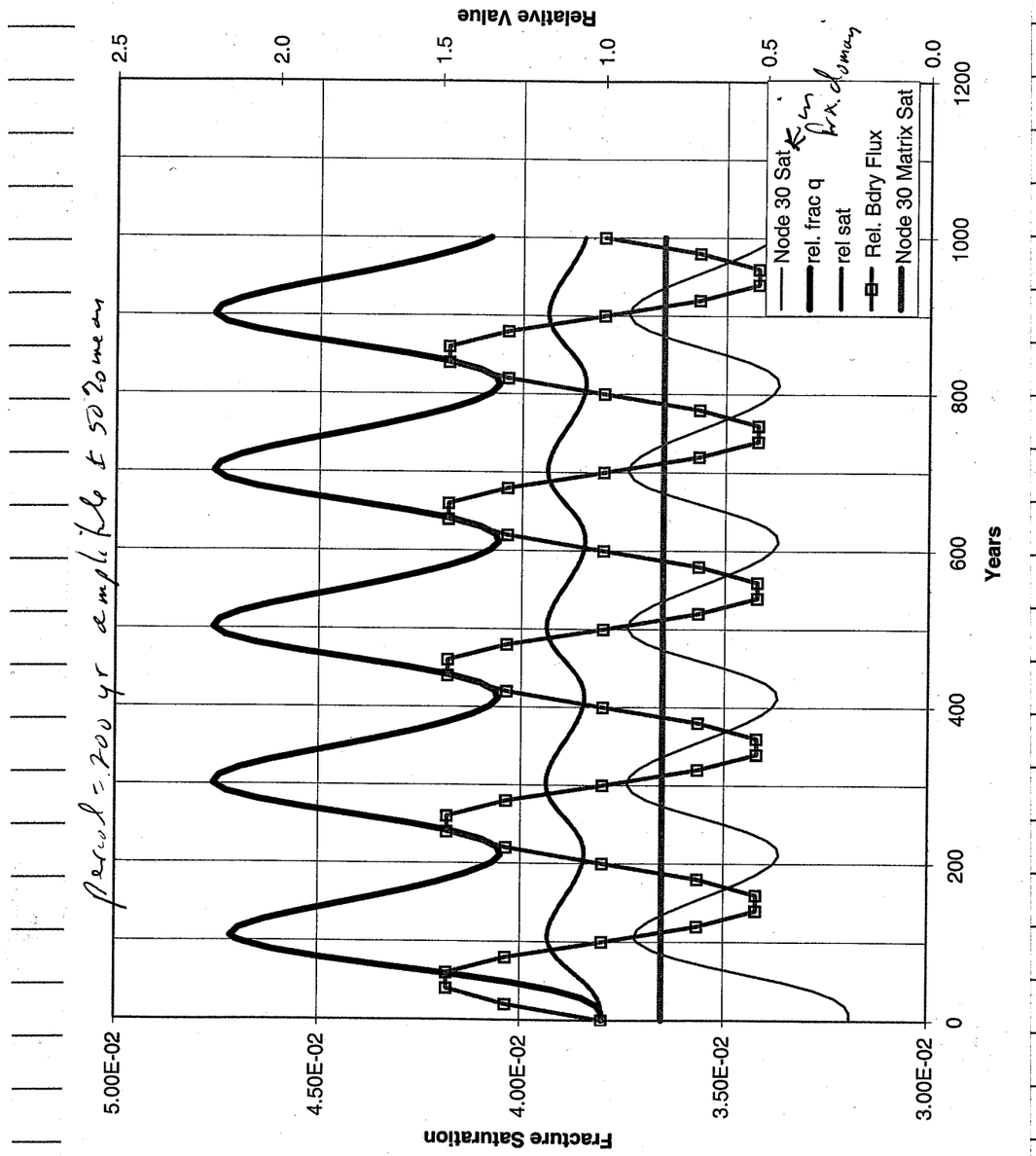
4/25/03



period = 100 yrs, amp ± 50% Node 30

shown in the graph on page 28.

4/25/03



4/25/03

As would be expected for flow through ~~pro~~ porous media, the amplitude of the subsurface ~~q~~ flux increases with the period of the ~~oscillation~~ oscillation.

Now consider the effect of the active fracture model. Need to develop tables of capillary pressure vs. saturation and relative k vs saturation. To do this must first clarify terminology between multiflo documentation and Liu et al (WRR (34, No 10) active fracture paper

Multiflo Manual Eqn 2-24	Liu et al eqn 5
$S_e = [1 + (\alpha P)^m]^{-\lambda}$	
$S_e^{-1/\lambda} = 1 + (\alpha P)^m$	
$(S_e^{-1/\lambda} - 1) = (\alpha P)^m$	
$\frac{1}{\alpha}(S_e^{-1/\lambda} - 1)^{1/m} = P$	$\frac{1}{\alpha}(S_e^{-1/m} - 1)^{1/n} = P$ (eqn 5)
$m = 1 - 1/\lambda$ GW 6/19/03	$\lambda = m$ $m = n$
Active Fracture	Active Fracture
$P = \frac{1}{\alpha}(S_e^{[r-1]/\lambda} - 1)^{1/m}$ GW 6/19/03	$P = \frac{1}{\alpha}(S_e^{[r-1]/m} - 1)^{1/n}$

4/25/03 Cw

The active fracture relative permeability in multiflo nomenclature is given by

$$k_r = S_e^{(1+\gamma)/2} \cdot \left[1 - \left\{1 - S_e^{(1-\gamma)/\lambda}\right\}^{\lambda}\right]^2$$

Let the gas ~~relav~~ Cw 10/27/03 relative permeability be computed by the linear relationship

$$k_{rg} = 1 - k_{rl}$$

For our hypothetical analysis, use the values of γ reported in the calibrated properties model.

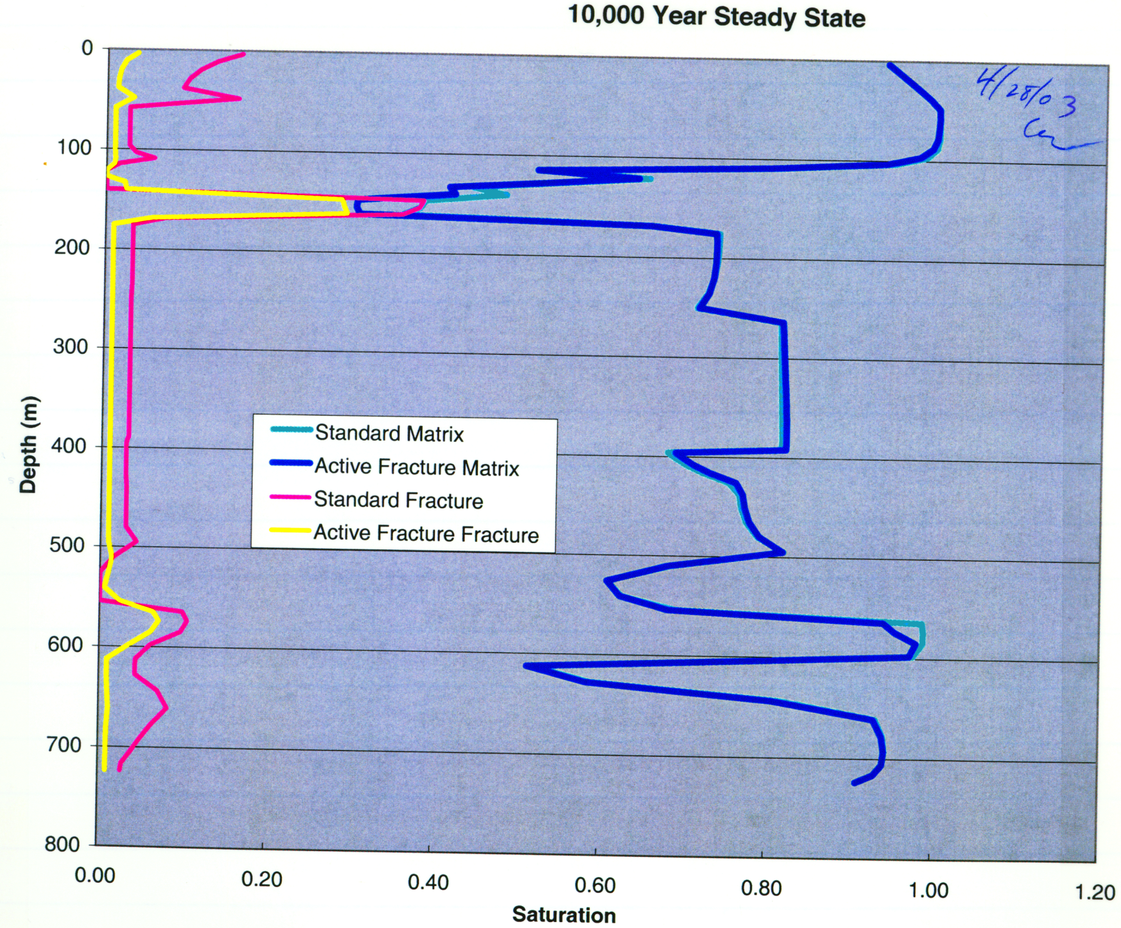
4/27/03 G. Walter

Constructed + excel spreadsheet with active fracture tables in
D:/multiflo/1d transient/active fracture/active fracture.xls

Copied tables to spock
multiflo_models/1d transient/active_fracture

April 28, 2003 G. Walter

Setup active fracture simulation based on longterm steady state simulation in spock multiflo_models/1d transient/sim2/longsim.dat
The vertical distribution of saturation for the standard model and active fracture model after 10^4 yrs are below.
~~below~~ Cw 9/12/03



4/28/03 Cw

The matrix saturation is almost the same for the two models which doesn't ~~seee~~ GW 10/27/03 seem to agree with the results reported by Liu et al 1998. The fracture saturation is lower for the active fracture model which does agree with Liu et al (1998). I am going to set-up a simple model to test the ~~sec~~ GW 10/27/03 behavior of the active fracture concept. The simple model will have only the following material types: Tcw12 1 GW 4/28/03 Ptn23, Tsw35, CHIVC, and BF3vb.

The files ~~fro~~ GW 10/27/03 for these simulations are in the subdirectory on spock called "simp6".

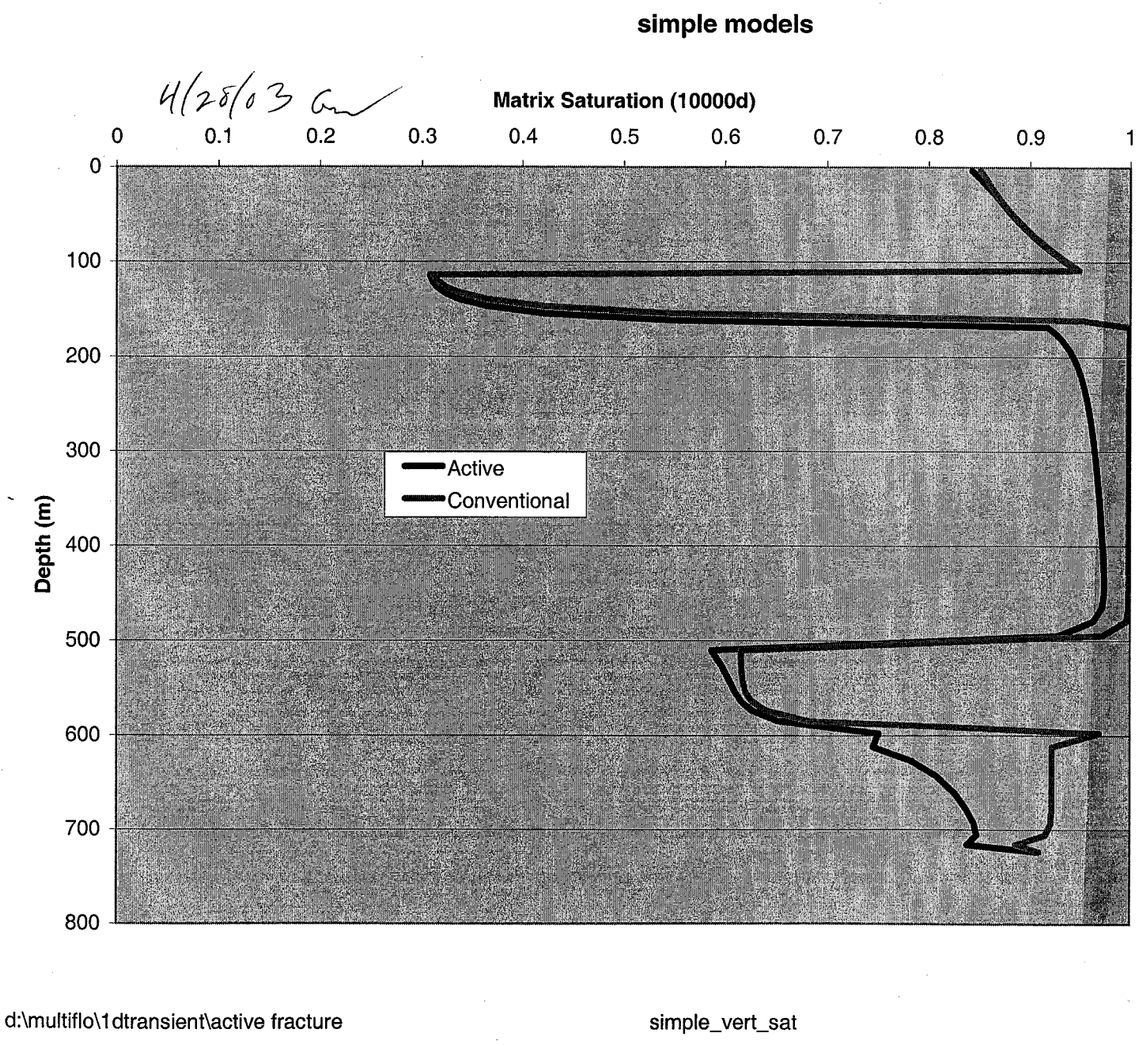
After talking to Scott Painter I realized that I may not have fully implemented the active fracture concept. Need to create tables to assign relative permeability for fracture/matrix flow. To do this, need to create new material tables that contain effective relative permeability for fracture/matrix flow where

$k_{rmf} = R k_{rm}$; k_{rmf} is relative perm. for fracture/matrix flow

and $R = S_e^{1+\gamma}$ (Liu et al eqn 18)

4/28/03 Cw

Set up two simulations
simple_active.dat simulates active fracture
simple_conv.dat " conventional model.
The results of these simulations shown below are more consistent with Liu et al



April 30, 2003

Set up periodic variation in infiltration simulation using simplified models. Will compare the results for the conventional and active fracture models.
Conventional frx Model = simple_conv_trans.dat
active frx model = simple_active_trans.dat

May 2, 2003 CW

Had some confusion about how to interpret the output from multiflo in terms of liquid fluxes. Outputs are intrinsic darcian ~~flow~~ velocities, that is, darcian velocity in the fracture. Unfortunately, ~~vel~~ multiflo only prints flows at discrete times and I want to see fine variation.

In spreadsheet analyze_flux, the active fracture flux computed using the multiflo saturation and gravity flow looks about right, but I can't get the calculations to work out for the conventional fracture sheet.

5/2/03 CW

Forgot to reset r in conventional model. Flux in fracture now looks about right at 24% of total 10 mm/yr the ~~rest~~ rest is in ~~the~~ matrix

5/6/03 C. Walter

Modified generate_3con.f to accept infiltration as mm/yr and volf to compute infiltration as kg/m^2-s. Assuming water with a unit specific gravity, the conversion is

$$1\ \frac{mm}{yr} \cdot \frac{10^{-3}\ m}{mm} \cdot \frac{1\ yr}{365\ d \cdot 86400\ s/d} \cdot \frac{10^3\ kg}{m^3} \rightarrow \frac{kg}{m^2\text{-}s}$$

This value is divided by volf to get the infiltration rate assigned to the fracture in Multiflo.

~~Before~~ I regenerated a boundary flux file (bc_10mm_200yr.txt) with a 10 mm/yr upper boundary flux with a period of 200 yrs. This was used to recalculate