308 - - - Q200002080007
Scientific Notebook # 236 (Continuation of Notebook # 150)

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308 - - - Q200002080007
Scientific Notebook # 236 (Continuation of Notebook # 150)

Ron Green
CNWRA #236

Ronald Green = RG

CNWRA
CONTROLLED
COPY 236

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REFLUX CALCULATIONS

NOTE - THIS NOTEBOOK IS A CONTINUATION OF WORK DESCRIBED IN NOTEBOOK #150. THE PORTIONS OF NOTEBOOK #150 THAT DISCUSS REFLUX DO ARE PAGES: 259-263, 275-280, 282-284, 289-290.

This is for George Rice RH 10/15/99

8-14-97 AR THE FOLLOWING IS A BRIEF DESCRIPTION OF REFLUXING AND THE EXPRESSIONS THAT ARE USED TO CALCULATE ITS COMPONENTS: AR 8-14-97

**Calculating Reflux of Condensate to the Boiling Zone**

Heat produced by the decay of spent fuel will cause waste package temperatures to exceed the boiling point of water. A portion of this heat may be consumed by vaporization of water dripping onto the packages, resulting in reduction of package temperature. A similar reduction in the temperature of the drift wall may be caused by vaporization of water in the surrounding rock. Water will vaporize as long as temperatures remain above boiling. The vapor will flow away from the boiling zone and condense where temperatures are below boiling. The condensate may then flow back to the boiling zone. This return of condensate to the boiling zone is called *refluxing*. A particular unit of water may participate in the reflux cycle many times. With every cycle, some portion of the refluxing water may escape and flow away from the heat source, possibly toward the water table.

Refluxing water may originate from two sources: 1) infiltration from ground surface, and 2) water boiled out of a dry-out zone in rock surrounding the waste package.

A method of calculating the amount of water that refluxes each year is presented below. However, it should be noted that some of the important variables that control refluxing are poorly constrained. Reliable estimates cannot be made until more precise values of these variables are obtained.

**Reflux Derived From Infiltration**

The amount of infiltration-derived water that refluxes in year 'N', is:

$$R_I = {}_{j=0,\,k=N}\Sigma^{1,\,N-1}\, I_k\,(1-L_I)^j\,]$$ (Note, j varies from 0 to N - 1, k from N to 1)

And for a constant infiltration rate:

$$R_I = {}_{j=0}\Sigma^{N-1}\, I\,(1-L)^j$$

Where:

$I_k$ = amount of infiltration in year N [m]
j, k = summation indices
N = years since start of refluxing
$L_I$ = fraction of infiltration that escapes the reflux cycle each year

Note: For constant I, $R_I$ converges to $I/L_I$. AR 8-14-97

**Reflux Derived From the Dry-Out Zone**

The total amount of water vaporized from the dry-out zone and available for refluxing is:

$$D = (T)\,(n)\,(S - S_r)$$

Where:

T = thickness of dry-out zone [m]
n = porosity of rock
S = liquid saturation
$S_r$ = residual saturation

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As with refluxing infiltration, some portion of refluxing dry-out zone water may escape the cycle each year ($L_D$). In addition, dry-out zone condensate may take more or less than a year to participate in a reflux cycle. The number of years required for water to complete one reflux cycle is 'P'. This gives rise to two cases:

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DESCRIPTION OF REFLUXING (CONT)

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**Case I. P >= 1.0**

The amount of dry-out zone water that refluxes in year 'N' is:

$$R_D = [\ (D)\ (P-L_D)^{N-1}\ ]\ /\ P^N$$

**Case II. P < 1.0**

In this case, the amount of dry-out zone water that refluxes in a given year is:

$$R_D = {}_{j=0}\Sigma^{1/P-1}\ D\ (1-L_D)^{1/P\,(N-1)+j}$$

**Total Reflux**

The total amount of refluxing water derived from both infiltration and the dry-out zone in year 'N' is:

$$R_T = R_I + R_D$$

For Case I with a constant infiltration rate this is:

$$R_T = {}_{j=0}\Sigma^{N-1}\ I\ (1-L_I)^j + [\ (D)\ (P-L_D)^{N-1}\ ]\ /\ P^N$$

For Case II with a constant infiltration rate:

$$R_T = {}_{j=0}\Sigma^{N-1}\ I\ (1-L_I)^j + {}_{j=0}\Sigma^{1/P-1}\ D\ (1-L_D)^{1/P\,(N-1)+j}$$

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The predominant source of refluxing water may change with time. At early times, refluxing water may be dominated by water derived from the dry-out zone. At later times, water derived from infiltration may dominate. If water escapes the reflux cycle, all dry-out zone water will eventually be lost and the amount of refluxing water will stabilize to the value of $R_I$ ($I/L_I$). If no losses occur, the amount of refluxing water will grow at a rate equal to 'I'. The reflux cycle will stop once waste package temperatures drop below boiling.

**Example Calculation**

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Calculate the amount of reflux occurring in year four. That is, four years after refluxing begins. Assume:

**Infiltration Derived Reflux**

- $I = 1X10^{-3}$ m (constant)
- $L_I = 0.1$

**Dry-Out Zone Derived Reflux**

- T = 20 m
- n = 0.15
- S = 0.9
- Sr = 0.0



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DESCRIPTION OF REFLUXING (CONT)

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Then:

D = (20 m) (0.15) (0.9 - 0.0) = 2.7 m.

- $L_D = 0.2$
- P = 1/3 (Case II)

In year 4, the amount of reflux due to infiltration and dry-out zone water is:

$$R_T = R_I + R_D = {}_{j=0}\Sigma^{N-1}\ I\ (1-L_I)^j + {}_{j=0}\Sigma^{1/P-1}\ D\ (1-L_D)^{1/P\,(N-1)+j}$$

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$$= {}_{j=0}\Sigma^{3}\ [(1X10^{-3})\ (1-0.1)^j] + {}_{j=0}\Sigma^{2}\ 2.7\ (1-0.2)^{9+j}$$

$$= 1X10^{-3}\ m\ [\ (0.9)^0 + (0.9)^1 + (0.9)^2 + (0.9)^3] + 2.7\ m\ [\ (0.8)^9 + (0.8)^{10} + (0.8)^{11}\ ]$$

$$= 1X10^{-3}\ m + 1X10^{-3}\ m\ [\ 2.44\ ] + 2.4\ m\ [\ 0.327\ ]$$

$$= 0.888\ m.$$

NOTE: this result represents the amount of refluxing water, not water escaping the reflux cycle.

**Derivation of Reflux Expressions**

**Infiltration Derived Reflux**

| Year | Infiltration | Reflux | Loss | Storage |
|---|---|---|---|---|
| 1 | $I_1$ | $I_1$ | $L_I I_1$ | $I_1 - L_I I_1 = I_1\ (1 - L_I)$ |
| 2 | $I_2$ | $I_2 + I_1\ (1 - L_I)$ | $L_I\ [I_2 + I_1\ (1 - L_I)]$ | $I_2 + I_1\ (1 - L_I) - L_I\ [I_2 + I_1(1 - L_I)] = [I_2\ (1-L_I) + I_1\ (1 - L_I)^2]$ |
| 3 | $I_3$ | $I_3 + [I_2\ (1-L_I) + I_1\ (1 - L_I)^2]$ | $L_I\ (\ I_3 + [I_2\ (1-L_I) + I_1\ (1 - L_I)^2])$ | $I_3 + [I_2\ (1-L_I) + I_1\ (1 - )^2] - L_I\ (\ I_3 + [I_2\ (1-L_I) + I_1(1 - L_I)^2]) = (\ I_3\ (1 - L_I) + [I_2\ (1-L_I)^2 + I_1\ (1 - L_I)^3])$ |

and so on ...

Thus, the amount of infiltration-derived water that refluxes in year four is:

$$R_I = I_4 + I_3\ (1-L_I)^1 + I_2\ (1-L_I)^2 + I_1\ (1-L_I)^3$$

$$R_I = {}_{j=0,\ k=N}\Sigma^{1,\ N-1}\ I_k\ (1-L_I)^j\ ]$$ (Note, j varies from 0 to N - 1, k from N to 1)

Or, if the infiltration rate is constant:

$$R_I = {}_{j=0,}\Sigma^{N-1}\ I\ (1-L_I)^j\ ]$$

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MR

DESCRIPTION OF REFLUXING (CONCL)
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**Dry-Out Zone Derived Reflux**

**Case II**

For P = 1/3

| Year | Cycle | Reflux | Loss | Storage |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | D |
| 1 | 1 | D | $L_oD$ | $D-L_oD = D(1-L_o)$ |
| | 2 | $D(1-L_o)$ | $L_oD(1-L_o)$ | $D(1-L_o)-L_oD(1-L_o) = D(1-L_o)^2$ |
| | 3 | $D(1-L_o)^2$ | $L_oD(1-L_o)^2$ | $D(1-L_o)^2-L_oD(1-L_o)^2 = D(1-L_o)^3$ |
| 2 | 1 | $D(1-L_o)^3$ | $L_oD(1-L_o)^3$ | $L_oD(1-L)^4$ |
| | 2 | $D(1-L_o)^4$ | $L_oD(1-L_o)^4$ | $L_oD(1-L)^5$ |
| | 3 | $D(1-L_o)^5$ | $L_oD(1-L_o)^5$ | $L_oD(1-L)^6$ |

and so on ...

Thus, the amount of dry-out zone water that refluxes in year 2 is:

$D [ (1-L_o)^3 + (1-L_o)^4 + (1-L_o)^5 ]$

$= {}_{j=0}\Sigma^{2} D (1-L_o)^{3+j}$

$= R_o = {}_{j=0}\Sigma^{1/P-1} D (1-L_o)^{1/P(N-1)+j}$

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MR

To: Sitakanta Mohanty

From: George Rice

Subject: TPA Code - Mass Balance for Reflux Module

Date: 8/21/97

Mass balance calculated as follows:

total reflux = total infiltration + dry-out water

Percent difference = [ total reflux - (total infiltration + dry-out water)] X 100
(total reflux + total infiltration + dry-out water)/2

Mass balances performed for three cases:

SEE PLOTS BELOW MR

1. "Moderate" conditions: Mass balance difference = 0.06%
   Thickness of dry-out zone = 20 m
   Period = 100
   Loss factor (infiltration) = 0.1
   Loss factor (dry-out) = 0.1

2. Reflux forced to occur at early times: Mass balance difference = 4.1%*
   Thickness of dry-out zone = 100 m
   Period = 1
   Loss factor (infiltration) = 0.9
   Loss factor (dry-out) = 0.9

3. Reflux forced to persist to late times: Mass balance difference = 0.9%
   (run = 20,000 yrs)
   Thickness of dry-out zone = 100 m
   Period = 100
   Loss factor (infiltration) = 0.01
   Loss factor (Dry-out) = 0.01

*Mass balance calculation can be improved by forcing TPA code to report output at earlier times.

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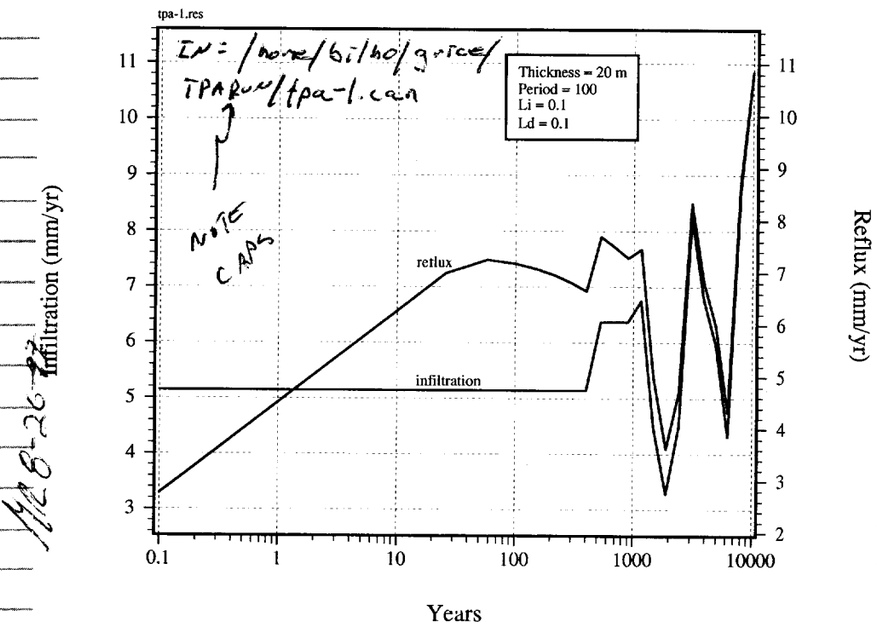
# Case 1, TPA Code Test - Reflux Module




MR 8-26-97

TPA CODE OUTPUT: infilper.res - MODIFIED - YEAR 0 → YEAR 0.1 SO RESULTS CAN BE PLOTTED ON LOG SCALE. NEW NAME = tpa-1.res
MR 8-26-97

Input file tpa.inp as supplied with TPA Version 3.1beta4 Code.
Not a basecase dataset. Use only for beta testing.
TPA 3.1beta4, Job started: Tue Aug 26 07:39:45 1997
Subarea Averaged Infiltration/Deep Percolation Including
After Reflux and Diversion - Values for Each Vector

IN: /home/bilbo/grice/TPARUN/tpa-1.res

| vector unitless | time yr | avinfil mm/yr | avreflux mm/yr | avdivert mm/yr |
|---|---|---|---|---|
| 1 | 0.1000000E+00 | 5.1448215E+00 | 2.7544821E+00 | 8.2634464E-01 |
| 1 | 2.5693704E+01 | 5.1448215E+00 | 6.9864341E+00 | 2.0959302E+00 |
| 1 | 5.8077611E+01 | 5.1448215E+00 | 7.2491623E+00 | 2.1747487E+00 |
| 1 | 9.8893734E+01 | 5.1448215E+00 | 7.1756778E+00 | 2.1527033E+00 |
| 1 | 1.5033768E+02 | 5.1448215E+00 | 7.0739401E+00 | 2.1221820E+00 |
| 1 | 2.1517675E+02 | 5.1448215E+00 | 6.9527686E+00 | 2.0858306E+00 |
| 1 | 2.9689880E+02 | 5.1448215E+00 | 6.8108273E+00 | 2.0432482E+00 |
| 1 | 3.9989989E+02 | 5.1448215E+00 | 6.6476912E+00 | 1.9943074E+00 |
| 1 | 5.2972070E+02 | 6.3738383E+00 | 7.6936522E+00 | 2.3080957E+00 |
| 1 | 6.9334463E+02 | 6.3738383E+00 | 7.4943494E+00 | 2.2483048E+00 |
| 1 | 8.9957344E+02 | 6.3738383E+00 | 7.2854446E+00 | 2.1856334E+00 |
| 1 | 1.1595007E+03 | 6.7496751E+00 | 7.4525303E+00 | 2.2357591E+00 |
| 1 | 1.4871086E+03 | 4.4886291E+00 | 4.9979532E+00 | 1.4993860E+00 |
| 1 | 1.9000200E+03 | 3.2858578E+00 | 3.6209015E+00 | 1.0862705E+00 |
| 1 | 2.4204465E+03 | 4.4947567E+00 | 4.7020430E+00 | 1.4106129E+00 |
| 1 | 3.0763831E+03 | 8.2302200E+00 | 8.3334861E+00 | 2.5000458E+00 |
| 1 | 3.9031145E+03 | 6.7801498E+00 | 6.8244343E+00 | 2.0473303E+00 |
| 1 | 4.9451126E+03 | 5.9622745E+00 | 5.9782781E+00 | 1.7934834E+00 |
| 1 | 6.2584292E+03 | 4.3152098E+00 | 4.3193102E+00 | 1.2957931E+00 |
| 1 | 7.9137110E+03 | 8.7454765E+00 | 8.7458956E+00 | 2.6237687E+00 |
| 1 | 1.0000000E+04 | 1.0847138E+01 | 1.0847239E+01 | 3.2541718E+00 |

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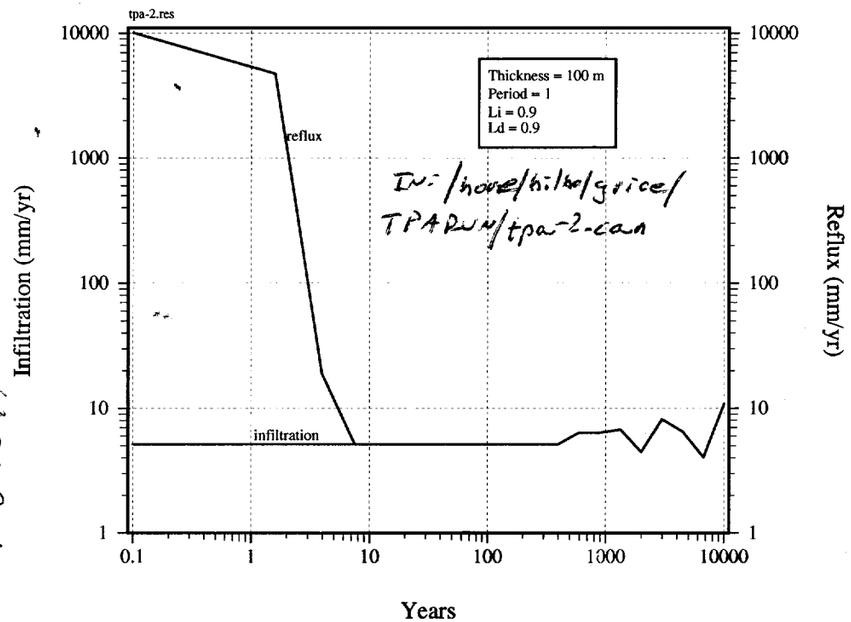
# Case 2, TPA Code Test - Reflux Module




AR 8-26-97

TPA OUTPUT = infilper.res - MODIFIED YEAR ϕ - FROM ϕ YRS TO 0.1 YRS SO IT WOULD PLOT ON LOG SCALE - NEW NAME = tpa-2.res

AR 8-26-97

Input file tpa.inp as supplied with TPA Version 3.1beta4 Code.
Not a basecase dataset. Use only for beta testing.
TPA 3.1beta4, Job started: Wed Aug 20 15:58:16 1997
Subarea Averaged Infiltration/Deep Percolation Including
After Reflux and Diversion - Values for Each Vector

IN: /home/bilbo/grice/TPARun/tpa-2.res

| vector unitless | | time yr | avinfil mm/yr | avreflux mm/yr | avdivert mm/yr |
|---|---|---|---|---|---|
| | 1 | 0.1000000E+00 | 5.1448215E+00 | 1.0084630E+04 | 3.0253891E+03 |
| | 1 | 1.5864169E+00 | 5.1448215E+00 | 4.7649273E+03 | 1.4294782E+03 |
| | 1 | 3.9585937E+00 | 5.1448215E+00 | 1.8980492E+01 | 5.6941475E+00 |
| | 1 | 7.5057209E+00 | 5.1448215E+00 | 5.1503133E+00 | 1.5450940E+00 |
| | 1 | 1.2809757E+01 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 2.0740907E+01 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 3.2600394E+01 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 5.0333941E+01 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 7.6850998E+01 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 1.1650208E+02 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 1.7579253E+02 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 2.6444982E+02 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 3.9701949E+02 | 5.1448215E+00 | 5.1448215E+00 | 1.5434464E+00 |
| | 1 | 5.9525154E+02 | 6.3738383E+00 | 6.3738383E+00 | 1.9121515E+00 |
| | 1 | 8.9166886E+02 | 6.3738383E+00 | 6.3738383E+00 | 1.9121515E+00 |
| | 1 | 1.3349031E+03 | 6.7496751E+00 | 6.7496751E+00 | 2.0249025E+00 |
| | 1 | 1.9976734E+03 | 4.4605153E+00 | 4.4573326E+00 | 1.3371998E+00 |
| | 1 | 2.9887169E+03 | 8.1609048E+00 | 8.1598405E+00 | 2.4479521E+00 |
| | 1 | 4.4706289E+03 | 6.4882750E+00 | 6.4876880E+00 | 1.9463064E+00 |
| | 1 | 6.6865391E+03 | 4.0380920E+00 | 4.0381627E+00 | 1.2114488E+00 |
| | 1 | 1.0000000E+04 | 1.0847138E+01 | 1.0847138E+01 | 3.2541414E+00 |

AR 8-26-97



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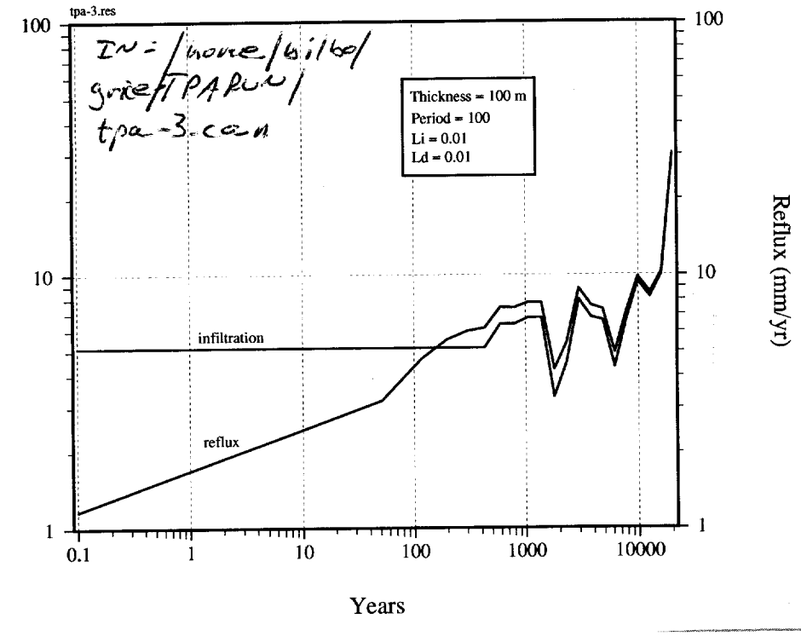
AR 8-26-97

# Case 3, TPA Code Test - Reflux Module

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TPA CODE OUTPUT = infilper.res - MODIFIED SO THAT YEAR ϕ = 0.1 - ALLOW TO BE PLOTTED ON log SCALE = tpa-3.res

AR 8-26-97

Input file tpa.inp as supplied with TPA Version 3.1beta4 Code.
Not a basecase dataset. Use only for beta testing.
TPA 3.1beta4, Job started: Thu Aug 21 07:48:15 1997
Subarea Averaged Infiltration/Deep Percolation Including
After Reflux and Diversion - Values for Each Vector

IN: /home/bilbo/grice/TPARun/tpa-3.res

| vector unitless | | time yr | avinfil mm/yr | avreflux mm/yr | avdivert mm/yr |
|---|---|---|---|---|---|
| | 1 | 0.1000000E+00 | 5.1448215E+00 | 1.1714482E+00 | 3.5143446E-01 |
| | 1 | 5.1387409E+01 | 5.1448215E+00 | 3.1896084E+00 | 9.5688251E-01 |
| | 1 | 1.1615522E+02 | 5.1448215E+00 | 4.6510457E+00 | 1.3953137E+00 |
| | 1 | 1.9778747E+02 | 5.1448215E+00 | 5.5381887E+00 | 1.6614566E+00 |
| | 1 | 3.0067536E+02 | 5.1448215E+00 | 5.9811515E+00 | 1.7943454E+00 |
| | 1 | 4.3035349E+02 | 5.1448215E+00 | 6.1496777E+00 | 1.8449033E+00 |
| | 1 | 5.9379761E+02 | 6.3738383E+00 | 7.4130562E+00 | 2.2239168E+00 |
| | 1 | 7.9979978E+02 | 6.3738383E+00 | 7.4057906E+00 | 2.2217372E+00 |
| | 1 | 1.0594414E+03 | 6.7496751E+00 | 7.7570221E+00 | 2.3271066E+00 |
| | 1 | 1.3866893E+03 | 6.7496751E+00 | 7.7247380E+00 | 2.3174214E+00 |
| | 1 | 1.7991469E+03 | 3.2858578E+00 | 4.2215254E+00 | 1.2664576E+00 |
| | 1 | 2.3190014E+03 | 4.4947567E+00 | 5.3830236E+00 | 1.6149071E+00 |
| | 1 | 2.9742172E+03 | 7.9682058E+00 | 8.7995807E+00 | 2.6398742E+00 |
| | 1 | 3.8000400E+03 | 6.7801498E+00 | 7.5461336E+00 | 2.2638401E+00 |
| | 1 | 4.8408930E+03 | 6.5916447E+00 | 7.2812782E+00 | 2.1843834E+00 |
| | 1 | 6.1527663E+03 | 4.3152098E+00 | 4.9206021E+00 | 1.4761806E+00 |
| | 1 | 7.8062290E+03 | 6.6288966E+00 | 7.1455931E+00 | 2.1436779E+00 |
| | 1 | 9.8902252E+03 | 9.3661355E+00 | 9.7828989E+00 | 2.9348697E+00 |
| | 1 | 1.2516858E+04 | 8.1726389E+00 | 8.4933898E+00 | 2.5480170E+00 |
| | 1 | 1.5827422E+04 | 1.0014201E+01 | 1.0245078E+01 | 3.0735235E+00 |
| | 1 | 2.0000000E+04 | 3.0054835E+01 | 3.0206411E+01 | 9.0619232E+00 |

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TPA Code Results
Mass Balance
Results From File 'infilper.res'

EXCEL SPREADSHEET FOR CALCULATING MASS BALANCE OF TPA RUNS - THIS IS FOR CASE 1, SEE pg 5.

Reflux Parameters:
Thickness = 20 m
Porosity = 0.14
Initial Saturation = 0.9
Residual Saturation = 0.1
Period = 100
Li = 0.1
Ld = 0.1

ON P.C. IN: C:/jonje/memos/reflux/tpa-1.xls

Amount of reflux derived from vaporized dry-out zone water:
20m(0.14)(0.9 - 0.1) = 2240 mm
Thus, For mass balance:
Total Reflux = Total Infiltration + 2240 mm

| Time (yr) | avinfil mm/yr | avreflux mm/yr | | total infil mm | total reflux mm |
|---|---|---|---|---|---|
| 0 | 5.1448 | 2.7545 | | 0 | 0 |
| 25.69 | 5.1448 | 6.9864 | | 132.169912 | 125.121861 |
| 58.08 | 5.1448 | 7.2492 | | 166.640072 | 230.545542 |
| 98.89 | 5.1448 | 7.1757 | | 209.959288 | 294.340085 |
| 150.3 | 5.1448 | 7.0739 | | 264.494168 | 366.285968 |
| 215.2 | 5.1448 | 6.9528 | | 333.89752 | 455.166415 |
| 296.9 | 5.1448 | 6.8108 | | 420.33016 | 562.24306 |
| 399.9 | 5.1448 | 6.6477 | | 529.9144 | 693.11275 |
| 529.7 | 6.3738 | 7.6937 | | 747.55714 | 930.75686 |
| 693.3 | 6.3738 | 7.4943 | | 1042.75368 | 1242.3784 |
| 899.6 | 6.3738 | 7.2854 | | 1314.91494 | 1524.52606 |
| 1160 | 6.7497 | 7.4525 | | 1708.6797 | 1918.87458 |
| 1487 | 4.4886 | 4.998 | | 1837.46205 | 2035.65675 |
| 1900 | 3.2859 | 3.6209 | | 1605.43425 | 1779.80285 |
| 2420 | 4.4948 | 4.702 | | 2022.982 | 2163.954 |
| 3076 | 8.2302 | 8.3335 | | 4173.8 | 4275.644 |
| 3903 | 6.7801 | 6.8244 | | 6206.75905 | 6267.79165 |
| 4945 | 5.9623 | 5.9783 | | 6638.7904 | 6670.2067 |
| 6258 | 4.3152 | 4.3193 | | 6747.17875 | 6760.3744 |
| 7914 | 8.7455 | 8.7459 | | 10814.2596 | 10817.9856 |
| 10000 | 10.847 | 10.847 | | 20434.9775 | 20435.3947 |
| | | | | | |
| Totals | | | | 67352.9546 | 69550.11622 |
| | | | | | |
| | Thickness | Porosity | Sat-Init | Sat-Resid | |
| | 20000 | 0.14 | 0.9 | 0.1 | |
| Dry-out: | 2240 | | | | |
| | | | | | |
| Mass | | | | | |
| Balance: | -42.792355 | = | -0.00061508 | | |

AR 8-26-97

$69550 - (67353 + 2240) = -6 \times 10^{-4}$

$[69550 + 67353 + 2240]/2$



9-2-97
AR

COMPARING REFLUX2 RESULTS - TPA CODE + MATHEMATICA - FOR CASE 1 - PAGE 5.
MATHEMATICA FILE IS IN:
/home/bilbo/grice/reflux/test-tpa-1.nb

AR 9-2-97

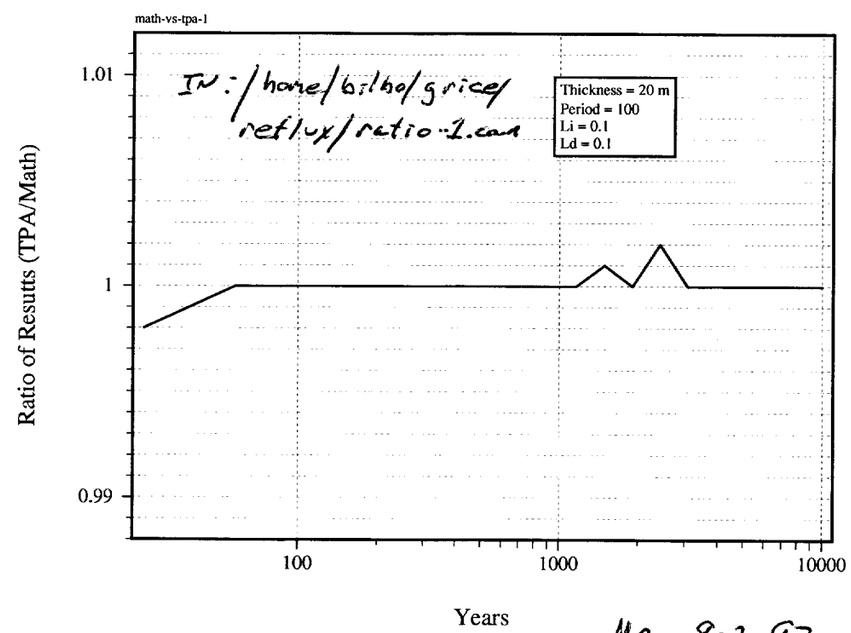
Comparison of reflux2 results obtained using Mathematica and the TPA code.
This comparison for "moderate" conditions (see page 5 of reflux notebook).

| Time(yrs) | TPA Code | Mathematica | Ratio(TPA/Math) |
|---|---|---|---|
| 26 | 6.986 | 6.997 | 0.998 |
| 58 | 7.249 | 7.249 | 1.000 |
| 215 | 6.953 | 6.953 | 1.000 |
| 400 | 6.648 | 6.648 | 1.000 |
| 900 | 7.285 | 7.285 | 1.000 |
| 1160 | 7.453 | 7.452 | 1.000 |
| 1487 | 4.998 | 4.995 | 1.001 |
| 1900 | 3.621 | 3.621 | 1.000 |
| 2420 | 4.702 | 4.694 | 1.002 |
| 3076 | 8.333 | 8.334 | 1.000 |
| 3903 | 6.824 | 6.825 | 1.000 |
| 4945 | 5.978 | 5.978 | 1.000 |
| 6258 | 4.319 | 4.319 | 1.000 |
| 7914 | 8.745 | 8.746 | 1.000 |
| 10000 | 10.85 | 10.85 | 1.000 |

IN: /home/bilbo/grice/reflux/math-vs-tpa-1

AR 9-2-97

# Reflux2 - TPA Code vs Mathematica, Case 1

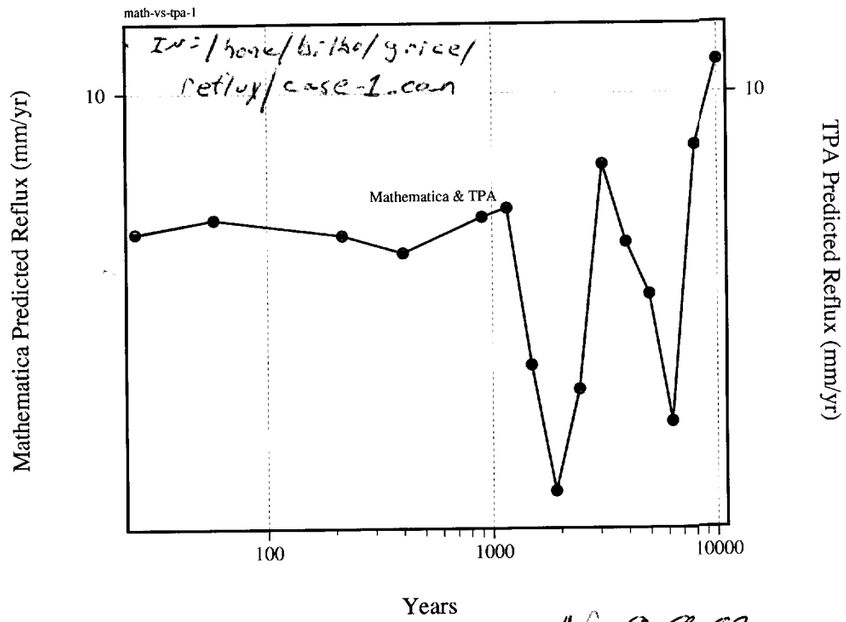



AR 9-2-97

9-9-97
MR

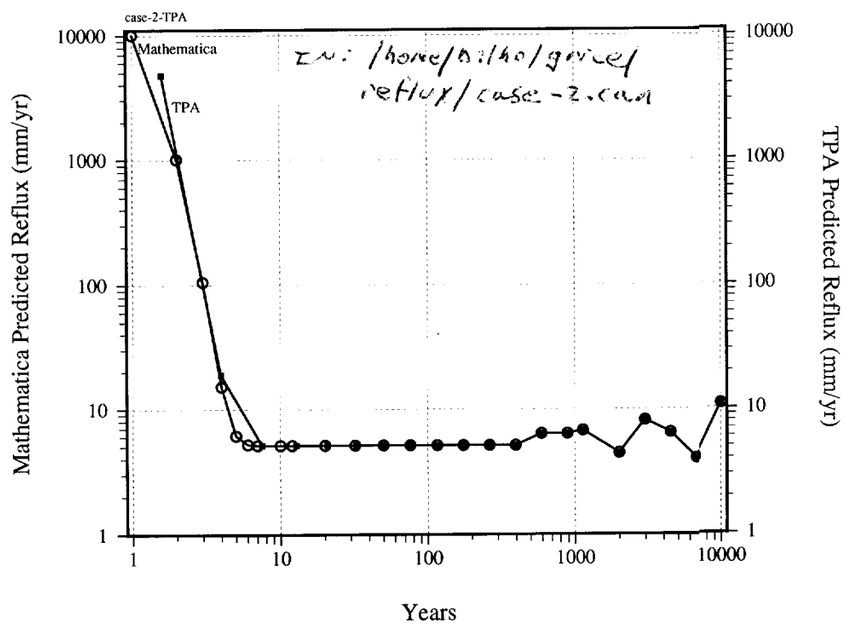
MR 9-9-97

# Reflux2 - TPA Code vs Mathematica, Case 1




AR 9-9-97

# Reflux2 - TPA Code vs Mathematica, Case 2




MR 9-9-97



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MR

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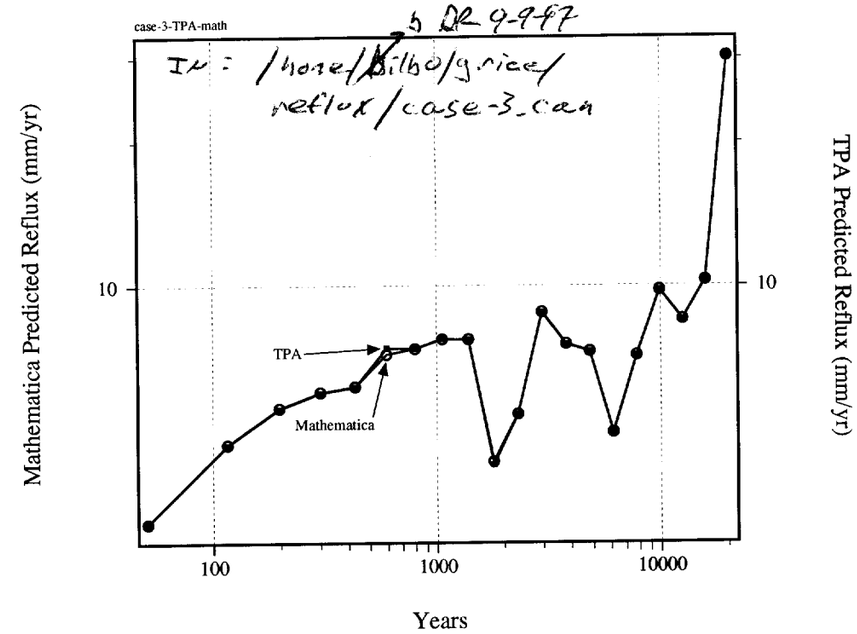
# Reflux2 - TPA Code vs Mathematica, Case 3




MR 9-9-97

9-11-97
MR

THE MATHEMATICA FILES USED TO PRODUCE THE PLOTS ON THIS AND THE PREVIOUS PAGE ARE IN:
~~/home/sneezy/~~ MR 9-11-97
/home/bilbo/grice/reflux:

test-tpa-1.nb
test-tpa-2.nb
test-tpa-3.nb

MR 9-26-97

9-26-97
MR

TPA CODE - REFLUX2 SENSITIVITY ANALYSES

- VARYING REFLUX2 PARMETERS [THICKNESS, PERIOD, LOSS-INFIL, LOSS-DRY] TO DETERMINE HOW LITTLE REFLUX WILL RESULT IN A RELEASE FROM THE WASTE PACKAGE.

ONLY VARYING REFLUX PARMETERS - USING BASE CASE INPUT FROM TPA3_11 - ALSO USING EXECUTABLE COMMAND:
/solapps/cnwra/tpa3_11/tpa.e. IN:
/home/bilbo/grice/tparun

NOTE - VOLCANO, SEISMO, AND FAULTO DO NOT APPEAR TO AFFECT RELEASES - COMPARE FILES SHOWN BELOW - BOTH USING tpa.inp FROM TPA3-11 - OUTPUTS ARE MODIFIED (ADDED HEADERS) cumrel.res FILES.

MR 9-26-97

Case 11:

Thickness = 500m
Period = 100
Li = 0.1
Ld = 0.1

Input file tpa.inp as supplied with TPA Version 3.1 Code.
Base case data set Rev 3.1.1 9/22/97
TPA 3.1, Job started: Thu Sep 25 13:34:22 1997
Cumulative Releases from EBS, UZ, and SZ by Nuclide
Summed Over All Subareas - Values for Each Vector

| vector unitless | nuclide unitless | ebscumrl Ci | uzcumrl Ci | szcumrl Ci |
|---|---|---|---|---|
| 1 | Cm246 | 8.2554E-04 | 8.2330E-04 | 6.5119E-04 |
| 1 | U238 | 1.5547E-04 | 1.5493E-04 | 1.2629E-04 |
| 1 | Cm245 | 6.9455E-03 | 6.9258E-03 | 5.5470E-03 |
| 1 | Am241 | 5.5657E-04 | 6.1891E-04 | 9.3470E-04 |
| 1 | Np237 | 3.0061E-01 | 3.0039E-01 | 2.8086E-01 |
| 1 | Am243 | 5.3941E-02 | 5.3786E-02 | 1.2038E-02 |
| 1 | Pu239 | 1.1925E-02 | 1.1904E-02 | 1.2526E-02 |
| 1 | Pu240 | 1.0244E-02 | 1.0219E-02 | 9.0347E-03 |
| 1 | U234 | 5.7879E-04 | 5.7680E-04 | 4.7026E-04 |
| 1 | Th230 | 3.2281E-02 | 3.2230E-02 | 2.6840E-02 |
| 1 | Ra226 | 2.1031E-02 | 2.1040E-02 | 8.2178E-03 |
| 1 | Pb210 | 2.0824E-02 | 2.0855E-02 | 8.0346E-02 |
| 1 | Cs135 | 1.1387E-01 | 1.1384E-01 | 8.4619E-16 |
| 1 | I129 | 3.4200E-02 | 3.4104E-02 | 3.1489E-02 |
| 1 | Tc99 | 1.3786E+01 | 1.3747E+01 | 1.2450E+01 |
| 1 | Ni59 | 1.9039E+00 | 1.8985E+00 | 1.3924E+00 |
| 1 | Cl4 | 4.6033E-01 | 2.2725E-01 | 2.1348E-01 |
| 1 | Se79 | 3.9441E-01 | 3.9335E-01 | 3.3591E-01 |
| 1 | Nb94 | 5.6708E-04 | 5.6565E-04 | 3.6040E-04 |
| 1 | Cl36 | 1.3250E-02 | 1.3213E-02 | 1.2418E-02 |

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MR 9-26-97

Case 13:

Thickness = 500m
Period = 100
Li = 0.1
Ld = 0.1

With seismo, faulto, and volcano

Input file tpa.inp as supplied with TPA Version 3.1 Code.
Base case data set Rev 3.1.1 9/22/97
TPA 3.1, Job started: Thu Sep 25 14:09:35 1997
Cumulative Releases from EBS, UZ, and SZ by Nuclide
Summed Over All Subareas - Values for Each Vector

| vector unitless | nuclide unitless | ebscumrl Ci | uzcumrl Ci | szcumrl Ci |
|---|---|---|---|---|
| 1 | Cm246 | 8.2554E-04 | 8.2330E-04 | 6.5119E-04 |
| 1 | U238 | 1.5547E-04 | 1.5493E-04 | 1.2629E-04 |
| 1 | Cm245 | 6.9455E-03 | 6.9258E-03 | 5.5470E-03 |
| 1 | Am241 | 5.5657E-04 | 6.1891E-04 | 9.3470E-04 |
| 1 | Np237 | 3.0061E-01 | 3.0039E-01 | 2.8086E-01 |
| 1 | Am243 | 5.3941E-02 | 5.3786E-02 | 1.2038E-02 |
| 1 | Pu239 | 1.1925E-02 | 1.1904E-02 | 1.2526E-02 |
| 1 | Pu240 | 1.0244E-02 | 1.0219E-02 | 9.0347E-03 |
| 1 | U234 | 5.7879E-04 | 5.7680E-04 | 4.7026E-04 |
| 1 | Th230 | 3.2281E-02 | 3.2230E-02 | 2.6840E-02 |
| 1 | Ra226 | 2.1031E-02 | 2.1040E-02 | 8.2178E-03 |
| 1 | Pb210 | 2.0824E-02 | 2.0855E-02 | 8.0346E-02 |
| 1 | Cs135 | 1.1387E-01 | 1.1384E-01 | 8.4619E-16 |
| 1 | I129 | 3.4200E-02 | 3.4104E-02 | 3.1489E-02 |
| 1 | Tc99 | 1.3786E+01 | 1.3747E+01 | 1.2450E+01 |
| 1 | Ni59 | 1.9039E+00 | 1.8985E+00 | 1.3924E+00 |
| 1 | Cl4 | 4.6033E-01 | 2.2725E-01 | 2.1348E-01 |
| 1 | Se79 | 3.9441E-01 | 3.9335E-01 | 3.3591E-01 |
| 1 | Nb94 | 5.6708E-04 | 5.6565E-04 | 3.6040E-04 |
| 1 | Cl36 | 1.3250E-02 | 1.3213E-02 | 1.2418E-02 |

MR 9-26-97

FOR THE BASECASE INPUT IN TPA3_11, THE SMALLEST AMOUNT OF REFLUX WATER THAT RESULTS IN A RELEASE FROM THE EBS IS ~~WHEN~~ MR 9-26-97 THE AMOUNT CORRESPONDING TO A THICKNESS OF 315 m.

MR 9-29-97

Case 27:

Thickness = 315m
Period = 200
Li = 0.1
Ld = 0.1

Input file tpa.inp as supplied with TPA Version 3.1 Code.
Base case data set Rev 3.1.1 9/22/97
TPA 3.1, Job started: Fri Sep 26 15:31:39 1997
Cumulative Releases from EBS, UZ, and SZ by Nuclide
Summed Over All Subareas - Values for Each Vector

| vector unitless | nuclide unitless | ebscumrl Ci | uzcumrl Ci | szcumrl Ci |
|---|---|---|---|---|
| 1 | Cm246 | 1.5665E-05 | 2.0437E-06 | 0.0000E+00 |
| 1 | U238 | 2.4817E-06 | 3.2434E-07 | 7.5370E-12 |
| 1 | Cm245 | 1.4653E-04 | 1.9131E-05 | 0.0000E+00 |
| 1 | Am241 | 1.1000E-05 | 1.7868E-06 | 0.0000E+00 |
| 1 | Np237 | 6.7626E-03 | 8.8381E-04 | 3.9537E-05 |
| 1 | Am243 | 1.1309E-03 | 1.4764E-04 | 0.0000E+00 |
| 1 | Pu239 | 2.5588E-04 | 3.3484E-05 | 1.8737E-06 |
| 1 | Pu240 | 1.9324E-04 | 2.5222E-05 | 1.3822E-06 |
| 1 | U234 | 9.2293E-06 | 1.2062E-06 | 2.8009E-11 |
| 1 | Th230 | 1.9545E-03 | 2.5542E-04 | 2.7588E-16 |
| 1 | Ra226 | 1.5254E-03 | 1.9967E-04 | 0.0000E+00 |
| 1 | Pb210 | 1.5193E-03 | 1.9913E-04 | 1.6956E-07 |
| 1 | Cs135 | 6.5881E-03 | 8.6104E-04 | 0.0000E+00 |
| 1 | I129 | 5.5586E-04 | 7.2650E-05 | 1.8469E-05 |
| 1 | Tc99 | 2.2437E-01 | 2.9322E-02 | 3.6192E-03 |

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SEE PREVIOUS PAGE.

MR 9-29-97

Case 29:

Thickness = 310m
Period = 200
Li = 0.1
Ld = 0.1

Input file tpa.inp as supplied with TPA Version 3.1 Code.
Base case data set Rev 3.1.1 9/22/97
TPA 3.1, Job started: Fri Sep 26 15:54:05 1997
Cumulative Releases from EBS, UZ, and SZ by Nuclide
Summed Over All Subareas - Values for Each Vector

| vector unitless | nuclide unitless | ebscumrl Ci | uzcumrl Ci | szcumrl Ci |
|---|---|---|---|---|
| 1 | Cm246 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | U238 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Cm245 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Am241 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Np237 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Am243 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Pu239 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Pu240 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | U234 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Th230 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Ra226 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Pb210 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Cs135 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | I129 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Tc99 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Ni59 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | C14 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Se79 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Nb94 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | Cl36 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

MR 9-29-97

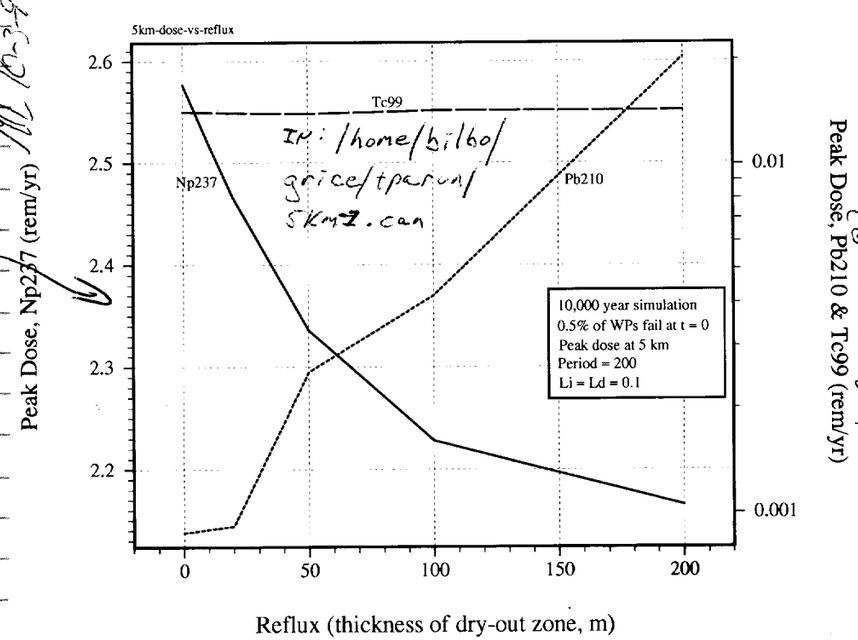
10-3-97

NOW USING NEW INPUT FILE - CHANGES RESULTS
FROM HERE ON, INPUT FILE IS: tpa.inp.meanvalues1

NOTE - THE OUTPUT FILES FROM WHICH THIS AND THE FOLLOWING 3 PLOTS WERE CREATED ARE IN: /home/bilbo/grice/tparun/npkdoset-1 THROUGH npkdoset-31.

MR 10-7-97

# TPA Code Sensitivity, Reflux vs Peak Dose

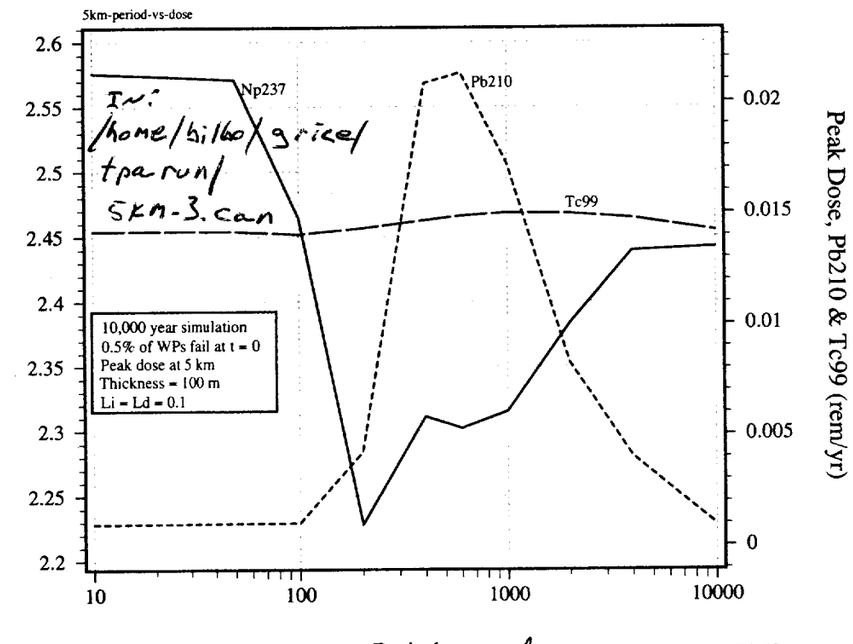



MR 10-7-97



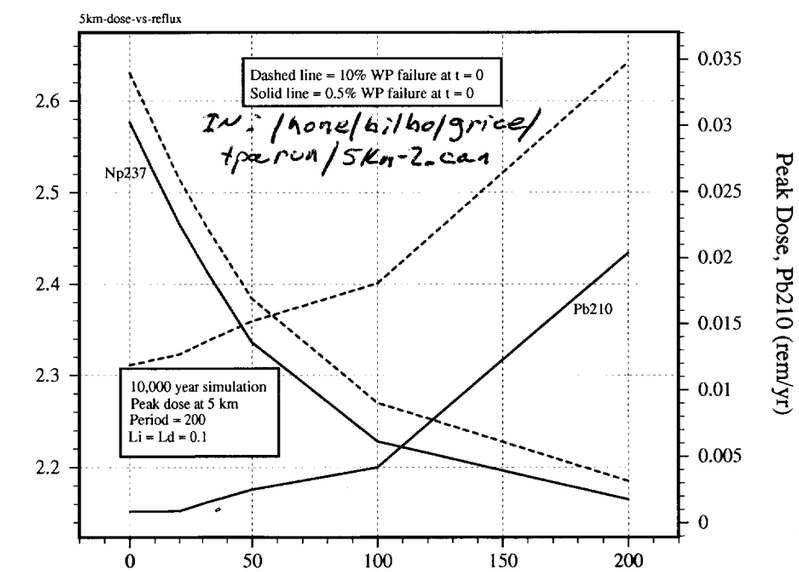
MR 10-7-97

# TPA Code Sensitivity to Reflux Period




MR 10-7-97

# TPA Code Sensitivity to WP Failure at t = 0




MR 10-7-97

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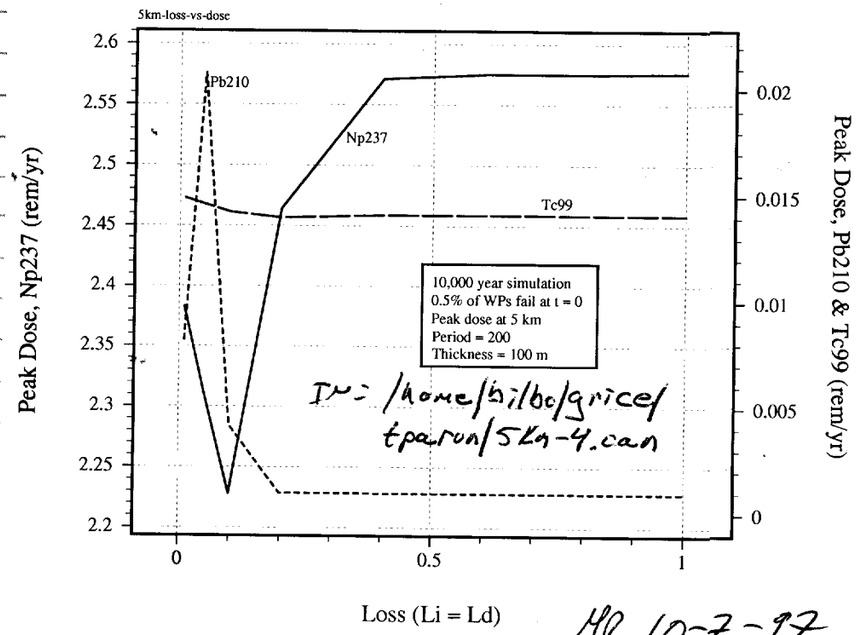
MR

# TPA Code Sensitivity to Reflux Loss Parameters




IN: /home/bilbo/grice/tparun/5km-4.can

MR 10-7-97

10-9-97
MR

RUNNING 100 REALIZATIONS OF REFLUX 1:

CHANGING CONSTANTS TO VARIABLES:

LENGTH OF REFLUX ZONE – UNIFORM – 10m – 200m
PERCHED BUCKET VOLUME – UNIFORM – 0.2 – 0.8

ALSO – FAULTFACTOR + FOWFACTOR MADE CONSTANTS, 1.0 + 0.05, RESPECTIVELY.
SUBAREAWET RETAINS UNIFORM DISTRIBUTION BUT VERY NARROW: 0.5 TO 0.50001 – PROGRAM WON'T RUN IF IT IS A CONSTANT.

RUN FOR 20,000 YRS – LOOK @ 5 KM

EXCEPT AS NOTED ABOVE, INPUT FILE SAME AS: tpa.inp.manualvcs1.

MR 10-7-97
~~TPA RO~~



10-10-97
MR

- RUN (TPA CODE) STARTED YESTERDAY CRASHED – MESSAGE ON SCREEN:
"logical unit 29 named 'diagnostic.out'
core dumped
istatus .ne. 0
istatus = sh("release.e > release.out")
istatus = 34304

- NOTE – 12 realizations WRITTEN TO OUTPUT FILE "infilper.res"

BUT – THE FILE "100 sample params" CONTAINS INFO ON 100 REALIZATIONS! – SIX VALUES FOR EACH VECTOR.

BUT – FILE "gwpkdos.res" ONLY CONTAINS OUTPUT FOR 12 VECTORS (REALIZATIONS)

– RE-RUN SAME INPUT – SEE WHAT HAPPENS:

THIS RUN IS IN: /home/bilbo/grice/tparun

REFLUX1 – SEE NOTES ON PREVIOUS PAGE

REFLUX2:

RUNNING 100 REALIZATIONS FOR 20,000 YEARS – LOOKING AT DOSE AT 5 KM. CHANGED FAULTFACTOR, FOWFACTOR, + SUBAREAWET TO CONSTANTS: 1.0, 0.05, + 0.5; RESPECTIVELY. TO DO SO – HAD TO COMMENT OUT REFERENCES TO CORRELATIONS IN ~ LAST 30 LINES OF tpa.inp.
IN: /home/bilbo/grice/tparun2

REFLUX2 PARAMETERS:
Reflux2Thickness – UNIFORM – 10.0 – 200.0m
Reflux2Period – UNIFORM – 1.0 – 100
Reflux2LossI – UNIFORM – 0.0 – 1.0
Reflux2LossD – UNIFORM – 0.0 – 1.0

10-13-97
MR

BOTH REFLUX1 + REFLUX2 RAN SUCCESSFULLY.
HOWEVER — THE sp.tpa FILE FOR REFLUX2
LISTS 2 REFLUX1 PARAMETERS AS VARIABLES —
THIS SHOULDN'T OCCUR — WILL DISCUSS
w/ SITAKANTA MOHANTY.

- RE-RUNNING REFLUX2 WITH REFLUX1 PARAMETERS
COMMENTED OUT.

10-14-97
MR

- REFLUX 2 RUN RAN SUCCESSFULLY — NOW RUNNING
ISOTECH RUN FOR 10,000 YRS.

OUTPUT OF SUCCESSFULL RUNS PUT INTO FILES
OF FORM:

REFLUX2 - 20Ky - 5Km - *.res AND:
REFLUX1 - 20Ky - 5Km - *.res

IN: /home/bilbo/grice/tparun2 + tparun,
RESPECTIVELY.

NEW RUN: REFLUX2 - SAME AS ABOVE BUT
RUN FOR 100,000 YRS; ELIMINATE DOSE @ 20 Km.

NOTE - FOR RUNS DISCUSSED ON THIS +
PREVIOUS PAGE:

Fmolt Factor = CONSTANT = 1.0
Fox Factor = CONSTANT = 0.05
Sub Run Wet = CONSTANT = 0.5

RUN ON SISYPHUS MR

IN: /sisyphus/home/bilbo/grice/tpatester

10-15-97
MR

NOTE - 10,000 YR REFLUX 2 RUN STARTED YESTERDAY DID
NOT WRITE TO MOST *.res FILES. RUNNING IT
AGAIN.



10-16-97
MR

NEW RUN - REFLUX1, 100,000 YR @ 20Km
IN: /home/bilbo/grice/tparun

DONE

10-17-97
MR

COMPLETED RUN WITH ALL VARIABLES HELD
CONSTANT EXCEPT THICKNESS OF DRY-OUT
ZONE FOR REFLUX2 — PURPOSE — NRC (JOHN
POHLE etal) ASKED TO SEE EFFECT OF
REFLUX PARAMETERS ON AMOUNT OF WATER
PASSING THROUGH REPOSITORY HORIZON.
IN:
/home/bilbo/grice/rflx-vs-div

FILES NAMED: reflux2-period-*

NOTE - MISNAMED - SHOULD BE CALLED THICKNESS

RUNNING NEW TPA RUN ON SISYPHUS. SAME AS ABOVE EXCEPT
ALL VARIABLES HELD CONSTANT EXCEPT PERIOD FOR
REFLUX 2. IN:
/home/bilbo/grice/rflx-vs-div

10/20/97
MR

100,000 YEAR RUNS @ 20Km DONE FOR REFLUX1 +
REFLUX 2. REFLUX2 OUTPUT IN:
/home/bilbo/grice/tpatester. FILES CALLED:
reflux2-100Ky-20Km-*.res.

NAME CHANGE: RUN FOR REFLUX2 WHERE ALL
VARIABLES HELD CONSTANT — OUTPUT NOW
CALLED: MR EXCEPT THICKNESS
reflux2-THICKNESS-*.res, etc

OUTPUT GIVING AMOUNT OF FLUID PASSING THROUGH REPOSITORY FOR REFLUX2 RUN

RUN WHERE ALL HELD CONSTANT EXCEPT PERIOD
reflux2-PERIOD-*.res

IN: /home/bilbo/grice/rflx-vs-div

OUTPUT GIVING VALUES OF 'avdivart' FROM infilper.res IN raw3.txt. MR 10-20-97

10/26/97
MR

- NEW TPA CODE SENSITIVITY RUN -
ALL VARIABLES HELD CONSTANT EXCEPT
LOSSD FOR REFLUX2. IN:
/home/bilbo/grice/rflx-vs-div

10-26-97
MR

Re: RUN WITH ONLY LOSSD VARYING (DRY-OUT-ZONE LOSS).
RUN COMPLETED. OUTPUT SAVED AS:
reflux2-lossd-*.res IN:
/home/bilbo/grice/rflx-vs-div

NOW RUNS TARTED - REFLUX1 WITH ONLY
LENGTH OF REFLUX ZONE VARYING, IN:
/home/bilbo/grice/tparun

"avdivert" VALUES FROM infilper.res IN
FILE raw4.txt.

10-22-97
MR

RUN WITH ONLY LOSSI VARYING (INFILTRATION LOSS) COMPLETED
OUTPUT SAVED AS:
reflux2-lossi-*.res IN:
/home/bilbo/grice/rflx-vs-div. 'avdivert' VALUES
FROM infilper.res IN RAW5.txt.

10-27-97
MR

REFLUX1 RUNS - OUTPUT IN:
~~home/sa~~ MR /home/bilbo/grice/tparun

RUN FOR 20,000 YRS, OUTPUT @ 5 KM DOWN GRADIENT:
"reflux1-20ky-5km-*.res"

100,000 YRS, 20 KM:
"reflux1-100ky-20km-*.res"

RUNS VARYING ONLY ONE REFLUX PARAMETER AT A TIME:

VARYING ONLY LENGTH - ALL OTHER TPA CODE PARAMETERS = CONSTANT:
"reflux1-length-*.res", raw6.txt



10-27-97
MR

RUN VARYING ONLY PERCHED BUCKET VOLUME:
"reflux1-bucket-*.res", raw7.txt

RUN VARYING ONLY MAXIMUM FLUX:
"reflux1-flux-*.res", raw8.txt

REFLUX2 RUNS - OUTPUT IN:
/home/bilbo/grice/tparun2 AND:
/home/bilbo/grice/rflx-vs-div
NOTE - ALL OUTPUT NOW IN DIRECTORY ...tparun2.

OUTPUT IN ...tparun2:

RUN FOR 20,000 YRS, 5 KM:
reflux2-20ky-5km-*.res
RUN FOR 10,000 YRS, 5 KM:
reflux2-10ky-5km-*.res
RUN FOR 100,000 YRS, 20 KM:
reflux2-100ky-20km-*.res

RUN WHERE ONLY THICKNESS VARIED - ALL OTHER
PARAMETERS HELD CONSTANT:
reflux2-thickness-*.res
RUN WHERE ONLY PERIOD VARIED:
reflux2-period-*.res
RUN WHERE ONLY LOSS-DRYOUT ZONE VARIED:
reflux2-lossd-*.res
RUN WHERE ONLY LOSS-INFILTRATION VARIED:
reflux2-lossi-*.res

MR
10-27-97

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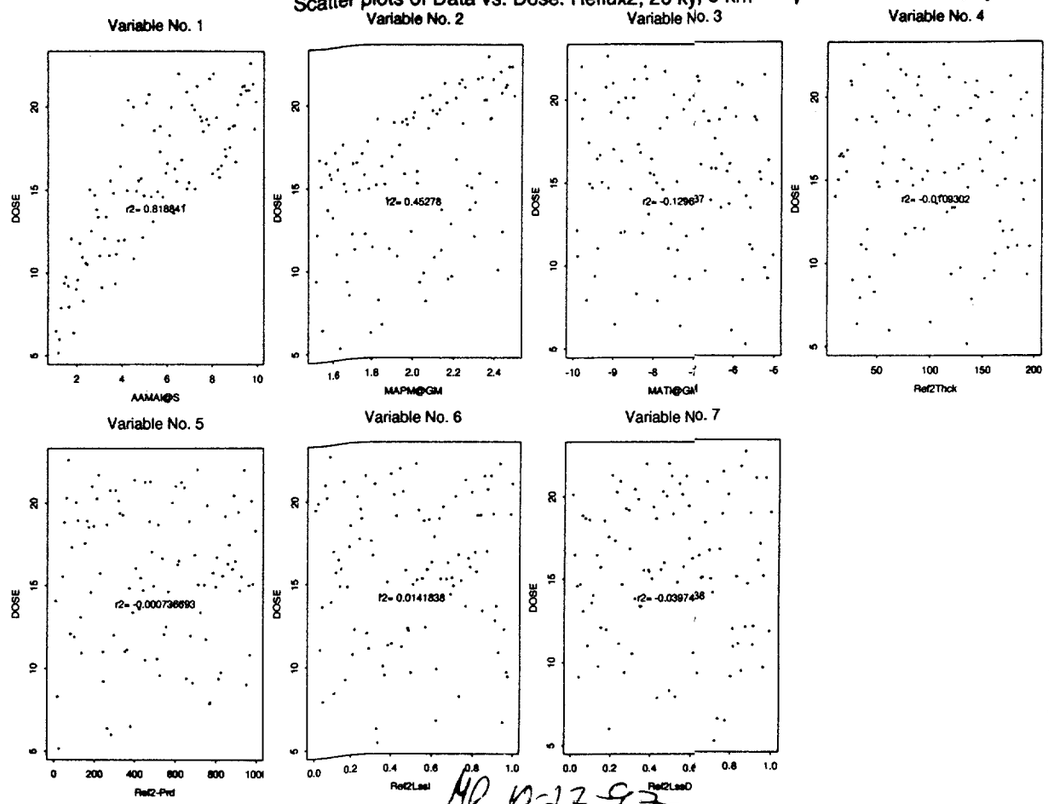
MR

THE PLOT BELOW, AND THE PLOTS ON THE FOLLOWING PAGES ARE RESULTS OF TPA CODE SENSITIVITY RUNS. THE RESULTS OF THE RUNS ARE IN THE DIRECTORIES SPECIFIED ON PAGES 20 + 21.

THESE RESULTS WERE PLOTTED USING Splus.

MR 10-27-97

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REFLUX2, 20Ky, 5Km

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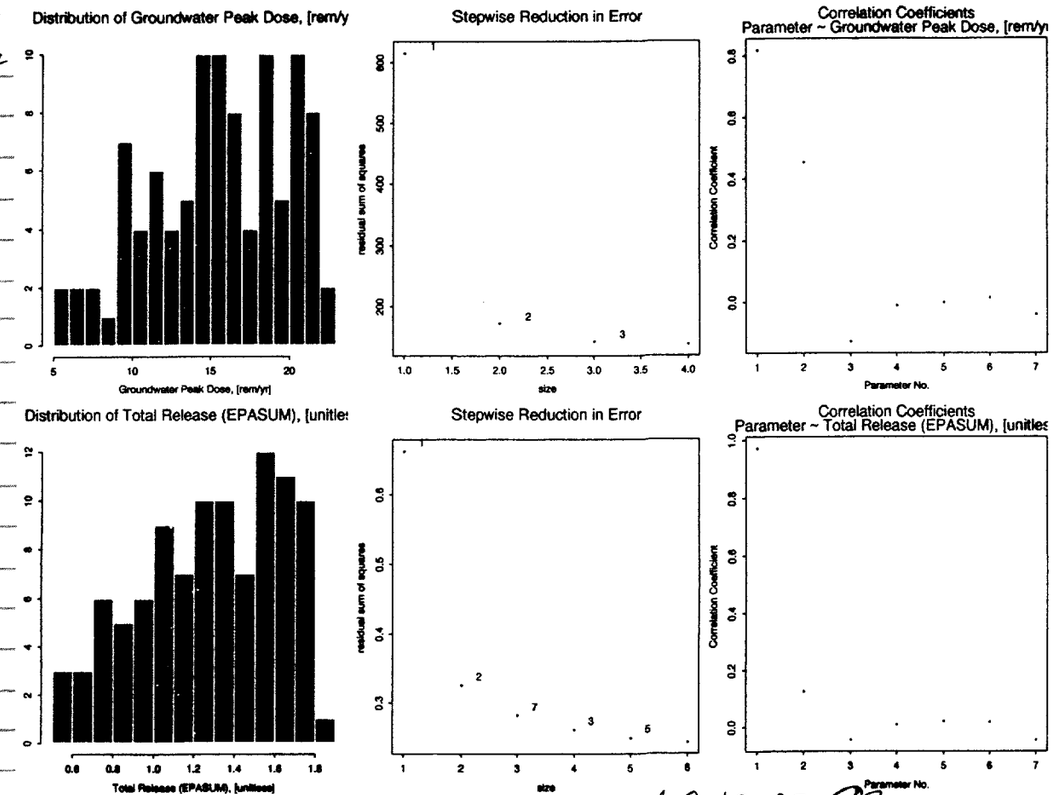
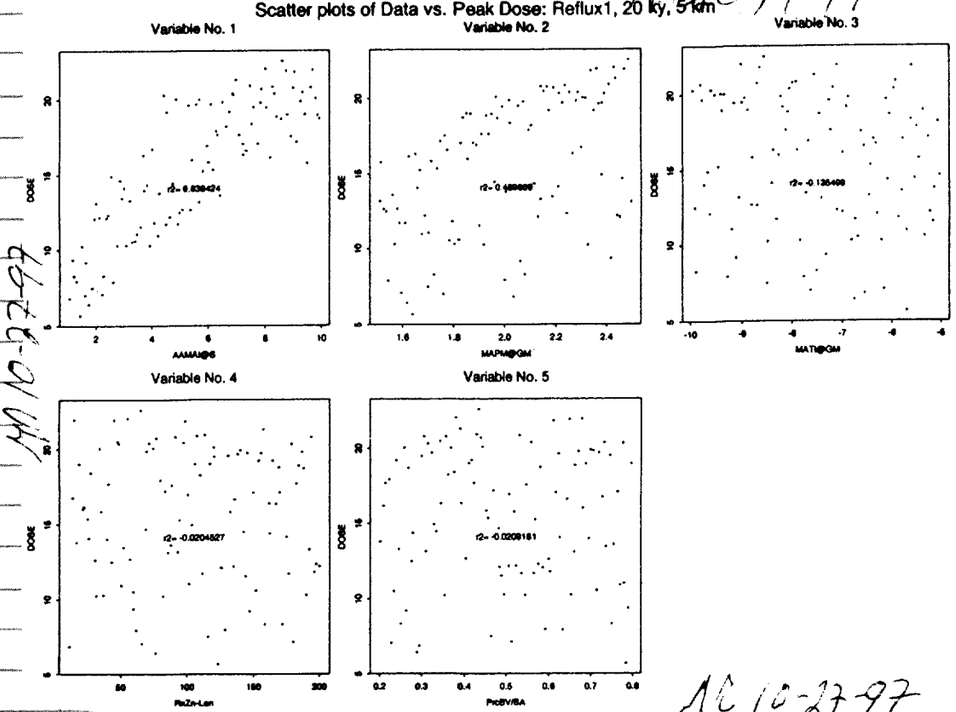
MR




MR 10-27-97

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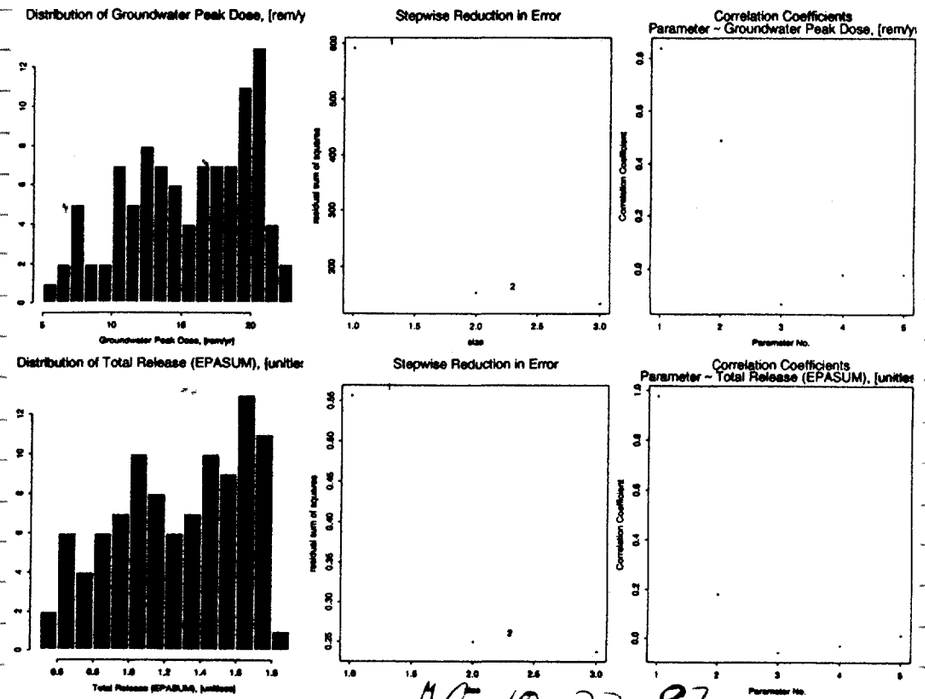
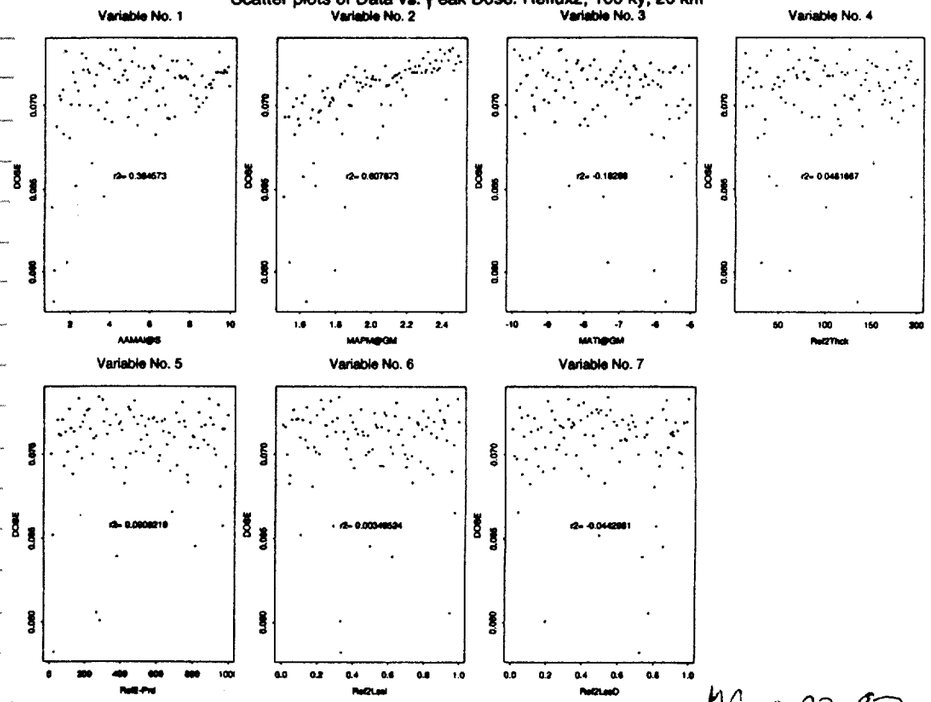
MR 10-97-27
Reflux1, 20Kg, 6Km




MR 10-27-97

Scatter plots of Data vs. Peak Dose: Reflux2, 100 ky, 20 km

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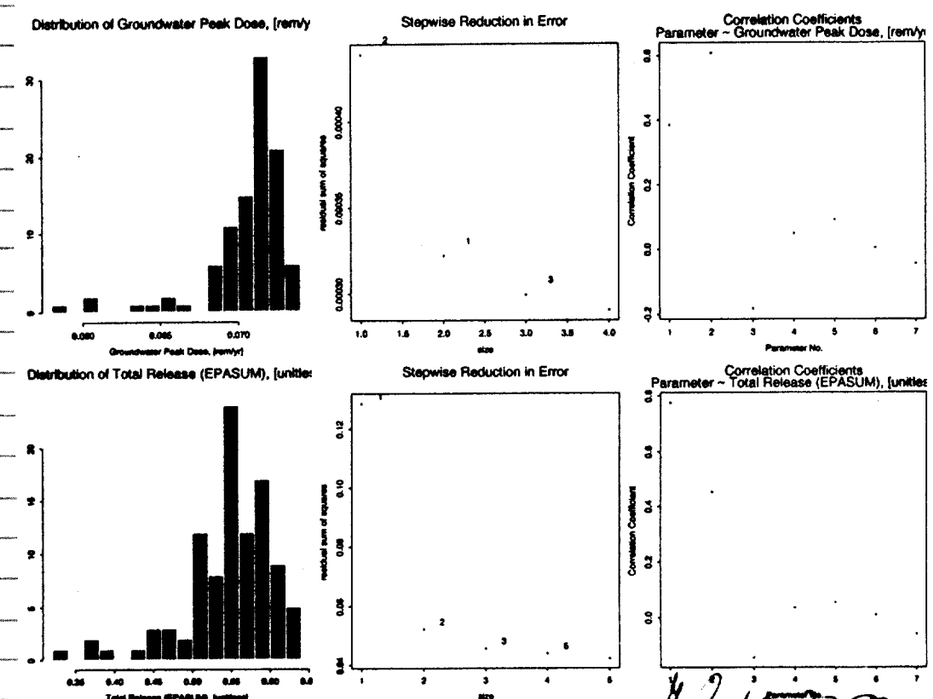
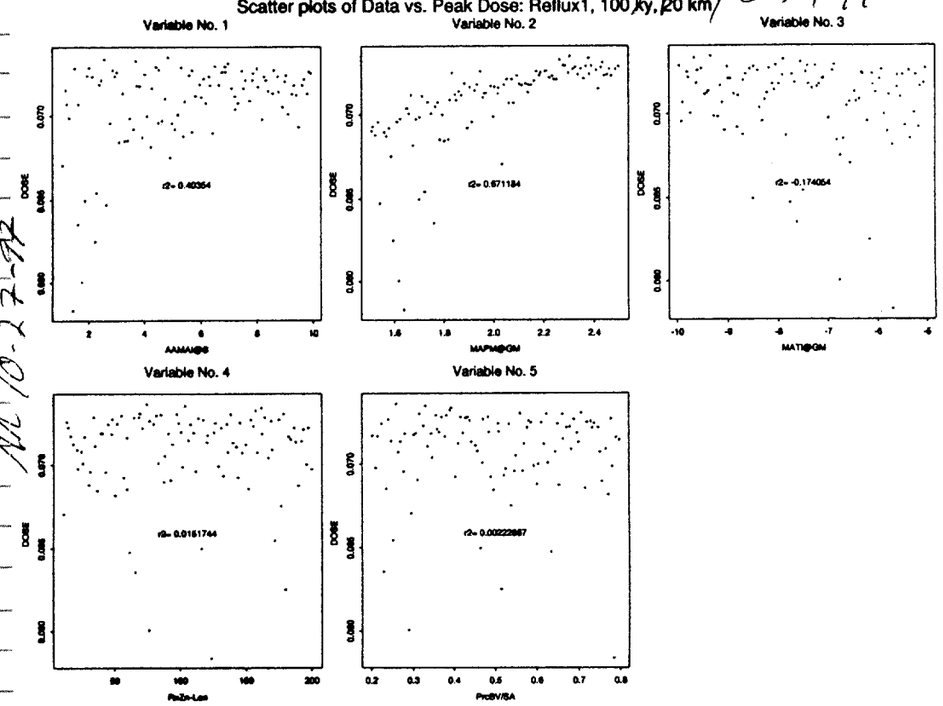
Reflux2, 100Ky, 20Km MR 10-27-97




MR 10-27-97

Scatter plots of Data vs. Peak Dose: Reflux1, 100 ky, 20 km

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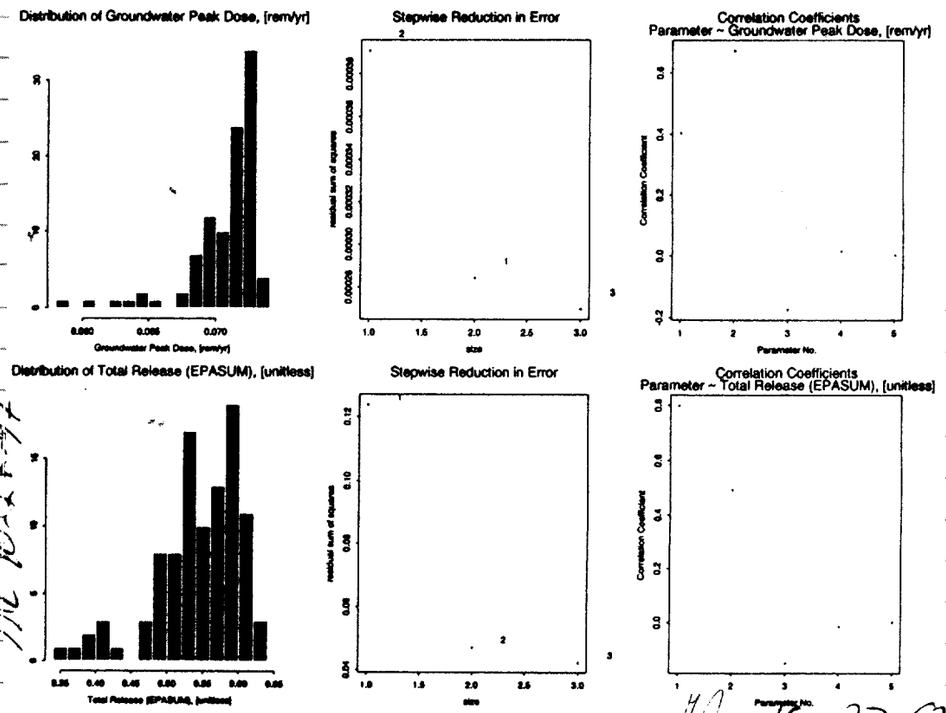
Reflux2, 100ky, 20km MR 10-27-97

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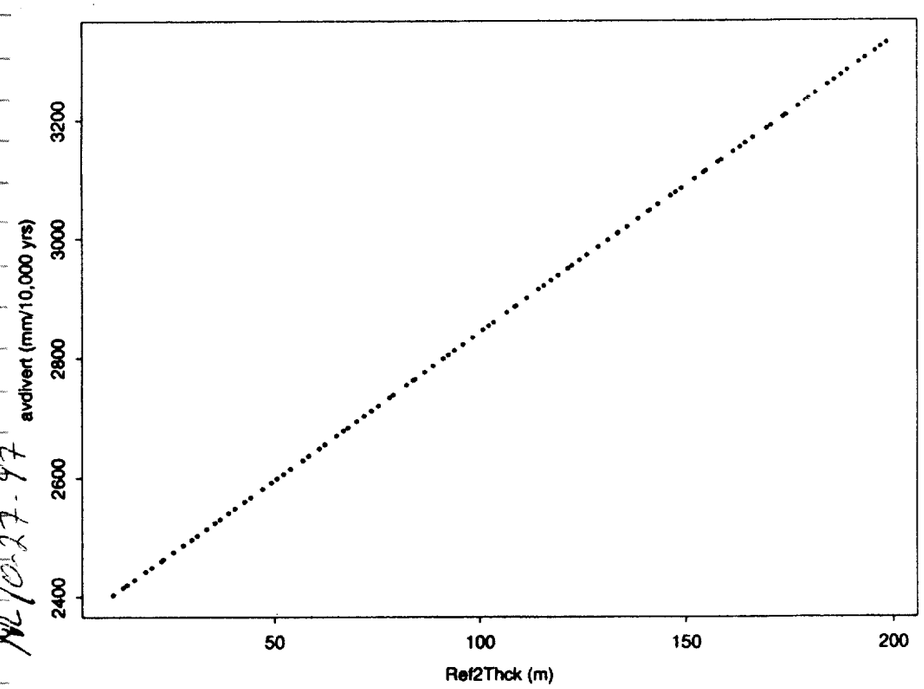
Effect of Reflux2 parameter 'Ref2Thck' on avdivert

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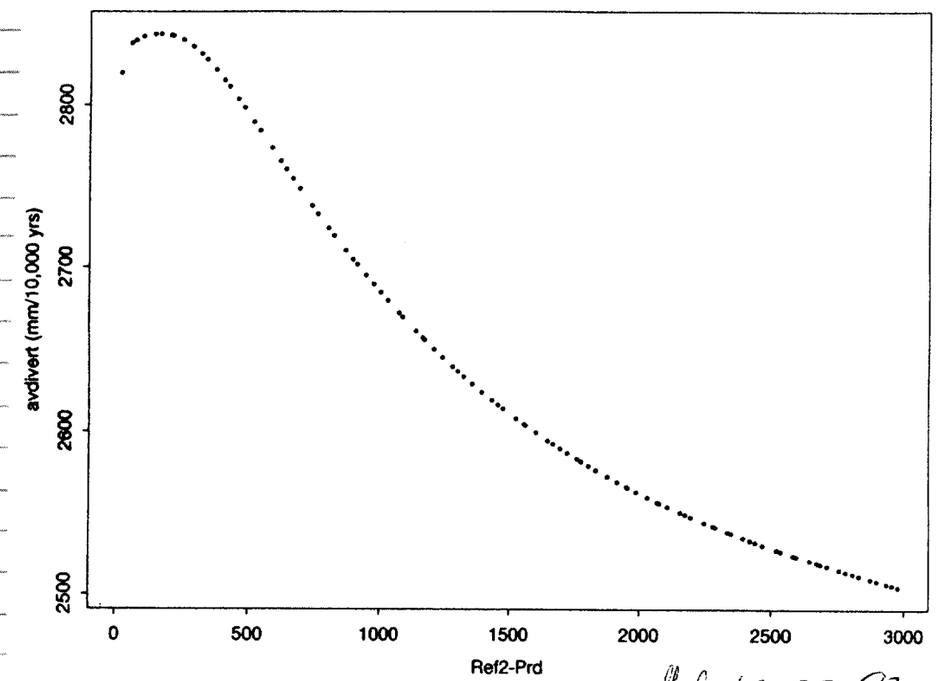
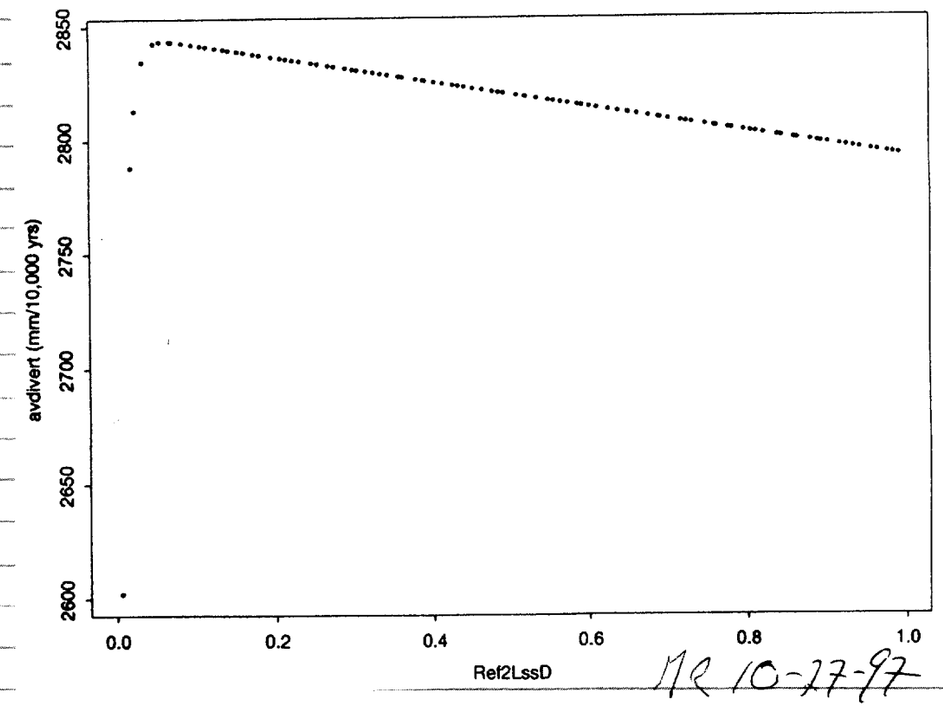
Effect of Reflux2 parameter 'Ref2-Prd' on avdivert




MR 10-27-97

Effect of Reflux2 parameter 'Ref2LssD' on avdivert

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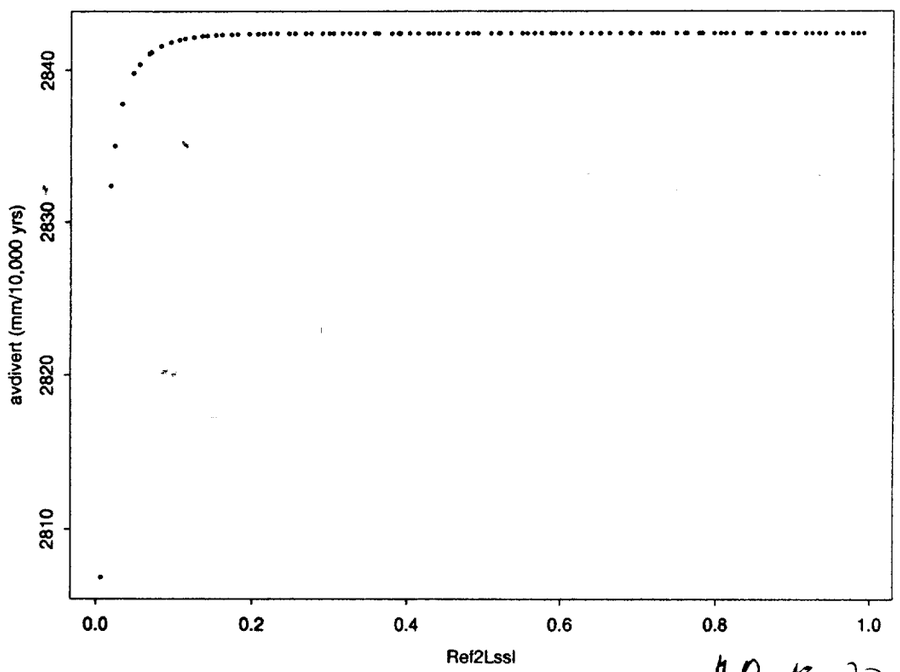
Effect of Reflux2 parameter 'Ref2Lssl' on avdivert

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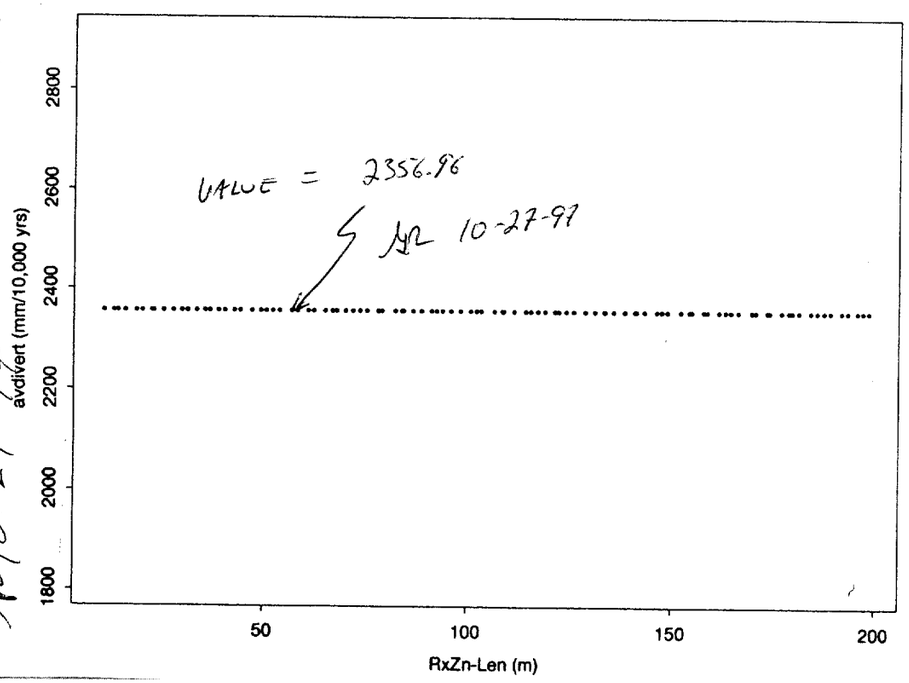
Effect of Reflux1 parameter 'RxZn-Len' on avdivert




VALUE = 2356.96
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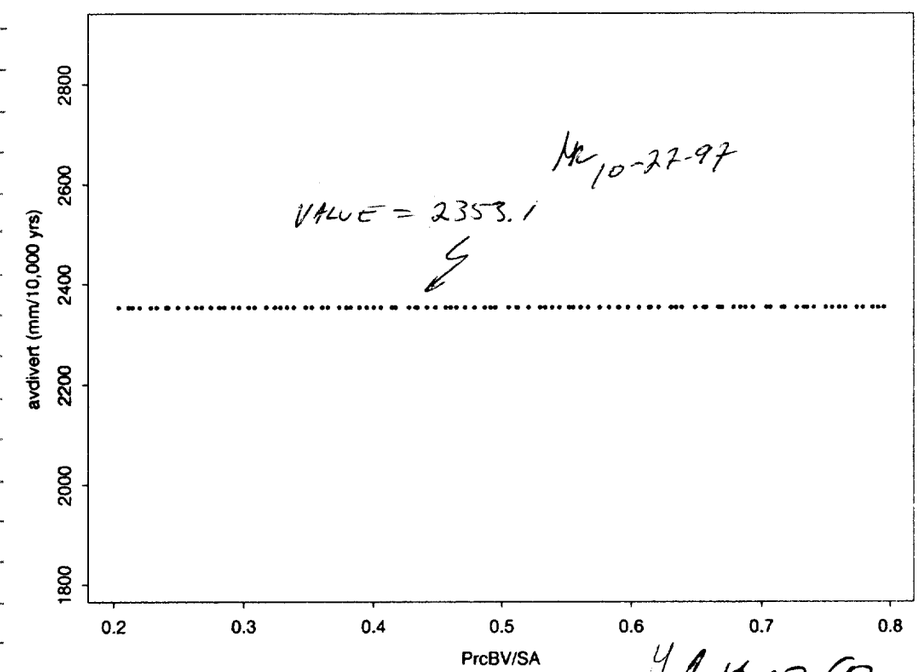
Effect of Reflux1 parameter 'PrcBV/SA' on avdivert




MR 10-27-97
VALUE = 2353.1

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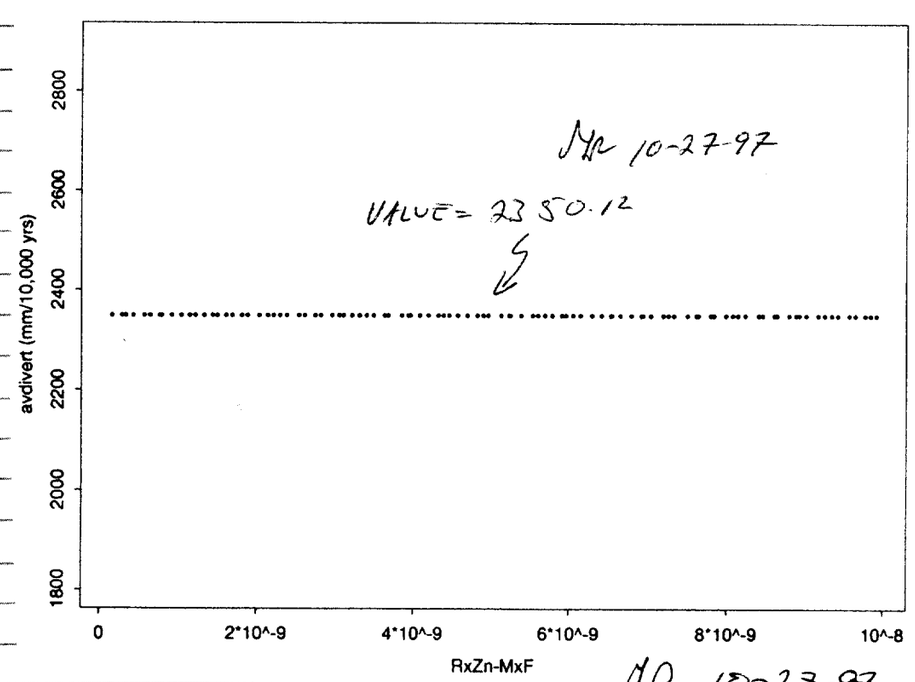
Effect of Reflux1 parameter 'RxZn-MxF' on avdivert




MR 10-27-97
VALUE = 2350.12

MR 10-27-97

11-12-97 RUNNING THE TPA CODE WITH TEMPERATURE-HUMIDITY TABLES GENERATED BY METRA.

3 METRA RUNS WERE PERFORMED:

"1.0-old.dat", 5.5-old-1.dat", AND "10.0-old-1.dat"

THESE RUNS IN: /home/bilbo/grice/3d/oldbase

THE TEMPERATURE & HUMIDITY OUTPUT PRODUCED BY METRA WAS CONVERTED TO THE FORM REQUIRED BY THE TPA CODE USING THE FORTRAN PROGRAM "tmp-rh-1.f" - THIS IS A SLIGHT MODIFICATION OF A CODE WRITTEN BY RUI CHEN.

FORTRAN CODE, MR 11-12-97

THE METRA RESULTS, AND TRANSFORMED OUTPUT ARE IN: /home/bilbo/grice/testcode

THE OUTPUT IN THE FORME REQUIRED BY THE TPA CODE IS:

"1-old-t-rh", "5.5-old-t-rh", AND "10-old-t-rh"

THE TPA RUNS THEMSELVES WERE DONE IN: /home/bilbo/grice/tparun

THE OUTPUT IS IN THE FILES

*-old-t-rh-gwpkdos
*-old-t-rh-npkdoset
*-old-t-rh-rel gwgs
*-old-t-rh-wpsfail
*-old-t-rh-cumrel

MR 2-18-98



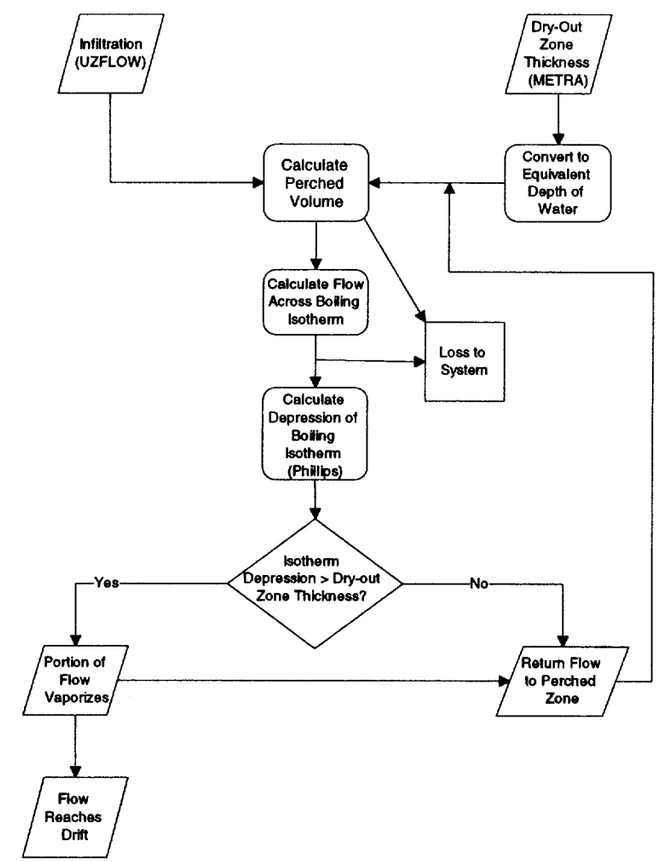
2-18-98 MR

NEW REFLUX SUBROUTINE TO BE INCORPORATED INTO NEXT VERSION OF TPA CODE. THIS IS MEANT TO REPLACE REFLUX2 AND REFLUX1 MODULES.

FLOWCHART OF NEW REFLUX MODULE. THIS IS FOLLOWED BY BOTH THE FORTRAN CODE AND THE EXCEL WORKSHEET PROVIDED ON THE PROCEEDING PAGES.

MR 2-18-98

Reflux Calculation
for one Time Step




MR 2-18-98

2-20-98
MR

REFLUX CODE - VERSION OF 2-18-98

MR 2-20-98

In: /home/bi/bo/gsice/refluxcode/reflux1_98.f

```
      PROGRAM REFLUX1_98
*
* By GRice January - February, 1998
*

*
* NOTE: this is a stand-alone program. Thus, it uses files and
* contains subroutines that will not be included in the final version.
* The final version will be a subroutine of the TPA code.
*

*****************************************************************
*****************************************************************
*                                                               *
* The OUTPUT of this program is 'reachDrift': the amount of water *
* that reaches the drift each year. The program reads two inputs: *
* infiltration and dry-out zone thickness as they vary with time. *
*                                                               *
*****************************************************************
*****************************************************************

      REAL Qm3PerYrinSA(100000), SAarea, thickness(100000)
      REAL interpQm3PerYrinSA(100000), interpThick(100000)
      INTEGER ntim,  nthick, iSA, timestep(100000), tim(100000)
      INTEGER interp_tim(100000)
      REAL MPrs_TSw, initSat, residSat
      REAL equivThick(100000), perchedVol(100000)
      REAL reachDrift(100000), loss(100000)

*
* Parameters:
*
*       cellLength - length of unit cell holding one waste package. Units - m.
*       cellWidth - width of unit cell holding one waste package. Units - m.
*       delEqTh - change in equivThick each year. Units - m.
*       delT - Thermal gradient in vicinity of boiling isotherm. CNWRA
*           experiment (Green et al.) indicated value of ~ 700. Units - none.
*       depress - distance boiling isotherm depressed by flow of water. Units - m
*       equivThick - Water equivalent of interpThick. Units - m.
*       h - enthalpy of phase change. Units - J/kg
*       initSat - initial satoration of TSW matrix.  Units - none
*       interpQm3PerYrinSA - Interpolated values of Qm3PerYrinSA created by interpolation
*           subroutine (maplist). Units - m^3/yr
*       interp_tim - array in which times go from 1 to end (e.g., 10000 years) in increments
*           one year. Created to allow interpolater (subroutine maplist) to create
*           interpolated values of infiltration (interpQm3PerYrinSA). Units - none
*       interpThick - Interpolated values of thickness created by interpolation
*           subroutine (maplist). Units - m
*       iSA - subarea (SA) number currently being evaluated. Passed from main.
*       kRock - Thermal conductivity of rock. Units - W/m-K
*       MPrs_TSw - matrix porosity of repository horizon - Topopah Springs tuff (TSw).
*           Units - none.
*       n2 - number of years for which interpolated values of Qm3PerYrinSA
*           and dry-out zone thickness (interpQm3PerYrinSA and interp_thick) will
*           be produced. Number of years in interp_tim.
*       nthick - number of values in table that gives thickness of dry-out zone vs time
*       ntim - number of times in ntim array. Passed from main.
*       perchedVol - Volume of water perched above dry-out zone
*           per unit cell (waste package). Units  - m^3.
*       Q - Steady flowrate, a function of perched volume. Flow that crosses boiling
*          isotherm. Units - m^3/s
*       Qm3PerYrinSA - water infiltrating from ground surface in a given year. Calculated
*           by UZFLOW and passed from main. Units - m^3/yr
*       reachDrift - amount of perched water that reaches the drift each year.
*          Units - m^3/yr.
```

MR 2-20-98

```
*       residSat - residual saturation of TSW matrix.  Units - none
*       rhoLiq - density of water at boiling isotherm. Units - kg/m^3
*       SAarea - area of subarea currently being evaluated. Passed from subroutine
*           gsarea. Units - m^2.
*       shed1Fact - fraction of perchedVol that dissappears from system each year. Mechanism
*           causing dissappearence not specified.
*       shed2Fact - fraction of 'Q' that dissappears from system each year. Mechanism
*           causing dissappearence not specified.
*       thickness - Thickness of dry-out zone above waste package. Read from file
*           'dry_thick.dat'. Units - m
*
*       tim - array containing times for which reflux is calculated. Passed from main
*           program. Units - years
*       vaporize - amount of water that crosses boiling isotherm but
*          vaporizes before reaching drift. Units - m^3/s.
*
```

MR 2-20-98



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MR

REFLUX CODE (CONT)

MR 2-20-98

```
      OPEN(12, FILE - 'out')
      OPEN(22, FILE - 'uzflow.res')
      OPEN(24, FILE - 'stop.i')
      OPEN(25, FILE - 'dry_thick.dat')

      ntim - 8
      nthick - 20
      n2 - 20

      MPrs_TSw - 0.14
      initSat - 0.90
      residSat - 0.00

*
* Subroutine to read timestep, tim, and Qm3PerYrinSA and thickness from files uzflow.res
* and dry_thick.dat. It then calls a subroutine that interpolates
* the infiltration and thickness data so that there are
* n2 years of values for infiltration and thickness.
* This subroutine also calls the subroutine that converts Qm3PerYrinSA
* from m^3/yr to m/yr.
*

      CALL INTERPOLATE (ntim, timestep, tim, Qm3PerYrinSA, n2,
     & interp_tim, interpQm3PerYrinSA, nthick, thickness,
     & interpThick, iSA)

*
* Subroutine that calculates the amount of water perched above the dry-out zone.
* The sources of this water are infiltration and water vaporized from the
* dry-out zone. Also calls subroutines that calculate losses to system and
* depression of boiling isotherm (Phillips).
*

      CALL PERCHED_VOL (n2, interpQm3PerYrinSA, interpThick,
     & MPrs_TSw, initSat, residSat, equivThick, perchedVol,
     & reachDrift, loss)

*
* Write results to file 'out'
*

      WRITE(12,101)
 101  FORMAT(1x, '  I', 3x, 'reachDrift')

      DO 20 I - 1, n2

        WRITE(12,102) I, reachDrift(I)
 102    FORMAT(1x, I3, 3x, F10.6)
```

MR 2-20-98

```
 20   CONTINUE

      CLOSE (UNIT - 12)
      CLOSE (UNIT - 22)
      CLOSE (UNIT - 24)
      CLOSE (UNIT - 25)

      STOP
      END

*****************************************************************-72
*****************************************************************-72

      SUBROUTINE INTERPOLATE (ntim, timestep, tim, Qm3PerYrinSA, n2,
     & interp_tim, interpQm3PerYrinSA, nthick, thickness,
     & interpThick, iSA)

      INTEGER ntim, nthick, n2
      REAL Qm3PerYrinSA(ntim), SAarea, thickness(nthick)
      REAL interpQm3PerYrinSA(n2), interpThick(n2)
      INTEGER interp_tim(n2), iSA, timestep(n2), tim(ntim)

*
* Subroutine to read timestep, tim, and Qm3PerYrinSA lists from data file uzflow.res
* This subroutine also calls the interpolating subroutine and the subroutine that
* converts Qm3PerYrinSA from m^3/yr tp m/yr.
*

      CALL uzflow_reader (ntim, timestep, tim, Qm3PerYrinSA,
     &      n2, interp_tim, interpQm3PerYrinSA)

*
* Subroutine that reads thickness of dry-out zone from data file. Also calls
* interpolating subroutine
*
```

MR 2-20-98

2-20-98 MR

NEW REFLUX CODE (CONT)

MR 2-20-98

```
      CALL thickness_reader ( nthick, timestep, tim, thickness,
     &     n2, interp_tim, interpThick)

      RETURN
      END

*************************************************************
*************************************************************

      SUBROUTINE uzflow_reader (ntim, timestep, tim, Qm3PerYrinSA,
     & n2, interp_tim, interpQm3PerYrinSA )

      REAL tim(ntim), Qm3PerYrinSA(ntim), interpQm3PerYrinSA(100000)
      REAL interp_tim(100000)
      INTEGER timestep(ntim), n2

 5    FORMAT(I3, X, f5.1, X, f5.4)

      DO 10 I = 1, ntim

         READ(22, 5) timestep(I), tim(I), Qm3PerYrinSA(I)

10    CONTINUE

*
* Subroutine that converts UZFLOW output from m^3/yr to m/yr.
*

      CALL convertUZ (iSA, ntim, Qm3PerYrinSA)
```

MR 2-20-98

```
* Create interp_tim array with n2 years.
*
      DO 20 I = 1, n2

        interp_tim(I) = I

20    Continue

*
* CALL subroutine to interpolate values of Qm3PerYrinSA for n2 years.
* This subroutine provided by Sitakanta Mohanty.
*

      CALL maplist (ntim, tim, Qm3PerYrinSA,
     &    n2, interp_tim, interpQm3PerYrinSA)

      RETURN
      END

*************************************************************
*************************************************************

      SUBROUTINE thickness_reader ( nthick, timestep, tim, thickness,
     & n2, interp_tim, interpThick )

      INTEGER  nthick, timestep(nthick), n2
      REAL tim( nthick), thickness(nthick),
     & interpThick(100000)
      REAL interp_tim(100000)

 5    FORMAT(I3, f7.1, f7.1)

      DO 10 I = 1,  nthick

         READ(25, 5) timestep(I), tim(I), thickness(I)

10    CONTINUE

*
* Create interp_tim array with n2 years.
*
      DO 20 I = 1, n2

        interp_tim(I) = I

20    Continue

*
* CALL subroutine to interpolate values of thickness for n2 years.
* This subroutine provided by Sitakanta Mohanty.
*
```

MR 2-20-98



2-20-98 MR

REFLUX CODE (CONT)

MR 2-20-98

```
      CALL maplist ( nthick, tim, thickness,
     &    n2, interp_tim, interpThick)

      RETURN
      END

c-----------------------------------------------------------------------
      subroutine maplist(n1, x1, y1, n2, x2, y2)
c-----------------------------------------------------------------------

c map data in first list into second list
c given the first set of {x,y}, and the second set of {x}, find the
c second set of {y}
```

MR 2-20-98

```
c
c n1  = input, integer,  dimesion of first array lists
c x1[n1] = input, double precision,  array of x-values in first list
c y1[n1] = input, double precision,  array of y-values in first list
c n2  = input, integer,  dimesion of second array lists
c x2[n2] = input, double precision,  array of x-values in second list
c y2[n2] = output, double precision,  array of y-values in second list
c          values of y2 based on linear interpolation to of first list
c
*      implicit double precision (a-h,o-z)

      dimension x1(n1), y1(n1)
      dimension x2(n2), y2(n2)

      external ainterl

      if( n1 .le. 0 ) then
        print *, ' '
        print *, ' ***>>> Error in maplist <<<*** '
        print *, '     n1 .le. 0 '
        print *, ' n1 = ', n1
        print *, ' x1 = ', x1
        print *, ' y1 = ', y1
        print *, ' n2 = ', n2
        print *, ' x2 = ', x2
        print *, ' y2 = ', y2
        INCLUDE 'stop.i'
      elseif( n2 .le. 0 ) then
        print *, ' '
        print *, ' ***>>> Error in maplist <<<*** '
        print *, '     n2 .le. 0 '
        print *, ' n1 = ', n1
        print *, ' x1 = ', x1
        print *, ' y1 = ', y1
        print *, ' n2 = ', n2
        print *, ' x2 = ', x2
        print *, ' y2 = ', y2
        INCLUDE 'stop.i'
      elseif( n1 .eq. 1 ) then
        do k = 1, n2
          y2(k) = y1(1)
        enddo
      else
        do k = 1, n2
         y2(k) = ainterl( n1, x1, y1, x2(k) )
        enddo
      endif

      return
      end

c-----------------------------------------------------------------------
      function ainterl( n, t, v, tin )
c-----------------------------------------------------------------------

c LINEAR interpolation in list of {time, value} data
c to find value at given time.
c
c n     = input, integer, length of array values
c t[n]  = input, double precision, array of times,
c                 assumed to be in ascending order
c v[n]  = input, double precision, array of values
c tin   = input, double precision, time at which interpolated
c                 value of "v" is requested
c ainterl = output, double precision, interpolated value
c                 if tin < t(1), then ainterl = v(1)
```

MR 2-20-98

MR 2-20-98

2-20-98 ML

REFLUX CODE (CONT)

ML 2-20-98

```
c                 if tin > t(n), then ainterl = v(n)
c
*      implicit double precision (a-h,o-z)
      dimension t(n)
      dimension v(n)

      if( n .le. 0 ) then
        print *, ' '
        print *, ' ***>>> Error in ainterl <<<*** '
        print *, ' n = ', n
        INCLUDE 'stop.i'
      elseif( n .eq. 1 ) then
        ainterl = v(1)
        return
      elseif( tin .le. t(1) ) then
        ainterl = v(1)
        return
      elseif( tin .ge. t(n) ) then
        ainterl = v(n)
        return
      else
        do k = 2, n
          if( tin .lt. t(k) ) then
            denom  =  (t(k)-t(k-1))
            if( denom .lt. 1.0d-30 ) denom = 1.0d-30
            frac = (tin - t(k-1))/ denom
            ainterl = v(k-1) +frac*(v(k)-v(k-1))
            return
          endif
        enddo
      endif
      print *, ' '
      print *, ' ***>>> Error in ainterl <<<*** '
      print *, ' should never get here '
      print *, ' n = ', n
      print *, ' tin = ', tin
      do i = 1, n
        write(*,100) i, t(i), v(i)
100     format( 'i,t,v=', 3e13.4 )
      enddo
      INCLUDE 'stop.i'
      end

*****************************************************************
*****************************************************************

      SUBROUTINE convertUZ (iSA, ntim, Qm3PerYrinSA)

      REAL SAarea, Qm3PerYrinSA(ntim)
      INTEGER iSA, ntim

      CALL gsarea (iSA, SAarea)

      DO 10 I=1, ntim

         Qm3PerYrinSA(I) = Qm3PerYrinSA(I) / SAarea

10    CONTINUE

      RETURN
      END

*****************************************************************
*****************************************************************

      SUBROUTINE gsarea (iSA, SAarea)
```

ML 2-20-98

ML 2-20-98

```
      REAL SAarea
      INTEGER iSA

      SAarea = 1.0

      RETURN
      END

*****************************************************************************-72
*****************************************************************************-72

      SUBROUTINE PERCHED_VOL (n2, interpQm3PerYrinSA,
     & interpThick, MPrs_TSw, initSat, residSat,
     & equivThick, perchedVol, reachDrift, loss)
```



2-20-98 ML

REFLUX CODE (CONT)

ML 2-20-98

```
      INTEGER n2
      REAL interpQm3PerYrinSA(n2), interpThick(n2)
      REAL perchedVol(n2), cellWidth, cellLength, cellArea
      REAL MPrs_TSw, initSat, residSat, equivThick(n2)
      REAL maxThick, delEqTh(100000), loss(100000)
      REAL reachDrift(n2)

      cellWidth = 22.0
      cellLength = 19.0
      cellArea = cellWidth * cellLength

*
* The equivalent thickness of water perched above the dry-out zone is
* a function of the maximum dry-out zone thickness. When the dry-out zone
* thickness decreases, the maximum amount (minus losses calculated below)
* derived from the dry-out zone remains perched and available to flow toward
* the drift.
*

      DO 10 I=1, n2

        IF(interpThick(I) .GT. maxThick) THEN
          maxThick = interpThick(I)
        ENDIF

        equivThick(I) = maxThick * (MPrs_TSw * (initSat
     &                    - residSat))

        IF (I .GT. 1) THEN
           delEqTh(I) = equivThick(I) - equivThick(I-1)
           IF (delEqTh(I) .LT. 0.0) THEN
              delEqTh(I) = 0.0
           ENDIF
        ENDIF

   10 CONTINUE

      DO 20 I=1, n2

*
* Calculate volume of water perched above the dry-out zone. After the
* first year, losses are subtracted from the amount perched.
*

      IF (I .EQ. 1) THEN
        perchedVol(I) = (interpQm3PerYrinSA(I)
     &                  + equivThick(I)) * cellArea
      ELSE
        CALL LOSSES (I, n2, perchedVol, interpThick, loss,
     &                  reachDrift)
```

ML 2-20-98

```
        perchedVol(I) = perchedVol(I-1) + ((interpQm3PerYrinSA(I)
     &                  + delEqTh(I)) * cellArea) - loss(I)
      ENDIF

   20 CONTINUE

      RETURN
      END

*****************************************************************************-72
*****************************************************************************-72

      SUBROUTINE LOSSES (I, n2, perchedVol, interpThick, loss,
     &                  reachdrift)

      INTEGER I, n2
      REAL perchedVol(n2), loss(n2), shed1(100000), shed2(100000)
      REAL interpThick(n2), reachDrift(n2), shed1Fact
      REAL vaporize(100000)

      shed1Fact = 0.01

*
* Shed1 is a loss to the system (mechanism undefined) that
* occurs every year.
*

      shed1(I) = perchedVol(I-1) * shed1Fact

*
* Shed2, vaporize, and reachDrift are functions of flow beyond
* the boiling isotherm (Q). No flow occurs the first year.
*
```

ML 2-20-98

2-20-98 MR

REFLUX CODE (CONCL)

MR 2-20-98

```
      shed2(1) = 0.0
      vaporize(1) = 0.0
      reachDrift(1) = 0.0

      IF(I .GT. 1)THEN

*
* Call subroutine that calculates 3D depression of boiling isotherm at
* long times with steady-state flow rate. One year assumed to be long time.
* Governing equation from O.M. Phillips, "The Infiltration of a Liquid
* Finger Down a Fracture into Superheated Rock", for CNWRA, 1994
*

        CALL PHILLIPS_3D (I, n2, interpThick, perchedVol,
     &                    reachDrift, shed1, shed2, vaporize)
      ENDIF

*
* Total amount of water lost to system:
*

      loss(I) = shed1(I) + shed2(I) + reachDrift(I)

      RETURN
      END

*****************************************************************************72
*****************************************************************************72

      SUBROUTINE PHILLIPS_3D (I, n2, interpThick, perchedVol,
     &                        reachDrift, shed1, shed2, vaporize)


      INTEGER I, n2
      REAL interpThick(n2), perchedVol(n2), reachDrift(n2),
     &     depress(100000), Q(100000), kRock, shed2Fact,
     &     shed1(n2), shed2(n2), vaporize(n2)

*
* Calculate amount of water that flows across the boiling isotherm. It
* depends on the amount of water that was perched the previous year.
*

      Q(I) = ((perchedVol(I-1)-shed1(I)) / (86400 * 365)) * 0.01

      rhoLiq = 958
      h = 2.432E+06
      kRock = 2.1
      delT = 100.0

*
* Calculate depression of boiling isotherm.
*


      depress(I) = SQRT( (rhoLiq * Q(I) * h) / (kRock * delT) )

      shed2Fact = 0.01
      shed2(I) = Q(I)*shed2Fact

*
* Calculate amount of flow (Q) that reaches the drift. Flow reaches drift
* only if the boiling isotherm is depressed more than the thickness of the
* dry-out zone. Amount of flow reaching drift is reduced by amount that
* vaporizes in transit and by an undefined loss: shed2. Shed2 (like shed1)
* represents water that leaves the system. It is lost even if no flow reaches
* the drift.
*

      IF(depress(I) .GT. interpThick(I)) THEN
        vaporize(I) = (interpThick(I)/depress(I)) * Q(I) *
        reachDrift(I) = (Q(I)- shed2(I) - vaporize(I)) * 86400 * 365
        shed2(I) = shed2(I) * 86400 * 365
      ELSE
        reachDrift(I) = 0.0
        shed2(I) = shed2(I) * 86400 * 365
      ENDIF

      RETURN
      END
```

MR 2-20-98

* SEE NOTE ON PAGE 42

MR 2-24-98



2-20-98 MR

EXCEL CODE USED TO CHECK RESULTS OF FORTRAN CODE:

MR 2-20-98

New Reflux
2/98
Incorporating Dry-out Zone Thickness and
Depression of Boiling Isotherm

| Year | Infiltration (m) | Thickness (m) | Thick Diff (m) | Max Fact |
|---|---|---|---|---|
| 1 | 0.003 | 5 | 5 | 1.00 |
| 2 | 0.003 | 10 | 5 | 1 |
| 3 | 0.003 | 100 | 90 | 1 |
| 4 | 0.004 | 80 | -20 | 0 |
| 5 | 0.005 | 60 | -20 | 0 |
| 6 | 0.004 | 20 | -40 | 0 |
| 7 | 0.003 | 2 | -18 | 0 |
| 8 | 0.003 | 2 | 0 | 0 |
| 9 | 0.003 | 2 | 0 | 0 |
| 10 | 0.003 | 2 | 0 | 0 |
| 11 | 0.003 | 2 | 0 | 0 |
| 12 | 0.003 | 2 | 0 | 0 |
| 13 | 0.0035 | 2 | 0 | 0 |
| 14 | 0.004 | 2 | 0 | 0 |
| 15 | 0.0045 | 2 | 0 | 0 |
| 16 | 0.005 | 2 | 0 | 0 |
| 17 | 0.004 | 2 | 0 | 0 |
| 18 | 0.003 | 1 | -1 | 0 |
| 19 | 0.002 | 1 | 0 | 0 |
| 20 | 0.001 | 0 | -1 | 0 |

EXCEL WORKSHEET ON WORKING DISK IN BLDG 51 IN C/JOBS/reflux/newreflux.XLS 2-98 MR

Step 1
Calculate volume of water perched above dry-out zone
This depends on infiltration and dry-out zone thickness
as well as values calculated in steps 2 and 4.

| Year | Porosity | Saturation | Add Eqv - Thick (m) | Unit Area (m^2) | Perched Vol (m^3) |
|---|---|---|---|---|---|
| 1 | 0.14 | 0.9 | 0.63 | 418 | 264.594 |
| 2 | 0.14 | 0.9 | 0.63 | 418 | 526.5159 |
| 3 | 0.14 | 0.9 | 11.34 | 418 | 5262.573 |
| 4 | 0.14 | 0.9 | 0 | 418 | 5211.098 |
| 5 | 0.14 | 0.9 | 0 | 418 | 5160.561 |
| 6 | 0.14 | 0.9 | 0 | 418 | 5110.116 |
| 7 | 0.14 | 0.9 | 0 | 418 | 5033.663 |
| 8 | 0.14 | 0.9 | 0 | 418 | 4958.55 |
| 9 | 0.14 | 0.9 | 0 | 418 | 4884.754 |
| 10 | 0.14 | 0.9 | 0 | 418 | 4812.25 |
| 11 | 0.14 | 0.9 | 0 | 418 | 4741.014 |
| 12 | 0.14 | 0.9 | 0 | 418 | 4671.023 |
| 13 | 0.14 | 0.9 | 0 | 418 | 4602.463 |
| 14 | 0.14 | 0.9 | 0 | 418 | 4535.307 |
| 15 | 0.14 | 0.9 | 0 | 418 | 4469.529 |
| 16 | 0.14 | 0.9 | 0 | 418 | 4405.106 |
| 17 | 0.14 | 0.9 | 0 | 418 | 4341.384 |
| 18 | 0.14 | 0.9 | 0 | 418 | 4267.297 |
| 19 | 0.14 | 0.9 | 0 | 418 | 4194.172 |
| 20 | 0.14 | 0.9 | 0 | 418 | 4111.126 |

MR 2-20-98

Step 2
Calculate first loss to system and volume of flow crossing
boiling isotherm

| Year | Perched Vol (m^3) | First Loss Factor | Q Factor | First Loss (m^3/yr) | Q (m^3/yr) |
|---|---|---|---|---|---|
| 1 | 264.594 | 0.01 | 0.01 | 2.64594 | 0 |
| 2 | 526.5158652 | 0.01 | 0.01 | 5.265159 | 2.619481 |
| 3 | 5262.572581 | 0.01 | 0.01 | 52.62573 | 5.212507 |
| 4 | 5211.097861 | 0.01 | 0.01 | 52.11098 | 52.09947 |
| 5 | 5160.560984 | 0.01 | 0.01 | 51.60561 | 51.58987 |
| 6 | 5110.116478 | 0.01 | 0.01 | 51.10116 | 51.08955 |

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MR

| | | | | | | |
|---|---|---|---|---|---|---|
| 7 | 5033.662598 | 0.01 | 0.01 | 50.33663 | 50.59015 | |
| 8 | 4958.550059 | 0.01 | 0.01 | 49.5855 | 49.83326 | |
| 9 | 4884.753997 | 0.01 | 0.01 | 48.84754 | 49.08965 | |
| 10 | 4812.250016 | 0.01 | 0.01 | 48.1225 | 48.35906 | |
| 11 | 4741.01419 | 0.01 | 0.01 | 47.41014 | 47.64128 | |
| 12 | 4671.023053 | 0.01 | 0.01 | 46.71023 | 46.93604 | |
| 13 | 4602.462586 | 0.01 | 0.01 | 46.02463 | 46.24313 | |
| 14 | 4535.30657 | 0.01 | 0.01 | 45.35307 | 45.56438 | |
| 15 | 4469.529292 | 0.01 | 0.01 | 44.69529 | 44.89954 | |
| 16 | 4405.105537 | 0.01 | 0.01 | 44.05106 | 44.24834 | |
| 17 | 4341.383575 | 0.01 | 0.01 | 43.41384 | 43.61054 | |
| 18 | 4267.29704 | 0.01 | 0.01 | 42.67297 | 42.9797 | |
| 19 | 4194.17211 | 0.01 | 0.01 | 41.94172 | 42.24624 | |
| 20 | 4111.126085 | 0.01 | 0.01 | 41.11126 | 41.5223 | |

MR 2-20-98

**Step 3**
**Calculate distance boiling isotherm depressed**
**(Phillip's 3-D Method)**

| Year | Q (m^3/s) | rhoLiq (kg/m^3) | h (J/kg) | Therm K Rock (W/m-K) | Delta T (K/m) | Depress (m) |
|---|---|---|---|---|---|---|
| 1 | 0 | 958 | 2.43E+06 | 2.1 | 100 | 0 |
| 2 | 8.30632E-06 | 958 | 2.43E+06 | 2.1 | 100 | 0.959973 |
| 3 | 1.65288E-07 | 958 | 2.43E+06 | 2.1 | 100 | 1.354175 |
| 4 | 1.65206E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.281227 |
| 5 | 1.6359E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.260237 |
| 6 | 1.62004E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.239529 |
| 7 | 1.6042E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.218758 |
| 8 | 1.5802E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.18708 |
| 9 | 1.55662E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.155722 |
| 10 | 1.53346E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.124683 |
| 11 | 1.51069E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.093957 |
| 12 | 1.48833E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.063543 |
| 13 | 1.46636E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.033436 |
| 14 | 1.44484E-06 | 958 | 2.43E+06 | 2.1 | 100 | 4.003726 |
| 15 | 1.42375E-06 | 958 | 2.43E+06 | 2.1 | 100 | 3.974409 |
| 16 | 1.40311E-06 | 958 | 2.43E+06 | 2.1 | 100 | 3.945482 |
| 17 | 1.38288E-06 | 958 | 2.43E+06 | 2.1 | 100 | 3.916944 |
| 18 | 1.36288E-06 | 958 | 2.43E+06 | 2.1 | 100 | 3.88851 |
| 19 | 1.33962E-06 | 958 | 2.43E+06 | 2.1 | 100 | 3.855189 |
| 20 | 1.31666E-06 | 958 | 2.43E+06 | 2.1 | 100 | 3.822014 |

MR 2-20-98

**Step 4**
**Compare dry-out zone thickness with isotherm depression. If thickness less than depression, Q (minus loss and fraction that vaporizes) reaches drift. Otherwise, Q (minus loss) returned to perched zone - added to perched volume.**

| Year | Second Loss Factor | Second Loss (m^3/yr) | Thick (m) | Depress (m) | IF - Result | Vaporize (m^3/yr) | Reach Drift (m^3/yr) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 5 | 0 | 0 | 0 | 0 |
| 2 | 0.01 | 0.026195 | 10 | 0.959973 | 0 | 0 | 0 |
| 3 | 0.01 | 0.052125 | 100 | 1.354175 | 0 | 0 | 0 |
| 4 | 0.01 | 0.520995 | 80 | 4.281227 | 0 | 0 | 0 |
| 5 | 0.01 | 0.515899 | 60 | 4.260237 | 0 | 0 | 0 |
| 6 | 0.01 | 0.510896 | 20 | 4.239529 | 0 | 0 | 0 |
| 7 | 0.01 | 0.505902 | 2 | 4.218758 | 1 | 23.98344 | 26.10082 |
| 8 | 0.01 | 0.498333 | 2 | 4.18708 | 1 | 23.80335 | 25.53158 |
| 9 | 0.01 | 0.490896 | 2 | 4.155722 | 1 | 23.62506 | 24.97367 |
| 10 | 0.01 | 0.483591 | 2 | 4.124683 | 1 | 23.44862 | 24.42685 |
| 11 | 0.01 | 0.476413 | 2 | 4.093957 | 1 | 23.27395 | 23.89091 |
| 12 | 0.01 | 0.46936 | 2 | 4.063543 | 1 | 23.10105 | 23.36563 |
| 13 | 0.01 | 0.462431 | 2 | 4.033436 | 1 | 22.92989 | 22.8508 |
| 14 | 0.01 | 0.455644 | 2 | 4.003726 | 1 | 22.76099 | 22.34775 |
| 15 | 0.01 | 0.448995 | 2 | 3.974409 | 1 | 22.59432 | 21.85622 |
| 16 | 0.01 | 0.442483 | 2 | 3.945482 | 1 | 22.42988 | 21.37598 |
| 17 | 0.01 | 0.436105 | 2 | 3.916944 | 1 | 22.26764 | 20.9068 |
| 18 | 0.01 | 0.429797 | 1 | 3.88851 | 1 | 11.053 | 31.4969 |
| 19 | 0.01 | 0.422462 | 1 | 3.855189 | 1 | 10.95828 | 30.8655 |
| 20 | 0.01 | 0.415223 | 0 | 3.822014 | 1 | 0 | 41.10708 |

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SEE NOTE ON PAGE 42
MR 2-24-98

EXCEL RESULTS - COMPARE FORTRAN RESULTS ON FOLLOWING PAGE.

MR 2-20-98



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MR

| | | | |
|---|---|---|---|
| 1 | 1.0 | 0.003 |
| 2 | 3.0 | 0.003 |
| 3 | 5.0 | 0.005 |
| 4 | 7.0 | 0.003 |
| 5 | 12.0 | 0.003 |
| 6 | 16.0 | 0.005 |
| 7 | 18.0 | 0.003 |
| 8 | 20.0 | 0.001 |

FORTRAN CODE INFILTRATION INPUT

MR 2-20-98

MR 2-20-98

| | | |
|---|---|---|
| 1 | 1.0 | 5.0 |
| 2 | 2.0 | 10.0 |
| 3 | 3.0 | 100.0 |
| 4 | 4.0 | 80.0 |
| 5 | 5.0 | 60.0 |
| 6 | 6.0 | 20. |
| 7 | 7.0 | 2. |
| 8 | 8.0 | 2.0 |
| 9 | 9.0 | 2.0 |
| 10 | 10.0 | 2.0 |
| 11 | 11.0 | 2.0 |
| 12 | 12.0 | 2.0 |
| 13 | 13.0 | 2.0 |
| 14 | 14.0 | 2.0 |
| 15 | 15.0 | 2.0 |
| 16 | 16.0 | 2.0 |
| 17 | 17.0 | 2.0 |
| 18 | 18.0 | 1.0 |
| 19 | 19.0 | 1.0 |
| 20 | 20.0 | 0.0 |

FORTRAN CODE THICKNESS INPUT

MR 2-20-98

| | reachDrift |
|---|---|
| 1 | 0.000000 |
| 2 | 0.000000 |
| 3 | 0.000000 |
| 4 | 0.000000 |
| 5 | 0.000000 |
| 6 | 0.000000 |
| 7 | 26.100811 |
| 8 | 25.531572 |
| 9 | 24.973656 |
| 10 | 24.426840 |
| 11 | 23.890903 |
| 12 | 23.365627 |
| 13 | 22.850798 |
| 14 | 22.347736 |
| 15 | 21.856205 |
| 16 | 21.375971 |
| 17 | 20.906790 |
| 18 | 31.496881 |
| 19 | 30.865484 |
| 20 | 41.107059 |

FORTRAN CODE RESULTS. COMPARE W/EXCEL RESULTS ON PREVIOUS PAGE

UNITS = $M^3/YR$

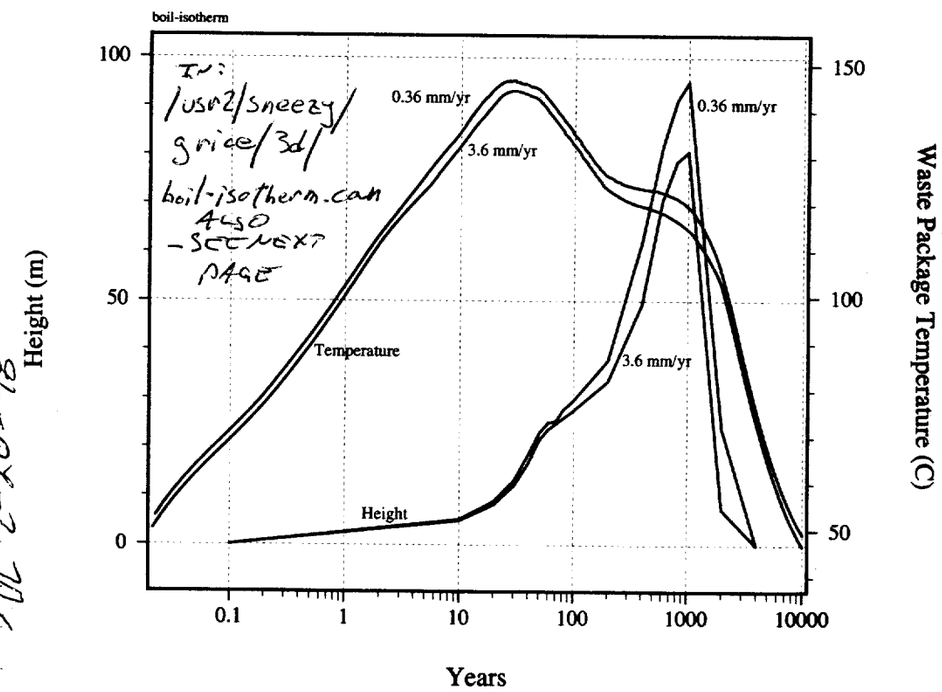
MR 2-20-98

MR 2-20-98

METRA OUTPUT - THICKNESS OF DRY-OUT ZONE

MR 2-20-98

## Height of Boiling Isotherm (100 C) Above Waste Package




MR 2-20-98

2-20-98

RESULTS OF METEA RUNS

ML 2-20-98

Height of boiling isotherm above waste package for 3.6 mm/yr and 0.36 mm/yr infiltration rates. Power = 83 kW/acre. Data from runs "3d-3.6-3.dat" and "3d-0.36.dat". Top of waste depth = 343.4 m.

| Time | 3.6 | 0.36 |
|---|---|---|
| .1 | 0 | 0 |
| 10 | 4.9 | 5.2 |
| 20 | 8.2 | 8.9 |
| 30 | 12.1 | 13.2 |
| 40 | 16.7 | 18.5 |
| 50 | 21.5 | 23 |
| 60 | 23.7 | 25.1 |
| 70 | 24.9 | 25.4 |
| 80 | 25.9 | 27.6 |
| 100 | 27.6 | 29.7 |
| 200 | 33.6 | 37.9 |
| 400 | 49.5 | 62.3 |
| 600 | 70.7 | 81.7 |
| 800 | 78.7 | 91.4 |
| 1000 | 80.7 | 95.1 |
| 2000 | 7.3 | 23.9 |
| 4000 | 0 | 0 |

IN:
/usr2/sneezy/grice/3d/
boil-isotherm

ML 2-20-98

3-13-98
ML

2-24-98 NOTE:
VAPORIZATION SHOULD BE CALCULATED AFTER THE LOSS (SHED2) IS DEDUCTED FROM THE FLOW (Q). OTHERWISE, THE SUBSEQUENT VALUE (REACHDRIFT) MAY BECOME NEGATIVE. (ESPECIALLY WHEN DEPRESS ≈ THICKNESS)

THE FORTRAN CODE HAS BEEN CORRECTED BY ALTERING THE LINE TO READ:

" VAPORIZE(I) = (INTERATHICK(I)/DEPRESS(I))
* (Q(I) - SHED2(I)) "

THE EXCEL CODE HAS ALSO BEEN CORRECTED

3-13-98
ML

MODIFICATION TO NEW REFLUX CODE (CALLING IT REFLUX3) - MASS BALANCE SUBROUTINE:



MASS BALANCE SUBROUTINE ADDED TO REFLUX3 CODE:

ML 3-13-98

```
*************************************************************************72
*************************************************************************72
      SUBROUTINE MASS_BALANCE (n2, interpQm3PerYrinSA, equivThick,
     &                         cellArea, perchedVol, reachDrift,
     &                         loss, massBal)

      INTEGER I, n2
      REAL interpQm3PerYrinSA(n2), equivThick(n2), cellArea
      REAL perchedVol(n2), reachDrift(n2), loss(n2)
      REAL totIn(100000), totOut(100000), delStore(100000)
      REAL delEqTh(100000), massBal(n2), relError(100000)

*
* Summ mass entering system
*

      totIn(1) = (interpQm3PerYrinSA(1) + equivThick(1))*cellArea

      DO 10 I=2, n2
        delEqTh(I) = equivThick(I) - equivThick(I-1)

        IF (delEqTh(I) .LT. 0.0) THEN
           delEqTh(I) = 0.0
        ENDIF

        totIn(I) = (interpQm3PerYrinSA(I) + delEqTH(I))*cellArea
     &             + totIn(I-1)
   10 CONTINUE

*
* Sum mass leaving system
*

      totOut(1) = loss(1)

      DO 20 I=2, n2
        totOut(I) = loss(I) + totOut(I-1)
   20 CONTINUE

*
* totIn - totOut should equal perchedVol
*

      DO 30 I=1, n2
        delStore(I) = totIn(I) - totOut(I)
        massBal(I) = delStore(I) - perchedVol(I)
        relError(I) = massBal(I)/((totIn(I)+totOut(I))/2)
   30 CONTINUE

      WRITE(21, 101)
  101 FORMAT(1x, 4x, 'I', 15x, 'totIn', 12x, 'totOut', 10x, 'perch',
     &       15x, 'massBal', 8x, 'relError')

      DO 40 I=1, n2
        WRITE(21, 102) I, totIn(I), totOut(I), perchedVol(I),
     &                 massBal(I), relError(I)
  102   FORMAT(1x, I5, 3x, 5(6x, F12.6))
   40 CONTINUE

      RETURN
      END

*************************************************************************72
*************************************************************************72
```

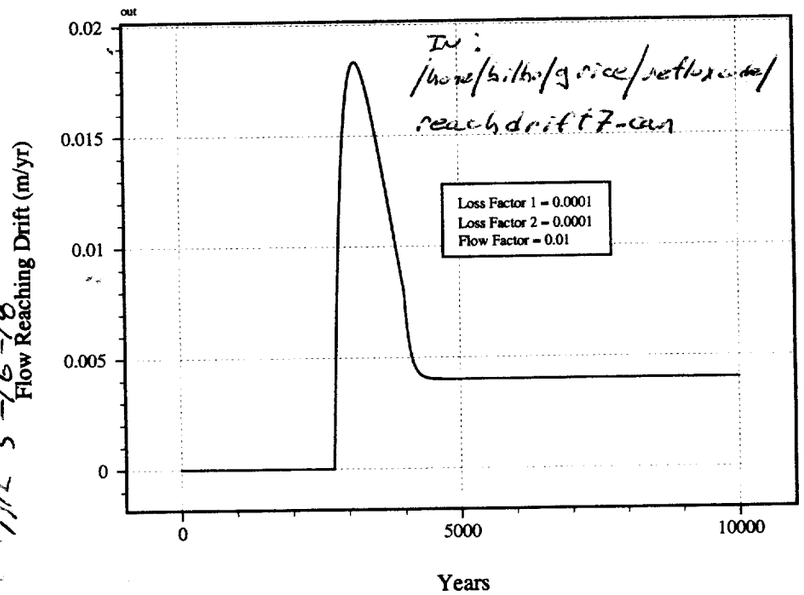
ML 3-13-98

ML 3-16-98

3-16-98
MR

NEW REFLUX - RESULTS + MASS BALANCE
MR 3-16-98

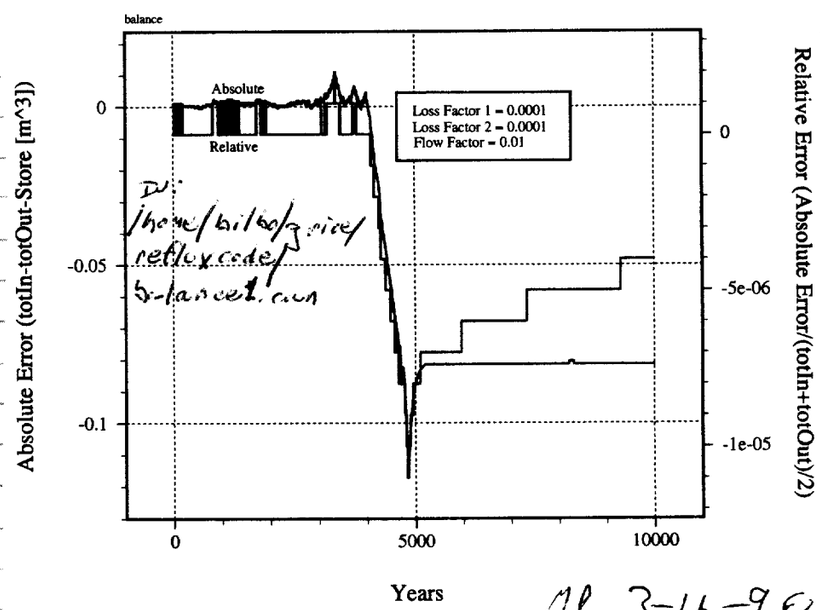
# New Reflux




MR 3-16-98

# REFLUX3 Mass Balance

MR 3-16-98




MR 3-16-98

NOTE - SEE PAGE 52 - THE DOUBLE PRECISION OF THE TPA CODE (INSTEAD OF SINGLE PRECISION) ELIMINATES ERRORS ALL TOGETHER

MR 7-13-98



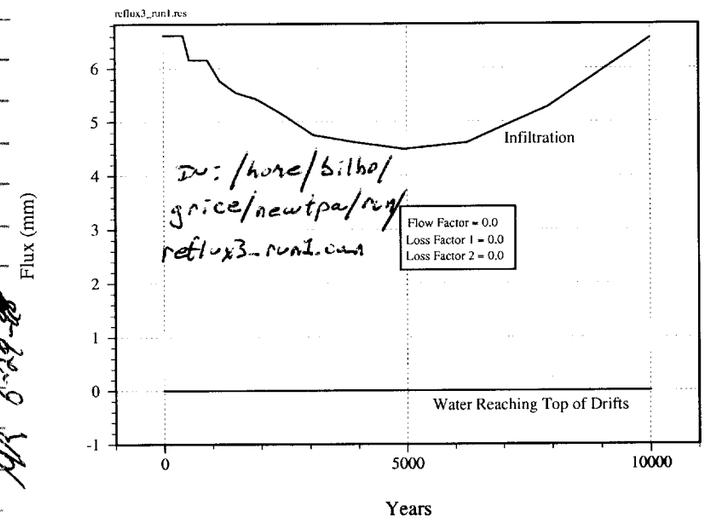
6-29-98
MR

TESTING TPA CODE VERSION OF REFLUX3 - ARE RESULTS REASONABLE?

TEST #1: NO WATER PERMITTED TO LEAVE SYSTEM - FLOW AND LOSS FACTORS SET TO ZERO.

MR 6-29-98

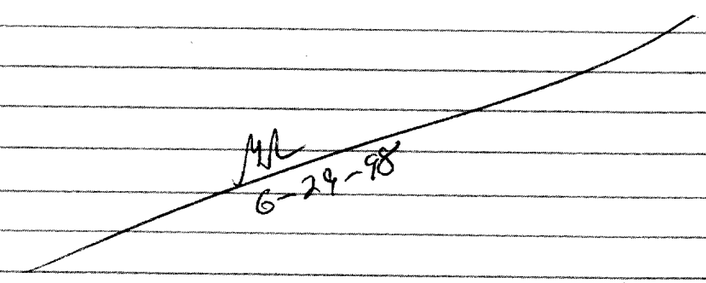
# TPA Code REFLUX3 Results




MR 6-29-98

TEST #1 RESULTS AS EXPECTED - NO WATER LEAVES SYSTEM.

TEST #2: NO DRY-OUT ZONE - ONLY WATER IS SYSTEM COMES FROM INFILTRATION:



MR 6-29-98

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MR

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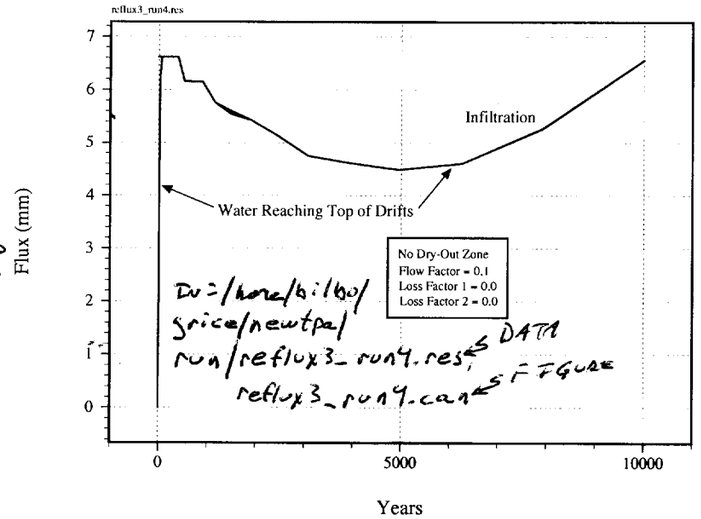
## TPA Code REFLUX3 Results

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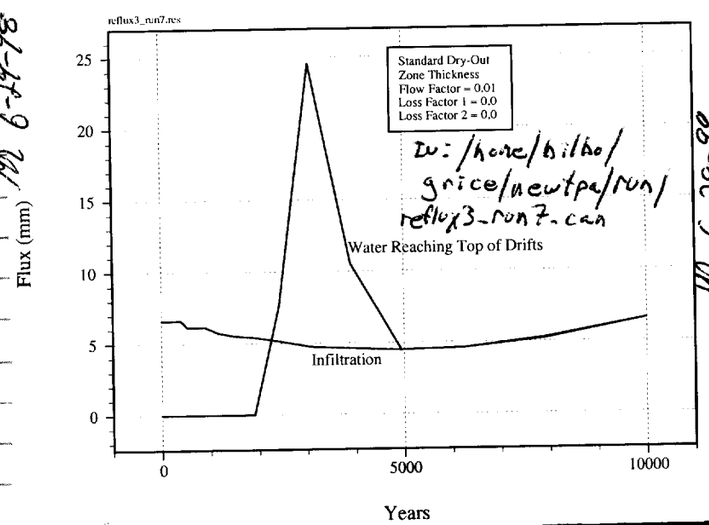
TEST #2 RESULTS AS EXPECTED: WITH NO WATER FROM DRY-OUT ZONE AND NO LOSSES, ALL INFILTRATION PASSES THROUGH SYSTEM AND WATER SOON REACHES DRIFTS AT INFILTRATION RATE. TIME THAT WATER REACHING DRIFTS + INFILTRATION RATE BECOME EQUAL DEPENDS ON FLOW FACTOR. MR 6-29-98

TEST #3 - TO COMPARE WITH TESTS #'s 4+5!

## TPA Code REFLUX3 Results

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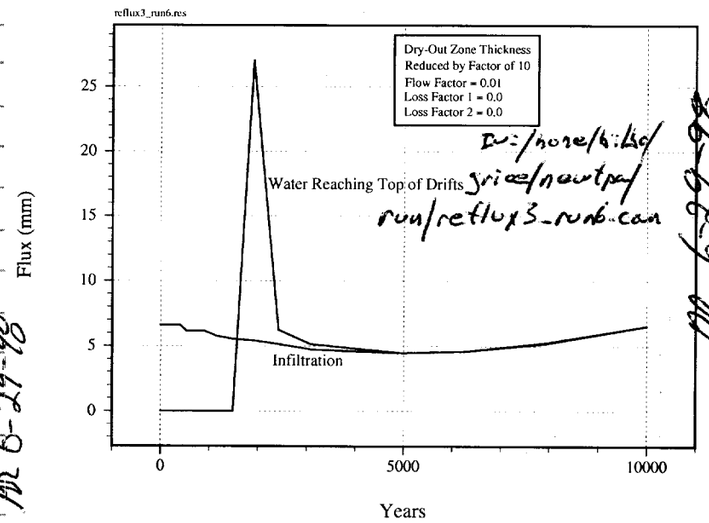
TEST #4 - SAME AS #3 BUT DRY-OUT ZONE THICKNESS ~~INCREASED~~ REDUCED BY FACTOR OF 10.

## TPA Code REFLUX3 Results

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RESULTS AS EXPECTED - AMOUNT OF WATER ~~REACHING~~ THAT REACHES DRIFTS IS REDUCED BY AMOUNT THAT VOLUME OF DRY-OUT ZONE WATER IS REDUCED: MR

REDUCTION IN DRY-OUT ZONE WATER (TOTAL VOLUME):

$$(80.7 - 8.07)(0.14)(0.9)(418)\ m^3$$

- (80.7 - 8.07): SEE PG 42 (m)
- 0.14: POROSITY
- 0.9: INIT SAT
- 418: AREA OF UNIT CELL ($m^2$)

TEST #5 - SAME AS #3 BUT WITH DRY-OUT ZONE THICKNESS INCREASED BY A FACTOR OF 10.

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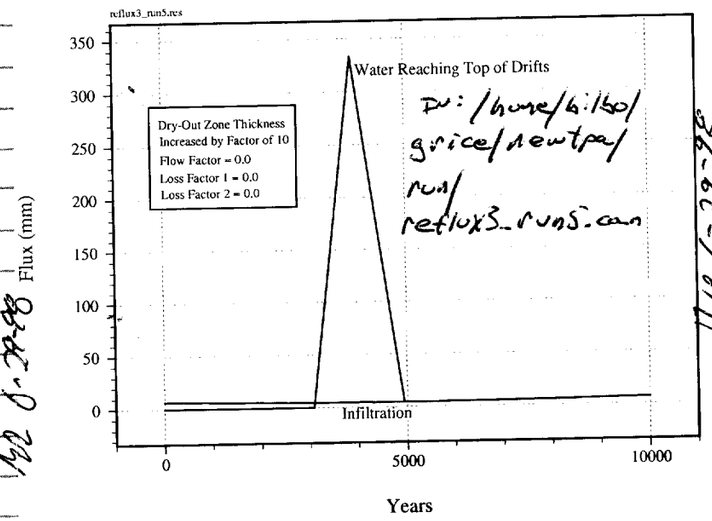
# TPA Code REFLUX3 Results




IN: /home/bilbo/grice/newtpa/run/reflux3_run5.com

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TEST #5 RESULTS AS EXPECTED - TOTAL AMOUNT OF WATER REACHING DRIFTS IS INCREASED BY AMOUNT VOLUME OF WATER CONTRIBUTED BY DRY-OUT ZONE IS INCREASED.

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INCREASE:

(807 m − 80.7 m) (0.14) 0.9 (418 m²)

INITIAL SATURATION

SEE PG 42

POROSITY

AREA OF UNIT CELL

NEW REFLUX3 VARIABLES IN TPA CODE.

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MR

RESULTS OF REFLUX3 RUNS THAT EXAMINE SENSITIVITY TO TEMPERATURE GRADIENT IN EXPRESSION DEVELOPED BY PITZLL ET AL (1996)

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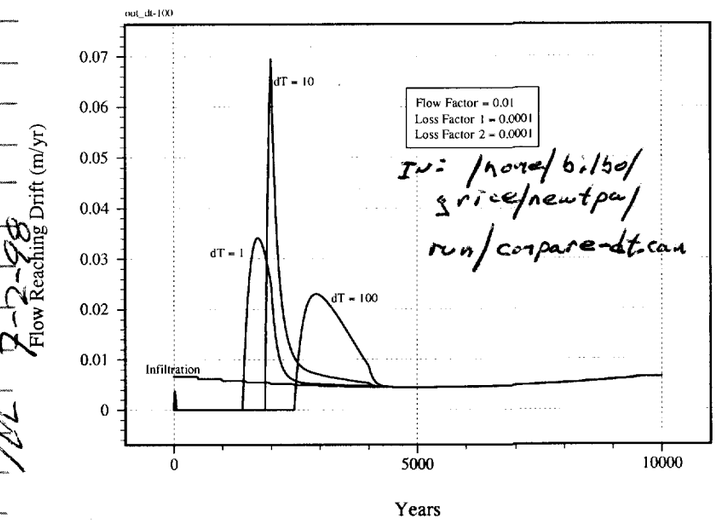
# REFLUX3: Effect of Tempertaure Gradient




IN: /home/bilbo/grice/newtpa/run/compare-dt.com

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- SEE NEXT PAGE

RESULTS OF MULTIPLE TPA RUNS (REALIZATIONS) TPA CODE AUTOMATICALLY CHANGES VARIABLES.

July 7, 1998

REFLUX3 Variables for NFENV table

| | | | | |
|---|---|---|---|---|
| constant | WPUnitCellWidth[m] | Width (m) of waste package unit cell | 22.5 | TRW Environmental Safety Systems, Inc. (1995) |
| loguniform | FractionOfCondensateRemoved | Fraction of water in condensation zone that is removed from system each year | 1.0e-8 - 1.0 | TEF team best estimate |
| loguniform | FractionOfCondensateTowardRepositoryRemoved | Fraction of water flowing from condensation zone toward repository that is removed from system each year | 1.0e-8 - 1.0 | TEF team best estimate |
| uniform | FractionOfCondensateTowardRepository | Fraction of water in condensation zone that flows toward repository each year | 0 - 1 | TEF team best estimate |
| constant | DensityOfWaterAtBoiling[kg/m³] | Density of water at boiling point (97 C, kg/m³) | 960.5 | Handbook of Chemistry and Physics (62nd Edition) |
| constant | EnthalpyOfPhaseChangeForWater[J/kg] | Enthalpy change, boiling water (J/kg) | 2.4E+6 | Handbook of Chemistry and Physics (62nd Edition) |
| uniform | TemperatureGradientInVicinityOfBoilingIsotherm[K/m] | Temperature gradient across boiling isotherm (K/m) | 1 - 100 | MULTIFLOW runs, laboratory-scale experiments |

jrjr/[illegible]/reflux3/table1.doc

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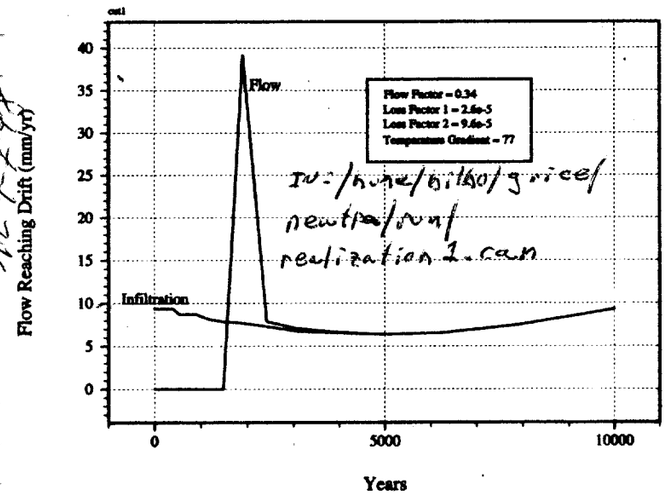
## REFLUX3 - Realization 1

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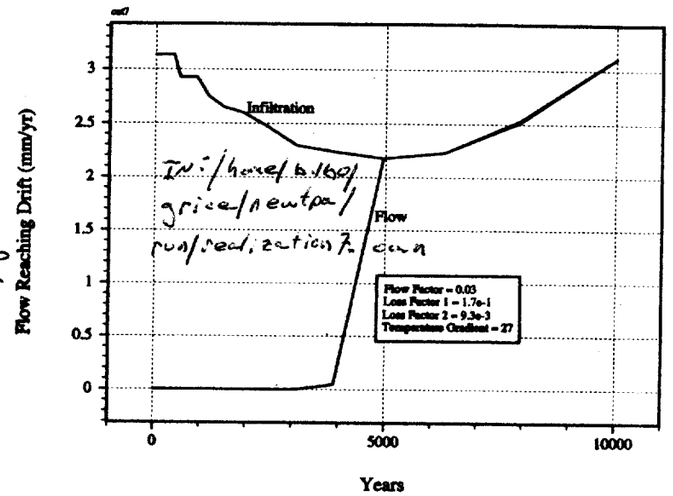
## REFLUX3 - Realization 7

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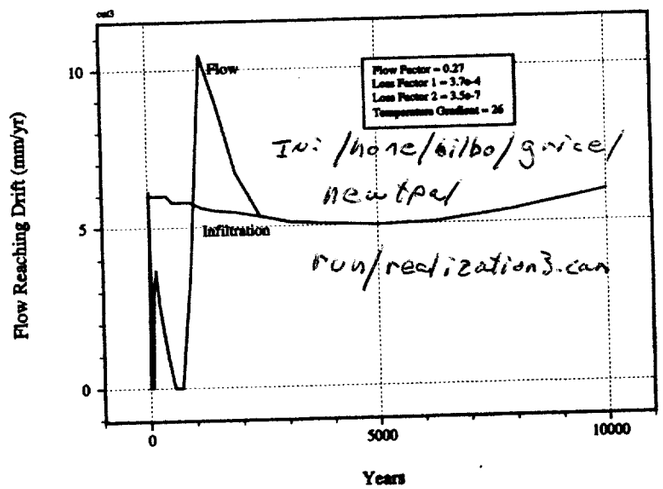
## REFLUX3 - Realization 3

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REFLUX3 MASS BALANCE - RESULTS OF STAND-ALONE VERSION.

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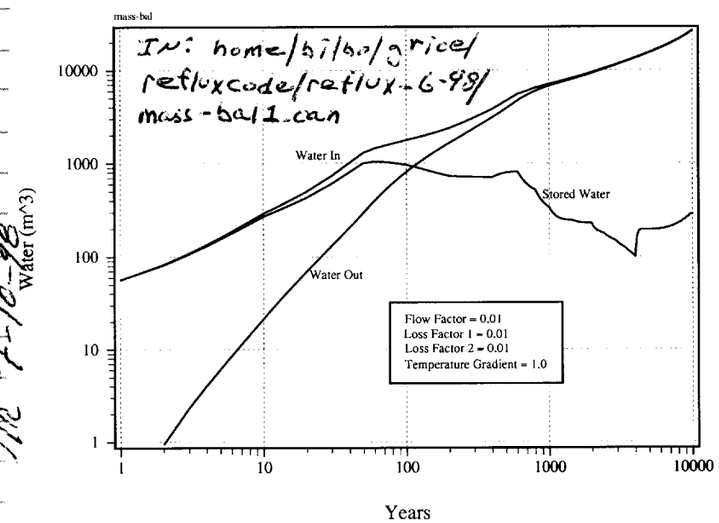
## REFLUX3 Mass Balance

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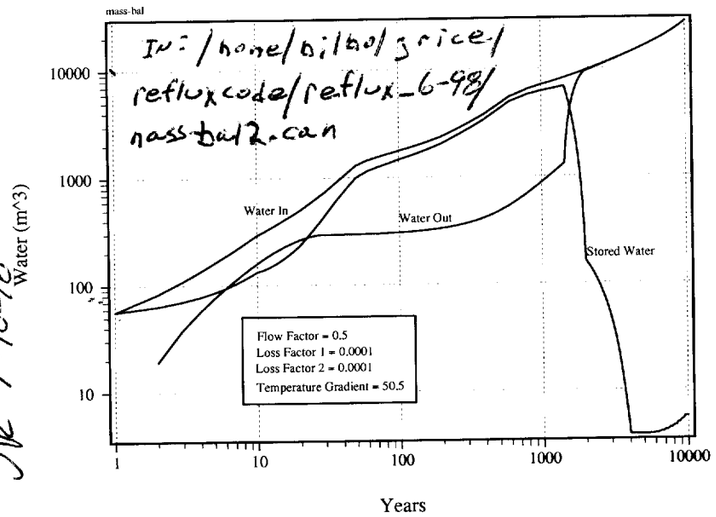
## REFLUX3 Mass Balance

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NOTE - THE FOLLOWING RUN DONE WITH THE CURRENT TPA CODE - DOUBLE PRECISION.

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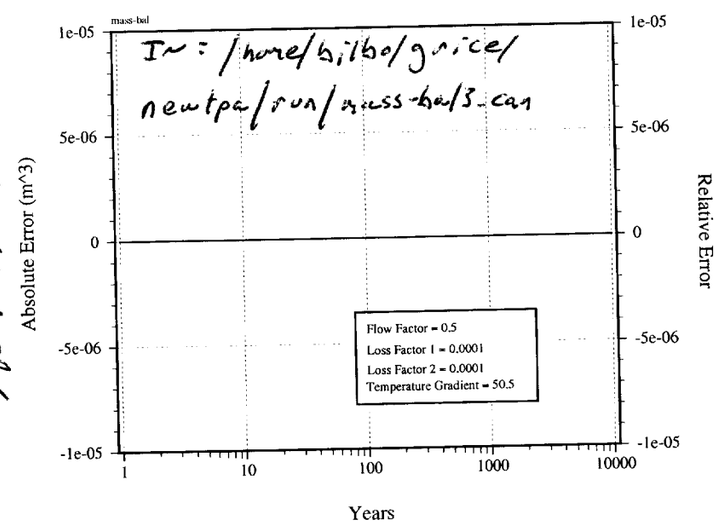
## REFLUX3 Mass Balance

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SEE NOTE ABOVE - ALSO SEE NOTE ON PG 44.

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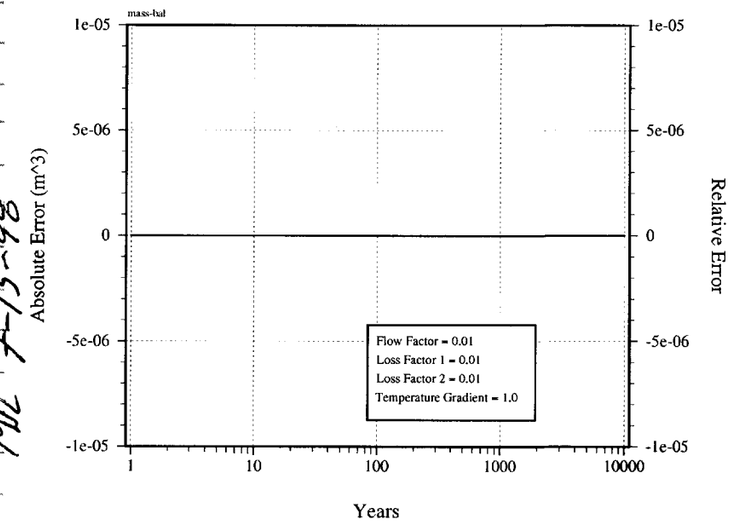
## REFLUX3 Mass Balance

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Final Entry:

This notebook appears to comply with QAP-001.

P. C. Gee
2/8/2000