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Scientific Notebook No. 227: graphical User Interface for Sub-Dividing Repository Area to Desired Vertical Columns (09/19/1997 through 07/30/2003)

#227

TPA

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Contents Page

TITLE: Graphical User Interface for Sub-dividing Repository Area to Desired Vertical Columns

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PROJECT:

One-dimensional modeling of each vertical column at Yucca Mountain is currently fixed at 7 columns. The ability to easily change the horizontal extent of each column is required for sensitivity analyses for unsaturated flow modeling. The top of each hydrostratigraphic unit, as well as the water table, must be determined for each new column. The underlying database for the stratigraphic information is stored in files with data resolution at 30 x 30 meter elements.

The graphical user interface (GUI) will be developed on a SUN workstation using libraries of X window calls. The libraries are referred to as tcl/tk language and it is supported by SUN. Versions of tcl/tk are available for IBM-compatible machines running WINDOWS or WINDOWS95. The GUI will be developed so as to allow the user to click on an area and have it subdivided horizontally in some restricted manner. Output will be the elevations of the hydrostratigraphic units for all of the new columns.

zip disks turned into QA with xerox copy of notebook
disk #1 bren:~/TPRUNS/* and bren:~/SUBAREA3/*
disk #2 /usr1/rfedors/*

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The following files were obtained from Stu Stothoff:

| | | | | |
|---|---|---|---|---|
| stu_cfmnn.xyz | 549869 | 4073999 | 603.042 | 59217 |
| | 547469 | 4083029 | 536.859 | |
| stu_cfun.xyz | 549959 | 4073999 | 761.737 | 59442 |
| | 547499 | 4083029 | 768.88 | |
| stu_chn1n2.xyz | 550019 | 4073999 | 820.987 | 59241 |
| | 547619 | 4083029 | 966.938 | |
| stu_n3ptn_all.xyz | 545010 | 4074000 | 1222.46 | 60400 |
| | 550980 | 4083030 | 1197.72 | |
| stu_ppw.xyz | 549989 | 4073999 | 800.705 | 59381 |
| | 547559 | 4083029 | 846.894 | |
| stu_tcbw.xyz | 549869 | 4073999 | 634.447 | 59499 |
| | 547499 | 4083029 | 592.044 | |
| stu_tiva_all.xyz | 545010 | 4079940 | 1420 | 51505 |
| | 550980 | 4083000 | 1268 | |
| stu_tptwtsw1_all.xyz | 550200 | 4074000 | 1109.62 | 54134 |
| | 547710 | 4083030 | 1259.93 | |
| stu_tsw23.xyz | 550169 | 4073999 | 1069.34 | 56939 |
| | 547709 | 4083029 | 1093.75 | |
| topo010.xyz | 545010 | 4074000 | 1127 | 60201 |
| | 550980 | 4083000 | 1268 | |

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The 1st numerical column is UTM coordinate east/west and the 2nd column is northing UTM coordinate. The 4th column is number of records (or grid points) in file. For each file, the The two records associated with the file (each file) are the upper-left and lower-right corners of the coverage within the file. The third column is the corresponding elevation in meters

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Note that eastings (UTM) get larger to the east & northings get larger to the north. UTM coordinates are in section/area 11.

The water table file is obtained from Danny Skelton who re-gridded out the water level data in EarthVision (Brit's latest water table):

→ 3d model-960905 ; file: waterelev_950912.dat

I named this file water.dat; headers need to be stripped & columns reformatted

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The order of the layers (from Stu Stothoff) are:

```
layers (top to bottom):

Tpcw
n3-Ptn
Tptn-TSw1
TSw2+3
CHn1n2
PPw
CFun
BFw

data files (top to bottom):

default map      (545025:30:550965)    (4074015:30:4082985)
topo010          (545010:30:550980)    (4074000:30:4083000)    (1107 1752)
60201
stu_tiva_all     (545010:30:550980)    (4074000:30:4083000)    (1107 1752)
51505
stu_n3ptn_all    (545010:30:550980)    (4074000:30:4083030)    (990.6 1461.8)
60400
stu_tptwtsw1_al  (545010:30:550980)    (4074000:30:4083000)    (950.4 1434.7)
54134
stu_tsw23        (545009:30:551009)    (4073999:30:4083029)    (857.3 1364.9)
56939
stu_chn1n2       (545009:30:551009)    (4073999:30:4083029)    (665.5 1212.3)
59241
stu_ppw          (545009:30:551009)    (4073999:30:4083029)    (518.9 1197.2)
59381
stu_cfun         (545009:30:551009)    (4073999:30:4083029)    (477.6 1072.6)
59442
stu_tcbw         (545009:30:551009)    (4073999:30:4083029)    (351.4 952.9)
59499
stu_cfmnn        (545009:30:551009)    (4073999:30:4083029)    (308.5 900.5)
59271
```

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The xyz files are stripped of headers and reformatted already. The *.dat files need to be stripped & reformatted.

Plus Stu Stothoff informed me that 6 of the files were gridded/shifted 1 meter off. The program used to shift the location entries is called junk.f (see top of next page). The files which need to be shifted are

stu_cfmnn.xyz
stu_cfun.xyz
stu_chn1n2.xyz
stu_ppw.xyz
stu tcbw.xyz
stu-tsw23.xyz

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```
Sep 15, 97 16:04                 jk2.f                          Page 1/1
      program junk
c Read in Stuart's data files for 30x30m pixel resolution.
c Shift location entries 1 meter (increase) both east and north.
c RFedors 5-30-97 CNWRA data manipiulation fortran code; modified 7-31-97


      parameter (max=80000)
      dimension x_east(max), y_north(max), elevat(max)
c     &           , xeast(max), ynorth(max), elev(max)
      character*20 infile, outfile

      write(6,*) 'Enter number of records: '
      read(5,*) nrec
      write(6,*) 'Enter input file name: '
      read(5,*) infile
c      write(6,*) 'Enter 1(shift) or 0(no shift): '
c      read(5,*) ishift
      write(6,*) 'Enter output file name: '
      read(5,*) outfile

      open(unit=8,file=infile,status='unknown')
      open(unit=9,file=outfile,status='unknown')

      do 50 i = 1,nrec
         read(8,*) x_east(i), y_north(i), elevat(i)
 50   continue

c Shift if needed.
c       if(ishift.eq.1) then
          do 80 i = 1,nrec
             x_east(i) = x_east(i) + 1.
             y_north(i) = y_north(i) + 1.
  80      continue
c       endif

c Write out different file
      do 200 i = 1,nrec
         write(9,'(i6,1x,i7,1x,f8.3)')  int(x_east(i)),
     &                         int(y_north(i)), elevat(i)
 200  continue

      stop
      end
```

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TO DO / Comments:

① The sort order changes between files. Some are column-oriented and some are row-ordered. This will be changed so as to get some consistency and allow a much simpler search algorithm which can assume a particular order.

② Still need to strip headers and reformat the water-level data

③ Create search algorithm and method to aggregate for new subarea delineations.

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Current tpa.inp.master has subarea polygons and their coordinates (seven subareas).

Copied files from /solapps/cnwra/tpa/tpa.inp.master
and /solapps/cnwra/tpa/data/*

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to /export2/rfedors/TPRUNS/AREAS/*

(also copied tpa.e to bren so as to run directly on bren for subarea testing).

To run tpa code need to add to .cshrc.local file
setenv TPA /export2/rfedors/TPRUNS

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The coordinates of the seven subareas are in the tpa.inp file. The other item to change for adjusting subareas ~~are~~ is the entry for each column, each layer for thickness [4 lines of entry (records) for each thickness value for each layer in each column; yes lots & lots of records]

There is also an entry for subarea area
inlet & outlet
(4 records for each subarea).

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General Outline of creating new Subareas

① Shift units of location 1 meter on some files per Stuart's request
(done, see previous pages)

② sort files and clip out an area which encompasses entire repository
(some files were apparently saved in column-ording and some in row-ordering, and a couple that have both)
My search for sub-dividing will be much more efficient if all files are consistently ordered.

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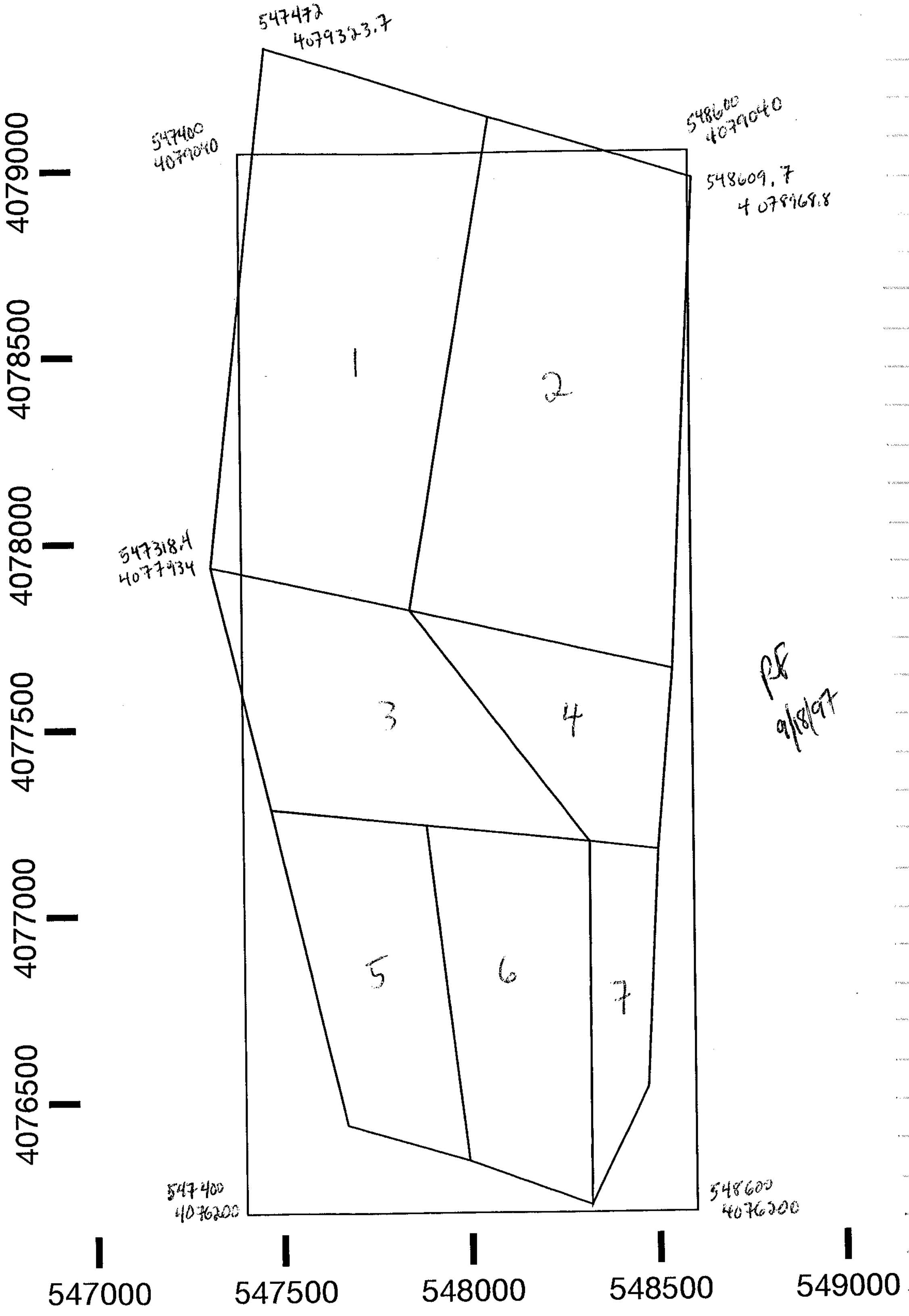
③ sub-dividing algorithm
- (i) create new polygons
- (ii) for each new polygon
  - a.) narrow the check area by determining $X_{min}$, $Y_{min}$ and $X_{max}$, $Y_{max}$
  - b.) for each pixel in the narrow area, determine if it is on the correct side of each face; this will be done by creating an equation for the line for each face
  - c.) Scanning line by line or column by column will allow one less face to be checked after the 1st face is crossed; and once both faces are crossed (either 2 opposite faces or 2 adjacent faces) the next row or column can be started.

I'm sure that all the graphics companies (computer graphics) have efficient search algorithms; but for what I need here, this brute force algorithm should suffice.

The tpa.inp.master of Sept 18, 1997 has the repository coordinates.

Tecplot display of the 1-area repository (rectangle)
and the 7-subarea repository is
attached to next page.
The minimum & maximum coordinates for the
repository areas are noted on the figure

PF
9/8/97



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./SUBAREAS/repository.lay
using { repository-1.pef
repository-7.pef

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PF

## Sort files & Clip Out Area of Entire Repository

Area to include plus 300 m buffer (UTM coord)
546990 to 548940 easting } defines nodes
4075890 to 4079640 northing. }
which for 30 m x 30 m resolution is 66 cells wide
by 126 cells tall
for a cell defined as the 30 x 30 area surrounding
each node (which then adds 15 m to entire area)

Input files included 8 lithologies and ground surface and water table; files which were shifted 1 m (*.xyz2) and reformatted (*.xyz1) for ease in reading files are listed in the small code which clips area and sorts by placing each node in its proper place in a matrix. Produces "sort.out" for later subdividing.

```
        program sort1
c Read in Stuart's data files for 30x30m pixel resolution;
c (the "2" at the end of filename signifies that I shifted coordinates 1 m.).
c Clip the large coverage files down to a manageable area which
c includes approx 300m extra on each side of current TPA3 repository 9-18-97.
c This is 546990 to 548940 easting and 4075890 to 4079640 northing.
c Sort into column major order by placing into a matrix; then write out a file.
c RFedors 9-19-97 CNWRA (UNIX-SUN) data manipiulation fortran code.

      parameter (maxx=66,maxy=126,ifiles=11,small=1.e-4)
      parameter(xmin = 546990.,xmax = 548940.)
      parameter(ymin = 4075890.,ymax = 4079640.)

      character*21 filein(ifiles), fileout
      integer i, j, k, kfile, ix, iy, nrec(ifiles)
      real  elev(maxx,maxy,ifiles)
      real xeast, ynorth, elevation

      fileout = 'sort.out'
      filein(1) = 'topo010.xyz1'
      filein(2) = 'stu_tiva_all.xyz1'
      filein(3) = 'stu_n3ptn_all.xyz1'
      filein(4) = 'stu_tptwtsw1_all.xyz1'
      filein(5) = 'stu_tsw23.xyz2'
      filein(6) = 'stu_chn1n2.xyz2'
      filein(7) = 'stu_ppw.xyz2'
      filein(8) = 'stu_cfun.xyz2'
      filein(9) = 'stu_tcbw.xyz2'
      filein(10) = 'stu_cfmnn.xyz2'
      filein(11) = 'water.xyz1'
      nrec(1) = 60201
      nrec(2) = 51505
      nrec(3) = 60400
      nrec(4) = 54134
      nrec(5) = 56939
      nrec(6) = 59241
      nrec(7) = 59381
      nrec(8) = 59442
      nrec(9) = 59499
      nrec(10) = 59217
      nrec(11) = 64722

c Set default value of matrix of stratigraphic layer tops to some flag.
      do 20 k = 1,ifiles
       do 20 j = 1,maxy
        do 20 i = 1,maxx
          elev(i,j,k) = -999.
 20   continue

      do 300 kfile = 1,ifiles
        open(unit=8,file=filein(kfile),status='unknown')
        write(6,*) kfile

        do 200 i = 1,nrec(kfile)
          read(8,'(i6,1x,i7,1x,f8.3)') ieast, inorth, elevation
          xeast = float(ieast)
          ynorth = float(inorth)

c Exclude if outside area of repository and 300 m buffer.
          if(xeast.lt.xmin-1..or.xeast.gt.xmax+1.) goto 200
          if(ynorth.lt.ymin-1..or.ynorth.gt.ymax+1.) goto 200
c Use column-ordering with start in lower left corner (SW).
c Determine matrix location by subtracting base value then divide by resolution.
c Add one to matrix location to avoid addressing zero location of matrix.
          if(mod(xeast,30.).lt.small.or.mod(ynorth,30.).lt.small) then
            ix = nint( (xeast-xmin) / 30. ) + 1
            iy = nint( (ynorth-ymin) / 30. ) + 1
           else
             write(6,*) 'El Problemo'
```

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```
             goto 500
           endif
c Load into appropriate position of matrix.
           elev(ix,iy,kfile) = elevation

 200     continue
         close(8)
 300  continue

c Write out different file in column-ordered format, origin in SW (lower-left).
      open(unit=9,file=fileout,status='unknown')
      ix = nint(xmin)
      iy = nint(ymin)
      write(9,1001) ix, nint(xmax)
      write(9,1003) iy, nint(ymax)
      write(9,1004)
      do 520 j = 1,maxy
       do 500 i = 1,maxx
         write(9,'(i6,i8,11f7.1)') ix, iy, ( elev(i,j,k), k = 1,ifiles )
         ix = ix + 30.
 500   continue
       ix = nint(xmin)
       iy = iy + 30.
 520  continue

 1001 format('# Origin in SW corner for',i7,' to ',i8,1x,'meters')
 1003 format('#',24x,i7,' to ',i8,1x,'meters')
 1004 format('# east  north ground  tiva n3ptn tptwtsw  tsw23'
     &      ,  ' chn1n2   ppw   cfun   tcbw  cfmnn  water')
      stop
      end
```

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"Sort.out" file (/export2/bren/rfedors/SUBAREA/Sort/sort.out)
Two problems noted with data

① ground surface (topo010.xyz) is not the highest surface in the southwest corner (546990, 4075890)
The Tiva unit is missing, and the "n3ptn" unit is higher (elevation)-wise than the groundsurface until the tiva unit appears, then everything is okay.
Ignore this problem for now since we've concerned with the units from the repository to the water table
(tsw23 to cfmnn)

② Isolated missing data points surrounded by good data points
A specific case is the cfmnn unit, column 548670
This is below the water table (at least in the sw corner

As a way to spot check the creation of "sort.out" I plotted the "elevdem.dat" file from the tpa input files (tpa/Data/), overlaid the outline of the area I clipped for the repository (and 300 m buffer), and compared the dependent variable elevation between the "sort.out" and the tecplot plot using the "prober" in tecplot. See figure on next page.

I also noted that the "elevdem.dat" file has its origin in the upper-left (NW) corner
(even though XLLCORNER = 545010 and YLLCORNER = 4074000 in the header lines of elevdem.dat)
and that the file is row-major ordered (c style, rather than fortran style).

The figure on the next page is mainly for visual reference.

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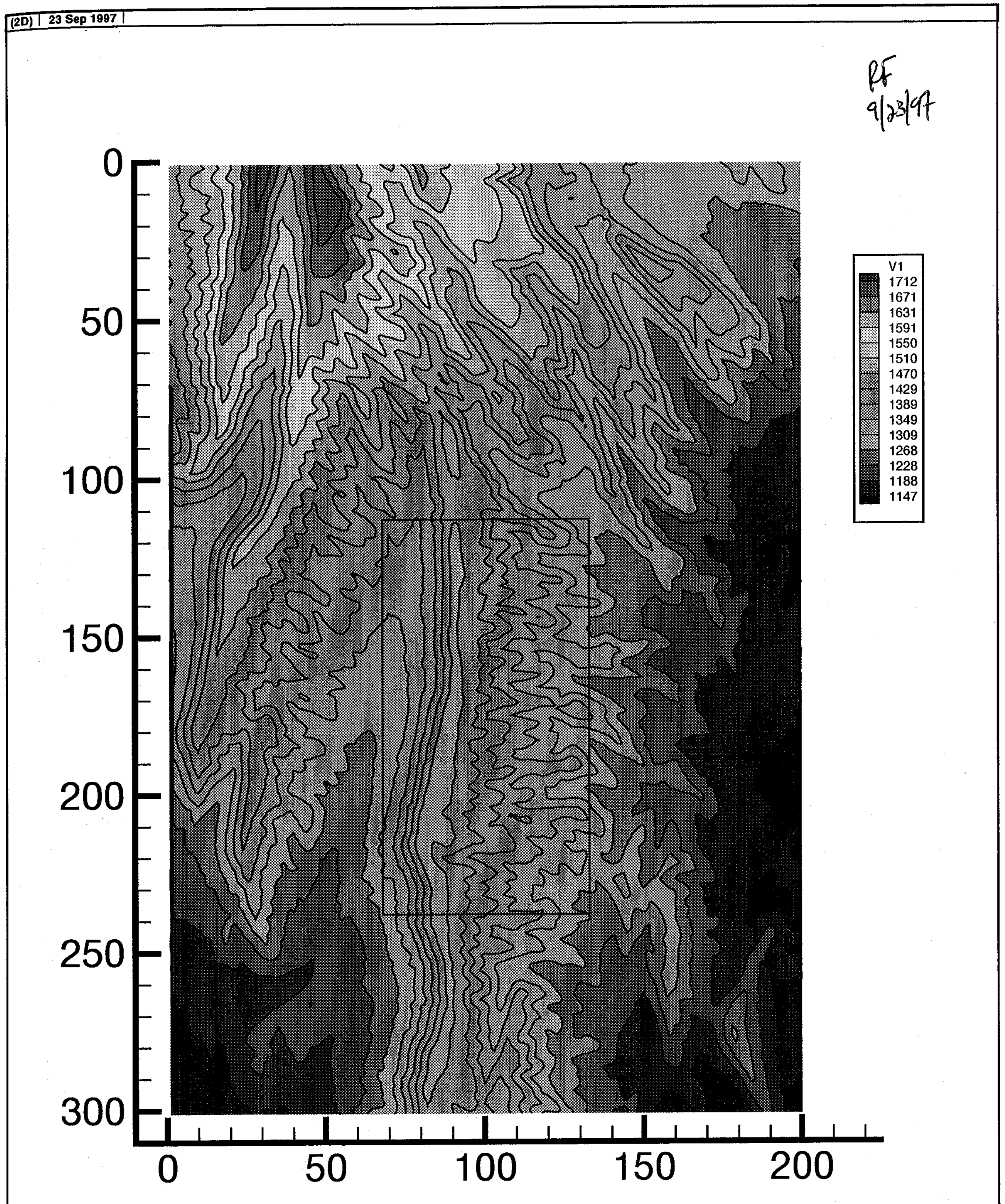

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30 m cells, 200 x 301; lower-left corner at 545010 and 4074000
The elemdem.dat origin is upper left corner; and is in row-major order.
Outline of repository area includes 300 m buffer.

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Repository Drift Outline - EDA II Design

New drift coordinates obtained from DOE. I extracted main and east block coordinates to text files (ascii) for PA folks. This work was put in scientific notebk #294 pages 58-60 instead of this notebook

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**Testing of TPA 4.0 UZFLOW and ITYM Preprocessor (March 21, 2000)**

I was volunteered to be the tester for the ITYM preprocessor, its linkage to UZFLOW, and for UZFLOW itself. UZFLOW is the module name in TPA 4.0 for climate and unsaturated zone flow. The ITYM preprocessor produces the *maidtbl.dat* file read in by UZFLOW and used as a basis for interpolation between sampled climate states.

**SETUP**

For TPA code testing, I copied the contents of /home/janetzke/tpa40betaK/data/* to /vscr1/rfedors/TPA4/data so that I could run tpa.e and change the *maidtbl.dat* as needed. This could not be done if I just set the environment variables to Ron Janetzke's home directory for the external files. Because vulcan loses scratchy's home directory mounting everytime vulcan is rebooted, Ron Janetzke had to email me the source code for ITYM for testing (otherwise, I could have gotten it directly from /export/home/janetzke/tpa/dev/). The source code was copied to vscr1/rfedors/src/* for use in process-level testing of the ITYM preprocessor. All testing is done on ds9 (SUN Ultra) and on vulcan (sure would be nice to have a home directory on vulcan). NOTE: all relative directory paths assume /vscr1/rfedors/ as the leading portion of the path.

NOTE: The TPA 4.0 directory ./data/* contains *soildem.dat* and *elevdem.dat*. These files no longer should be in the data for tpa; the updated versions of these files (along with other DEMs for ITYM) should now reside in the ITYM data directory. If those files are to remain in the ./data/ directory, then the other DEMs needed for ITYM should be added to that directory.

Working in ./RUNS/ directory TPA4 simulations, hence copied *tpa.inp* (the base case) to ./RUNS/ directory and changed permissions on it so that I could modify the file. I also set environment variables as follows and made an alias to make it easier to type the tpa executable command:

```
For TPA 4.0 testing:
setenv TPA_TEST /home/janetzke/tpa40betaK
setenv TPA_DATA /vscr1/rfedors/TPA4
For TPA 3.2.3 testing:
setenv TPA_TEST /solapps/cnwra/A_tpa3.2.3
setenv TPA_DATA /solapps/cnwra/A_tpa3.2.3
For both:
alias tpa $TPA_TEST/tpa.e
```

For ITYM testing, the code was run in the /vscr1/rfedors/ITYM and IYTM2.

**Code for Test 1 and Test 3**

A fortran code was developed to help test the subarea averaging and the climate interpolation in UZFLOW of TPA 4.0. The code is *maid.f* and its listing is included here. Various version of the code were used for particular tasks and testing; the variants of *maid.f* are of the form *maid*.f* where the asterisk stands for one or more characters that are shorthand for the specific test.

The code creates a *maidtbl.dat* file with special entries for the infiltration values. For the climate interpolation, the *maid.f* code creates DEMs with identical infiltration values for a particular climate state, but different values for different climate states. For the subarea averaging test, all values of infiltration are identical except for the nodes in a particular subarea. Visual inspection of the output from *maid.f* readily confirms that the code is working properly.

| | | |
|---|---|---|
| Pixels in the DEM that fall into Subarea 8 are: | Row 28, | column 23 |
| (120 m * 120 m cell size) | 29, | 23-26 |
| | 30, | 23-30 |
| | 31, | 23-30 |
| | 32, | 26-30 |
| | 33, | 30 |

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Program listing for *maid.f*

```
         program maid
c driver for writing maidtbl.dat file for testing
c creates maidtbl.dat with 2 precips and 2 temperature with
c subarea 8 having different values than the rest of the map
c  (define subarea 8 using if statements in the loops)
c RFedors  March 23, 2000

        integer iowrit, NCOLS, NROWS, i, j
        real XCORNER, YCORNER, CELLSIZE, NODATA, var1, var2
        real value1, value2

        iowrit = 8
        NCOLS = 49
        NROWS = 75
        XCORNER = 545010.000000
        YCORNER = 4074000.000000
        CELLSIZE = 120.000000
        NODATA = -9999.000000

c  initialize output file

        open(unit=iowrit,file='maid.dat',form='formatted')

        write(iowrit,'(a)')
     &  '# DEM table of expected MAI [mm/yr] for each pixel'
        write(iowrit,'(a)')
     & '# Table is a function of MAP [mm/yr] and MAT [C]'
        write(iowrit,'(a)')
     &   '# Coordinate system is UTM NAD27 [m]'
        write(iowrit,'(2a)') '# File generated on '

c  write DEM for first precip and temperature
        var1 = 100.
        var2 = 5.
        value1 = 0.
        value2 = 2.
c  write header
        write(iowrit, '(a,i8)') 'NCOLS',  NCOLS
        write(iowrit, '(a,i8)') 'NROWS',  NROWS
        write(iowrit, '(a,f16.6)') 'XLLCORNER', XCORNER
        write(iowrit, '(a,f16.6)') 'YLLCORNER', YCORNER
        write(iowrit, '(a,f16.6)') 'CELLSIZE', CELLSIZE
        write(iowrit, '(a,f16.6)') 'NODATA_VALUE', NODATA
        write(iowrit, '(a,1pe15.7)') 'VAR1',    var1
        write(iowrit, '(a,1pe15.7)') 'VAR2',    var2

        do 10 i = 1,NROWS
         do 10 j = 1,NCOLS
           if (i.eq.28.and.j.eq.23) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.29.and.j.ge.23.and.j.le.26) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.30.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.31.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.32.and.j.ge.26.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.33.and.j.eq.30) then
                          write(iowrit,'(1pe15.8)') value2
           else
                  write(iowrit, '(1pe15.8)') value1
           endif

 10     continue

c  write DEM for first precip and second temperature
        var1 = 100.
        var2 = 20.
        value1 = 0.
        value2 = 2.
c  write header
        write(iowrit, '(a,i8)') 'NCOLS',  NCOLS
        write(iowrit, '(a,i8)') 'NROWS',  NROWS
        write(iowrit, '(a,f16.6)') 'XLLCORNER', XCORNER
        write(iowrit, '(a,f16.6)') 'YLLCORNER', YCORNER
        write(iowrit, '(a,f16.6)') 'CELLSIZE', CELLSIZE
        write(iowrit, '(a,f16.6)') 'NODATA_VALUE', NODATA
        write(iowrit, '(a,1pe15.7)') 'VAR1',    var1
        write(iowrit, '(a,1pe15.7)') 'VAR2',    var2

        do 20 i = 1,NROWS
         do 20 j = 1,NCOLS
           if (i.eq.28.and.j.eq.23) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.29.and.j.ge.23.and.j.le.26) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.30.and.j.ge.23.and.j.le.30) then
```

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```
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.31.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.32.and.j.ge.26.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.33.and.j.eq.30) then
                          write(iowrit,'(1pe15.8)') value2
           else
                  write(iowrit, '(1pe15.8)') value1
           endif

 20     continue

c  write DEM for second precip and first temperature
        var1 = 600.
        var2 = 5.
        value1 = 0.
        value2 = 2.
c  write header
        write(iowrit, '(a,i8)') 'NCOLS',  NCOLS
        write(iowrit, '(a,i8)') 'NROWS',  NROWS
        write(iowrit, '(a,f16.6)') 'XLLCORNER', XCORNER
        write(iowrit, '(a,f16.6)') 'YLLCORNER', YCORNER
        write(iowrit, '(a,f16.6)') 'CELLSIZE', CELLSIZE
        write(iowrit, '(a,f16.6)') 'NODATA_VALUE', NODATA
        write(iowrit, '(a,1pe15.7)') 'VAR1',    var1
        write(iowrit, '(a,1pe15.7)') 'VAR2',    var2

        do 30 i = 1,NROWS
         do 30 j = 1,NCOLS
           if (i.eq.28.and.j.eq.23) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.29.and.j.ge.23.and.j.le.26) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.30.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.31.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.32.and.j.ge.26.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.33.and.j.eq.30) then
                          write(iowrit,'(1pe15.8)') value2
           else
                  write(iowrit, '(1pe15.8)') value1
           endif

 30     continue

c  write DEM for second precip and temperature
        var1 = 600.
        var2 = 20.
        value1 = 0.
        value2 = 2.
c  write header
        write(iowrit, '(a,i8)') 'NCOLS',  NCOLS
        write(iowrit, '(a,i8)') 'NROWS',  NROWS
        write(iowrit, '(a,f16.6)') 'XLLCORNER', XCORNER
        write(iowrit, '(a,f16.6)') 'YLLCORNER', YCORNER
        write(iowrit, '(a,f16.6)') 'CELLSIZE', CELLSIZE
        write(iowrit, '(a,f16.6)') 'NODATA_VALUE', NODATA
        write(iowrit, '(a,1pe15.7)') 'VAR1',    var1
        write(iowrit, '(a,1pe15.7)') 'VAR2',    var2

        do 40 i = 1,NROWS
         do 40 j = 1,NCOLS
           if (i.eq.28.and.j.eq.23) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.29,and.j.ge.23.and.j.le.26) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.30.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.31.and.j.ge.23.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.32.and.j.ge.26.and.j.le.30) then
                          write(iowrit,'(1pe15.8)') value2
           elseif (i.eq.33.and.j.eq.30) then
                          write(iowrit,'(1pe15.8)') value2
           else
                  write(iowrit, '(1pe15.8)') value1
           endif

 40     continue

c  finalize output file

        write(iowrit, '(a)')    'NCOLS 0'
        close(iowrit)

        stop
        end
```

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### Test 1- Interpolation of Climates in UZFLOW module

This is a hand calculation test of the interpolation in UZFLOW between climate states. An artificial *maidtbl.dat* file was created using the *maid.f* code that had infiltration of 1 for the present-day climate (162.8 mm/yr precipitation and 17.38 deg C temperature) and a higher value at a climate state of twice the precipitation but the same temperature. Two different tests were done, one with the future infiltration value set to 2 and one with the future infiltration value set to 20. The *tpa.inp* file was modified so that no sampling could occur for climate; this was done by setting the present day annual average infiltration parameter to a constant value of 1, the precipitation multiplier at full glacial to a constant value of 2, and the temperature shift at full glacial to a constant value of 0.

Testing output files are located in ./rfedors/TPA4/RUNS/Climate2 → case 1: future infiltration = 2 mm/yr
./ rfedors/TPA4/RUNS/Climate3 → case 2: future infiltration = 20 mm/yr

The values at 10,000 yrs reported in infilper.res (and in uzflow.rlt if the subarea area is divided out the units are converted to mm/yr from m/yr) are:

case 1: infiltration = 1.340 mm/yr
case 2: infiltration = 3.5444 mm/yr

The hand calculation first starts with interpolating the precipitation values for the tpa computational steps of 500 yr from the climato2.dat fractions of hard-wired modern precipitation, the full glacial multiplier, and fractions of full glacial. Next the interpolation weights to be used for infiltration values in the DEMs of *maidtbl.dat* are calculated between precipitation values of particular DEMs in maidtbl.dat and the modern and full glacial precipitation values:

| Year | fraction | precip mm/yr | log10 precip | wt1 | wt2 | Infiltration mm/yr |
|---|---|---|---|---|---|---|
| | modern | 162.8 | 2.211654 | | | 1 |
| 9,000 | .304244 | 212.331 | | | | |
| 9,500 | interpolate | 216.208 | 2.334872 | .590679 | .409321 | |
| 10,000 | .35188 | 220.086 | 2.342592 | .565032 | .434968 | |
| | full glacial | 325.6 | 2.512684 | | | 2 or 20 |

where the weights (wt1 and wt2) are calculated as follows:

$$wt1 = \frac{\text{log10 Precip Full Glacial} - \text{log10 Precip value at intermediate point}}{\text{log10 Precip Full Glacial} - \text{log10 Modern Precip}}$$

$$wt2 = 1 - wt1$$

The equation for wt1 is only true for the test case I chose because I put the modern and full glacial DEMs of infiltration into the *maidtbl.dat* file. Normally, this wouldn't be the case; the terms of the equation for wt1 would have to match the precipitation values in *maidtbl.dat*.

The weights can then used to calculate the infiltration values at each point in time. Then uzflow module calculates a cumulative infiltration over time followed by interpolation to the output times. The infiltration at the desired climate (precipitation only for this case since I made temperatures identical in the ITYM output) is calculated using the equation below and is reported in columns 2 and 4 in the following table. Thus, the value reported by tpa is an average with the previous time value (see columns 4 and 7 below).

$$\text{log10 Infiltration} = \text{log10 Infiltration}_{ITYM\ c\lim ate1} * \text{wt1} + \text{log10 Infiltration}_{ITYM\ c\lim ate2} * \text{wt2}$$

| Year | Case 1: full glacial infiltration at 2 mm/yr | | | Case 2: full glacial infiltration at 20 mm | | |
|---|---|---|---|---|---|---|
| | log10 infilt mm/yr | infiltration mm/yr | Average for 10,000 yr | log10 infilt mm/yr | infiltration mm/yr | Average for 10,000 yr |
| 9,500 | .123218 | 1.328 | | .532539 | 3.4083 | |
| 10,000 | .130938 | 1.35188 | 1.33994 | .565906 | 3.680497 | 3.5444 |

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These values agree with the tpa output mentioned above. Note that there is a minor inconsistency in that precipitation at each computational step is interpolated in natural arithmetic space, while the weights are calculated from log10 values of precipitation at the time steps. This issue may require further contemplation.

### Test 2- Checking Functionality of ITYM Preprocessor Options in *itym.dat* File

This series of tests were done to ensure that the ITYM preprocessor has the intended flexibility of (i) changing cell size (for aggregation of 30m-by-30m pixel regression estimates), (ii) changing precipitation and temperature ranges, (iii) changing the number of DEMs (number of different climate states for which a DEM is produced), and (iv) changing regression equation option.

While editing of *itym.dat* to create *maidtbl.dat* with the standard deviations set to zero for all sampled parameters, it was noted that Stothoff uses tab delimited data entries. Accidental deletion of tab, with spaces still present, will lead to bomb-outs in trying to run ITYM. This is a poor design feature for an input file that we will be editing by hand; this should be changed in the next round of TPA changes. Stothoff uses MATLAB to create this file so he does not have this problem (the TPA users should not be required to use MATLAB to edit this input file).

The directories where these tests were done are:

| | |
|---|---|
| ./TPA4/ITYM2/Aggreg | TPA 4.0 results when different aggregation used (cell size 240) pixel merge=8 |
| ./TPA4/RUNS/Table/ | *maidtbl.dat*: *tpa.inp* temperature set to higher value than in *maidtbl.dat* |
| ./TPA4/RUNS/Table2/ | *maidtbl.dat*: *tpa.inp* max temperature set to exactly the value highest value in *maidtbl.dat* |

1. The num_pixel_merge option produced *maidtbl.dat* files of the expected size and structure for values of 1, 4, and 8; all resulting *maidtble.dat* files were successfully read by UZFLOW. (Note: pixel merge values of 1 and 4 were used successfully in Test 1 for climate interpolation).
2. The input values for the range of precipitation and temperature were adjusted to something smaller than what the TPA simulation was expecting from the climate parameters in the *tpa.inp* file; UZFLOW properly rejected the *maidtbl.dat* file and stopped.
3. The number of DEMs for different temperatures (num_MAT_table) was changed from 4 to 2 to 1. ITYM produced the proper *maidtbl.dat* file and UZFLOW successfully read in the DEMs for num_MAT_table values of 4 and 2; ITYM did not produce a table with num_MAT_table set to 1. A *maidtbl.dat* file was created with *maid.f* with only one temperature; UZLOW properly rejected that *maidtbl.dat* (tpa.e stopped) when num_MAT_table was set to 1 (we do not presently allow for UZFLOW to interpolate between 1 value for temperature or 1 value for precipitation since this does not make sense).
4. The test for ITYM use of option TPA4 and TPA3 was successful and is reported as part of Test 6 results.

### Test 3 – Subarea Averaging in UZFLOW (Subarea 8)

This will test whether the aggregating to subarea averages is working properly. I have constant values (non-zero) for two climates with Subarea 8; the remaining modeling area (all other subareas) have infiltration set to zero for both climates. The code constructed to create such a *maidtbl.dat* file is called *maid.f* with variations called *maid??.f* for specific tests. This code was the same one as was used in Test 1 where the climate interpolation was checked. This code sets the appropriate cell locations to a non-zero values through the use of if-then statements for each row (and columns in that row) that subarea 8 covers.

Modify *tpa.inp* to have no change for climate (temperature shift = 0 and precipitation multiplier = 1). Since a problem was indentified (and later corrected) in the UZFLOW module for aggregating to subarea averages, simulations done in the directories noted below were simply done to probe for the algorithm error.

The directories where these tests were done are:

./TPA4/RUNS/Subarea8/ and variations of ./Subarea8-??/

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Screen output was used to judge the results of the test and was captured into a file called *std.out*, which is saved in each working directory. The screen output notes which subareas had all zero entries; hence if subarea 8 is **not** listed, and all of the other subareas are listed, then by default the test passes. When UZFLOW calculates subarea averages, it stops after calculating subarea averages when the average equals zero and prints messages to the screen. The captured screen output was inspected to make sure that only subarea 8 had a non-zero average.

This series of simulations done in the directories noted above indicate that UZFLOW is not properly aggregating the ITYM output into subarea averages. Re-testing after correction of this problem is reported later in this scientific notebook.

### Test 4 – Evaluate UZFLOW's Ability to Read *maidtbl.dat* With and Without Errors in the *maidtbl.dat* File

Tests were made using manipulated *maidtbl.dat* files that contained unusual or garbage information to check UZFLOW ability to bomb-out when passed bad information.

The directories where these tests were done are:

| | |
|---|---|
| ./TPA4/RUNS/Zero/ | *maidtbl.dat:* mostly zero infiltration entries |
| ./TPA4/RUNS/Zero1/ | *maidtbl.dat:* zero infiltration entries only for low temperature and precip DEM |
| ./TPA4/RUNS/Zero2/ | *maidtbl.dat:* some zero infiltration entries, but each subarea average > 0 (maid2.f) |
| ./TPA4/RUNS/Zero3/ | *maidtbl.dat:* some MAI > MAP (maid23.f) |
| ./TPA4/RUNS/Zero3a/ | *maidtbl.dat:* subarea average MAI > MAP (maid23a.f) |
| ./TPA4/RUNS/Garbage/ | *maidtbl.dat:* mostly zero infiltration entries |
| ./TPA4/RUNS/Garbage2/ | *maidtbl.dat:* gibberish entry in the infiltration field |
| ./TPA4/RUNS/Garbage/ | *maidtbl.dat:* cell size set to 30 but NCOLS=49 and NROWS=75 (maidG2.dat file) |
| ./TPA4/RUNS/Table/ | *maidtbl.dat*: *tpa.inp* temperature set to higher value than in *maidtbl.dat* |

1. It was shown that the comment lines added to the top of *maidtbl.dat* were properly read in by UZFLOW.

2. Some values of zero as infiltration are okay (some pixels may have evaporation equal to or greater than precipitation), however, subarea averages of zero infiltration are not likely. TPA 4.0 properly ran to completion when some entries were zero, and it properly bombed when a subarea average was zero for at least one climate state DEM. It was checked to see if infiltration values greater than the precipitation would cause UZFLOW to bomb; it only bombed when the subarea average MAI was greater than the precipitation, which is good. Screen capture of the simulation were checked to determine when the code bombed (stopped before completing a simulation).

3. The TPA 4.0 code stopped when gibberish entries (non-numeric entries for infiltration) and keyword errors (CELLSIZE) were manually put into the *maidtbl.dat* file. This part of the check was done in case someone manually alters the *maidtbl.dat* file instead of using ITYM to create it.

4. The TPA 4.0 code stopped when the *tpa.inp* file climate conditions were set to higher values than the climate range output in the *maidtbl.dat* file. Kind of tough to interpolate when you don't have a large enough range for the interpolation.

### Test 5 – Check Reasonableness of Output From ITYM

The reasonableness of ITYM output was checked 2 different ways. One, plots of the infiltration DEM for a couple different climates were made in Tecplot 7.0 and the magnitude and spatial variability were judged based on my knowledge of shallow infiltration at Yucca Mountain. Two, magnitudes of subarea averages and modeling domain averages were tracked over changes in climate. In addition, the number of realizations needed by ITYM for the expected values to stabilize was tracked. This was done to verify that the base case number of realizations was adequate to cover the uncertainty.

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Plot files are:
./c120-p100-t0.eps
./c120-p100-t0-full.eps
./c120-p200-t14-full.eps
./maidr1000-P200-T14.eps

Location of tests for number of realization:
./TPA4/ITYM/Real50/*
./TPA4/ITYM/Real100/*
./TPA4/ITYM/Real500/*
./TPA4/ITYM/Real1000/*

Shallow infiltration estimates from ITYM as extracted from captured screen output
(4 x 4 =16 climate states calculated for each realization number case [timings])

| Climate | Expected Means for Specified Number of Realizations (R) | | | |
|---|---|---|---|---|
| | R=50 | R=100 | R=500 | R=1000 |
| P=100, T=0 | 6.23 | 8.14 | 10.44 | 10.64 |
| P=200, T=7.3 | 25.19 | 24.99 | 22.40 | 22.35 |
| P=200, T=14.7 | 16.78 | 15.51 | 14.89 | 15.42 |
| P=400, T=14.7 | 56.21 | 48.77 | 48.18 | 50.46 |
| P=800, T=14.7 | 153.02 | 163.44 | 149.43 | 142.59 |
| Simulation Time, in response to question of why this is not run each tpa.e execution | | | | |
| Time (minutes) | 177.53 | 163.44 | 700.4 | 1387.2 |
| min/realization | 3.5 | 1.6 | 1.40 | 1.39 |

Note that for shorter simulations, lesser number of realizations, the timings are inconsistent. This is likely caused by the heavy usage of vulcan during Real50 and not during Real100. The overnight simulations (Real500 and Real1000) are more consistent (1 realization takes 1.4 minutes). The mean value infiltration=2.006 mm/yr is obtained for the *itym.dat-stdev0* simulation (all standard deviations set to zero, one realization) for climate modern climate of Precip=162.8 mm and Temperature=17.38 deg Celcius. This further illustrates the effect of using Monte Carlo averages rather than mean values in the input (the increase in predicted results).

Conclusion: ITYM preprocessor produces reasonable results that are consistent in spatial variability expected for the crest, ridgetop and steep hillslopes of Yucca Mountain. The magnitude of MAI for subareas were consistent with what was expected for different climate conditions and it illustrated the expected qualitative interplay between precipitation and temperature and their effect on shallow infiltration. Also, based any stability of mean values, the 1000-realization case should be used as the base case for TPA4.0 simulations.

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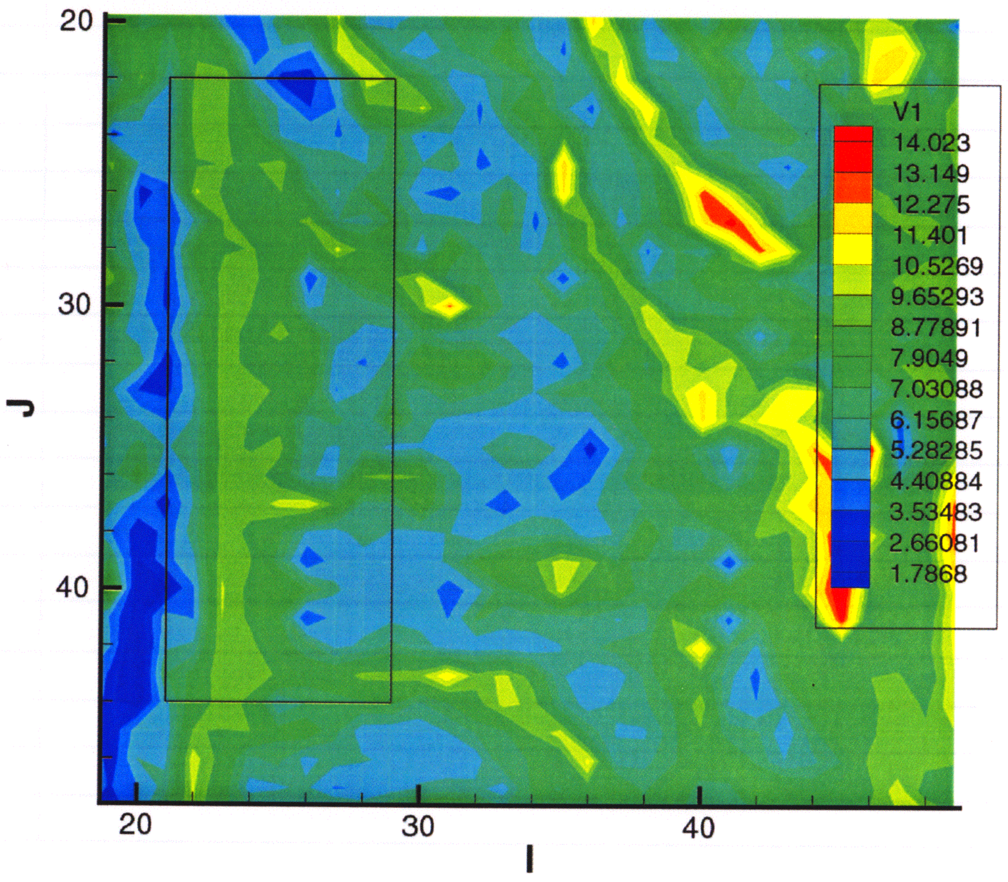
Cell size=120; Precipitation=100mm/yr; Temperature=0 deg C; Realizations=10
Only area near repository is plotted; approximate outline of repository in black.

(2D) | 22 Mar 2000 |



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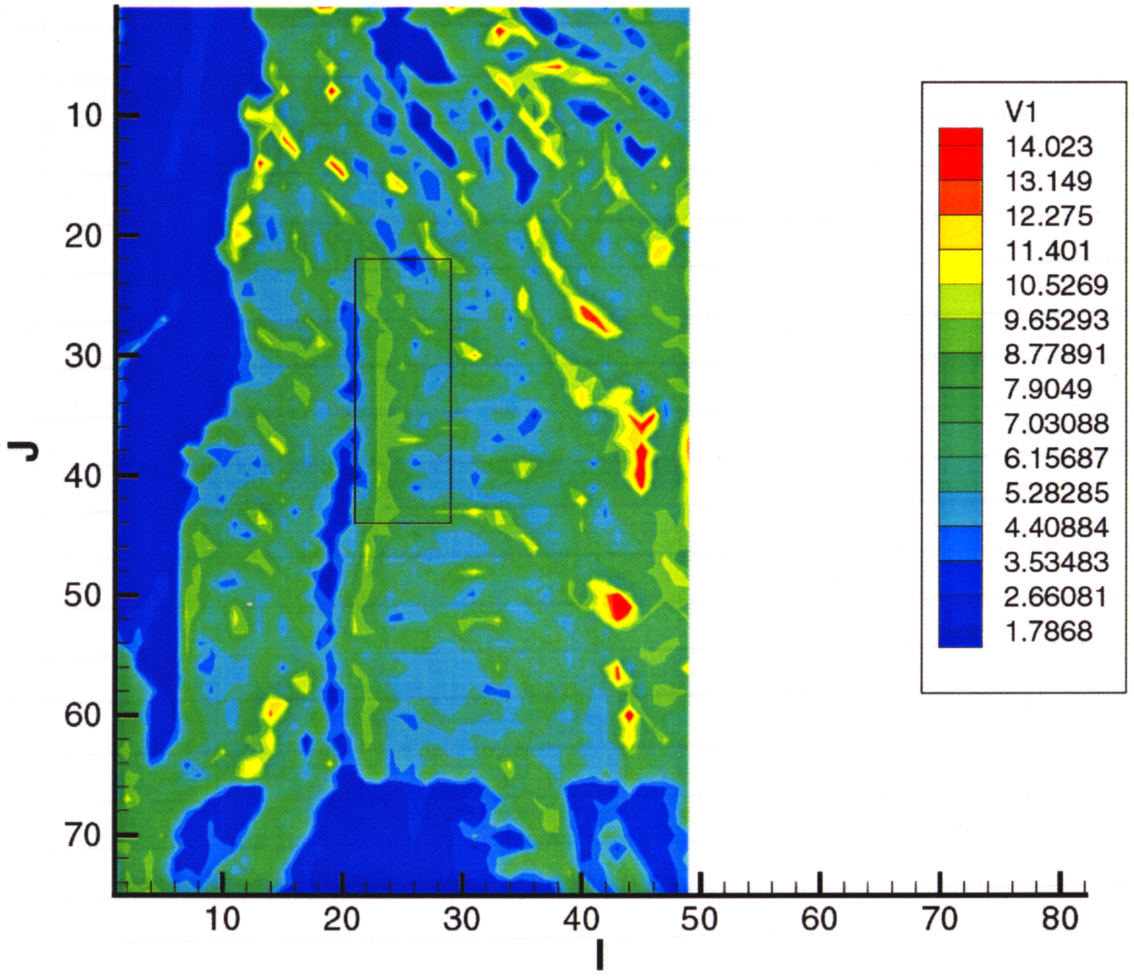
Cell size=120; Precipitation=100mm/yr; Temperature=0 deg C; Realizations=10
Entire modeling area; approximate outline of repository in black.

(2D) | 22 Mar 2000 |



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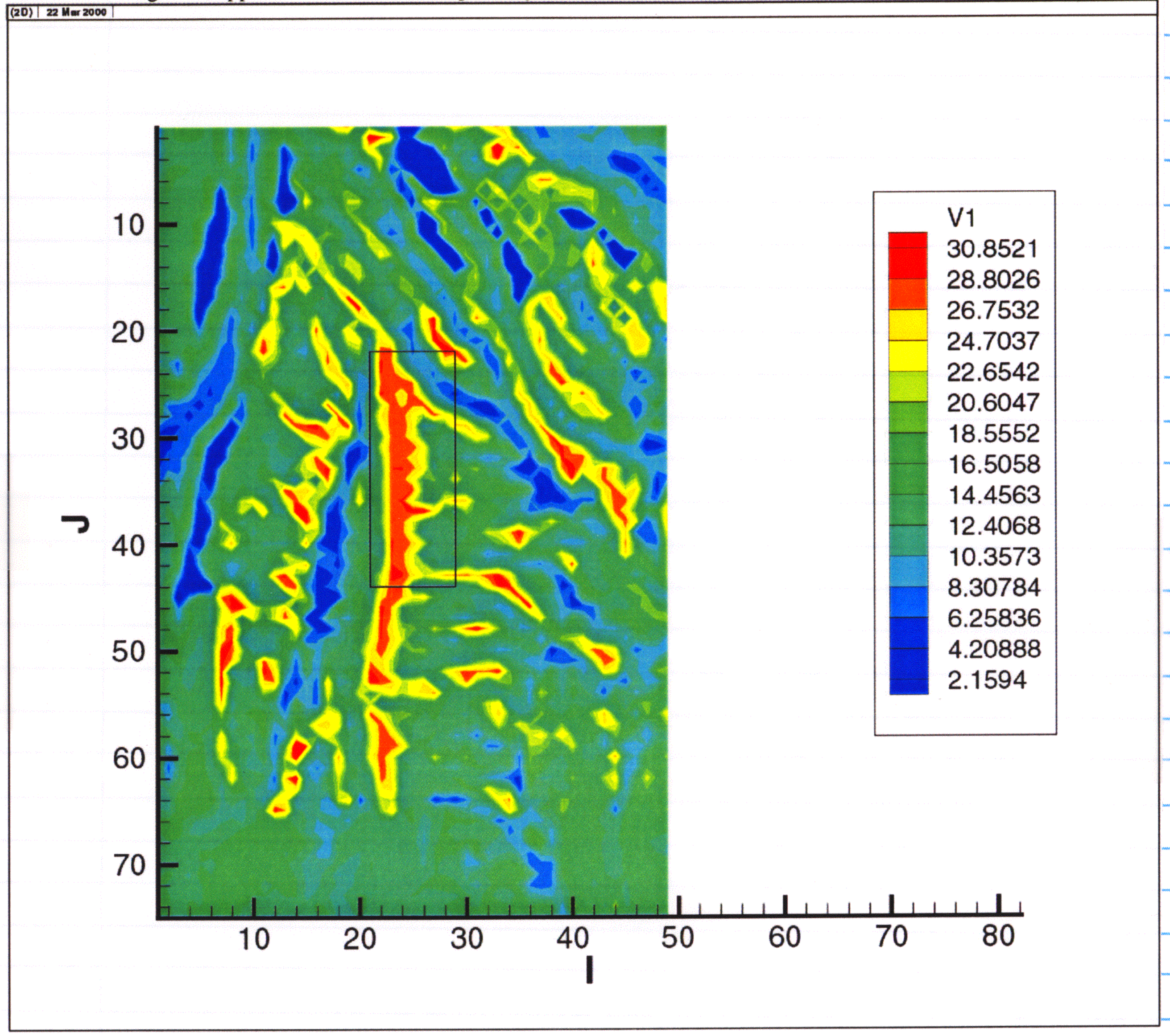
RF

Cell size=120; Precipitation=200mm/yr; Temperature=14.67 deg C; Realizations=10
Entire modeling area; approximate outline of repository in black.



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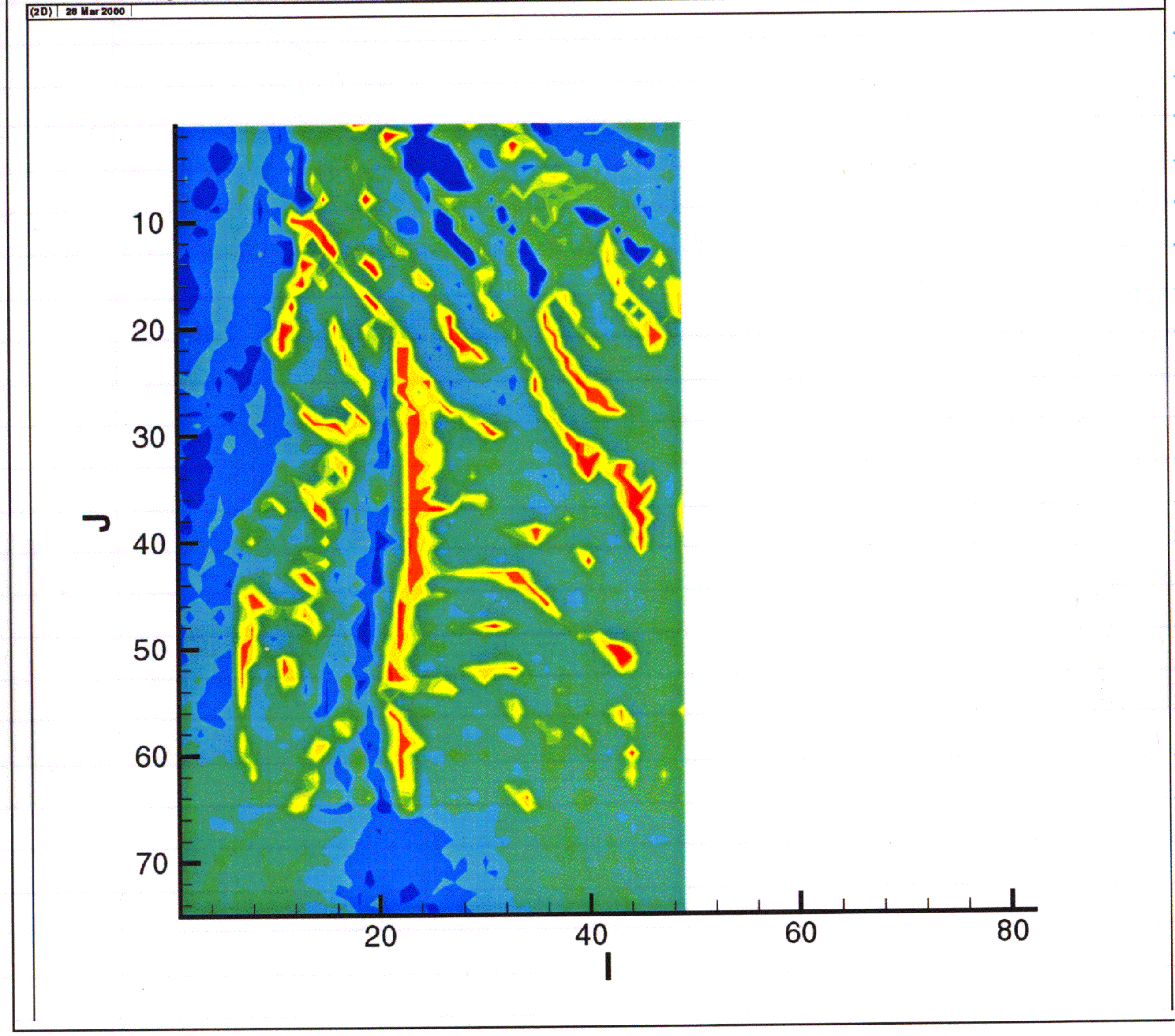
Cell size=120; Precipitation=200mm/yr; Temperature=14.67 deg C; Realizations=1000
Entire modeling area; approximate outline of repository in black.



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**Test 6 – Comparison of TPA 3.2.3 and TPA 4.0 Results**

Single realizations were created in using the ITYM preprocessor with standard deviations set to "0" in *itym.dat* so that a comparison could be made with TPA 3.2.3 results. The *itym.dat* file was edited to change all standard deviations throughout all the tables in the file. Using the mean values in ITYM should lead to similar results between TPA 3.2.3 results and TPA 4.0 (TPA3 option). Some small differences should be expected since the subarea delineations have changed slightly since TPA 3.x. The *itym.dat* file used to create the *maidtbl.dat* files are referenced below:

./TPA4/ITYM/TPA3/*itym.dat-stdev0*
./TPA4/ITYM/TPA3/*maidtbl.dat.tpa3-real1*
./TPA4/ITYM/TPA3/*maidtbl.dat.tpa4-real1*

The simulations were made in
./TPA3/Runs-1/*
./TPA4/RUNS/TPA3/*
./TPA4/RUNS/TPA3-4/*

The output *infilper.res* output file was checked in all cases and the results were tabulated for two times, time=0 and time step 201 (time = 10,000yrs).

| Infiltration output read from infilper.res output file, subarea flux (m3/yr) | | | | | | | |
|---|---|---|---|---|---|---|---|
| | TPA 3.2.3 Results | | TPA 4.0 (TPA3 option) | | TPA 4.0 (TPA4 option) | | |
| | time 0 yr | time 10000 | time 0 yr | time 10000 | time 0 yr | time 10000 | |
| Subarea | | | | | | | |
| 1 | 4187 | 16271 | 3867.6 | 9476.9 | 4007.8 | 11207 | |
| 2 | 4531.7 | 17495 | 4667.5 | 11180 | 4924.7 | 13503 | |
| 3 | 2520.7 | 9509.4 | 2133.3 | 5078.9 | 1367.3 | 4170.3 | |
| 4 | 1164.8 | 4586.8 | 1246.8 | 3029.2 | 1038 | 2928.3 | |
| 5 | 1893.3 | 7071.6 | 2159.5 | 5172.8 | 1927 | 5449 | |
| 6 | 2046.7 | 7803.9 | 2400.9 | 5563.4 | 2370.3 | 6691 | |
| 7 | 728.48 | 2824.8 | 768.88 | 1709.3 | 1066.5 | 2918.7 | |
| 8 | | | 1826.9 | 4659.5 | 2377.1 | 6467.7 | |

The differences between TPA 3.2.3 and TPA 4.0 (TPA3 option) appear to be reasonable and do not suggest any problem with the implementation in TPA 4.0. The large fluxes at time 10,000 years in TPA 3.2.3 results were not unexpected since we knew that this version was over-predicting infiltration for future climates.

While the values appear to be reasonable, and lead to reasonable infiltration flux values when the subarea areas values are separated out, it was surprising to find that the western subareas did not have larger fluxes than the eastern subareas (i.e., subareas 1 should have higher flux than subarea 2; subarea 5 should have higher flux than subarea 6, and subarea 6 should have higher flux than subarea 7). Note that TPA 3.2.3 did not appear to have this problem with subarea averaging (see Test 3 results).

The following table (next page) repeats the volumetric flux ($m^3$/yr) output reported in the table above, but has been converted to linear flux (mm/yr) rates by dividing out the areas of each subarea. The reduction in infiltration under a future climate as calculated using TPA 3.2.3 versus that calculated using TPA 4.0/TPA3 option is evident. The reduction was expected because of a bug-fix found in the TPA 3.x algorithm that lead to high future infiltration estimates.

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| Using same subarea areas for TPA 3.2.3 and TPA 4.0 (leads to small error) [FLUX mm/yr] | | | | | | |
|---|---|---|---|---|---|---|
| | TPA 3.2.3 Results | | TPA 4.0 (TPA3 option) | | TPA 4.0 (TPA4 option) | |
| | time 0 yr | time 10000 | time 0 yr | time 10000 | time 0 yr | time 10000 |
| Subarea | | | | | | |
| 1 | 5.79 | 22.49 | 5.35 | 13.10 | 5.54 | 15.49 |
| 2 | 5.77 | 22.29 | 5.95 | 14.25 | 6.28 | 17.21 |
| 3 | 6.46 | 24.36 | 5.46 | 13.01 | 3.50 | 10.68 |
| 4 | 5.61 | 22.10 | 6.01 | 14.59 | 5.00 | 14.11 |
| 5 | 5.00 | 18.66 | 5.70 | 13.65 | 5.08 | 14.38 |
| 6 | 4.82 | 18.37 | 5.65 | 13.09 | 5.58 | 15.75 |
| 7 | 4.44 | 17.23 | 4.69 | 10.43 | 6.51 | 17.80 |
| 8 | | | 4.64 | 11.84 | 6.04 | 16.44 |

**TESTING AFTER CHANGES TO UZFLOW MODULE (March 27, 2000)**

Initial testing (Tests 1-6) found a problem with the subarea averaging in UZFLOW. The following changes were made in the code. One of the changes is not related to the subarea issue, it allows for UZFLOW to input one climate from the *maidtbl.dat* and ITYM if a constant climate is needed for testing. The problem was a flip-flopping of indices so that at 3 locations in the *uzflow.f* code, the pointer definition was flipped between the x-direction and y-direction.

The code changes are listed on the following page. A summary of Test 3 and Test 6 test results that were re-run is included here. Portions of Test 3 and Test 6 were re-run to make sure that the changes in UZFLOW corrected the problem and did not cause any other unexpected problem to arise.

Re-testing was done in:
./TPA4/Sa8a/
./TPA4/Real1000/ using tpa40betaK/tpa.e
./TPA4/re-Real1000/ using ./TPA-Compile/tpa.e (later used for tpa40betaO version)
Note that Ron Janetzke recompiled tpa40betaO for me, but he forgot to include the changes to UZFLOW. Hence, I recompiled his /home/janetzke/tpa40betaO/*.f, except with the new *uzflow.f*, in the directory:
./TPA-Compile/

**Re-Test 3**

To check for proper subarea averaging, I again used the *maidtbl.dat* file with zero entries everywhere except in the pixels of subarea 8. This *maidtble.dat* file was created by compiling running the ./TPA4/ITYM/*maidsa8.f* code and creating the file called ./TPA4/ITYM/maidsa8.dat, which was then copied into the ./TPA_TEST/data directory to replace the *maidtbl.dat* file.

The ./TPA4/RUNS/*SA8a/std.out* output file shows that subareas 1 to 7 have zero averages, thus by default subarea 8 is the only subarea with non-zero averages.

The test shows that the bug fixes in UZFLOW have corrected the problem.

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Four Stothoff corrections per testing 3/27/00

```
>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
in subroutine calc_wp     insert code fragment

c% one entry only
        if (nvec .eq. 1) then
                if (abs(vec(1)-val) .lt. 1d-10) then
                        wgt1    = done
                        wgt2    = dzero
                        mpnt1   = 1
                        mpnt2   = 1
                                                        return
                endif
        endif

after
       INTEGER nvec, mpnt1, mpnt2
       INTEGER it1, m1, m2

>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
in subroutine load1DTBL
        data idDTBLids / mDTBLxll, mDTBLyll, mDTBLdx,
     &          mDTBLny, mDTBLnx, mDTBLbad, mDTBLv1, mDTBLv2 /

should be
        data idDTBLids / mDTBLxll, mDTBLyll, mDTBLdx,
     &          mDTBLnx, mDTBLny, mDTBLbad, mDTBLv1, mDTBLv2 /

>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
in subroutine DEMij_to_m
       mi       = (nint(DTBLStat(mDTBLny)) - my)
     &                  * nint(DTBLStat(mDTBLnx)) + mx

should be
        mi       = (my - 1) * nint(DTBLStat(mDTBLnx)) + mx

>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
in subroutine mapDTBL_to_SAs

after
        x0(1)    = DTBLStat(mDTBLxll)
        x0(2)    = DTBLStat(mDTBLyll)
        dx(1)    = DTBLStat(mDTBLdx)
        dx(2)    = DTBLStat(mDTBLdy)
        nx(1)    = nint(DTBLStat(mDTBLnx))
        nx(2)    = nint(DTBLStat(mDTBLny))

add
c% correct for flipped Y direction

        x0(2)    = x0(2) + (nx(2) - 1) * dx(2)
        dx(2)    = -dx(2)

also
           do it2 = irSA(1,1), irSA(1,2)
                xpt(1)   = x0(1) + dx(1) * dble(it2 - 1)
                do it3 = irSA(2,1), irSA(2,2)
                        xpt(2)   = x0(2) + dx(2) * dble(it3 - 1)

should be
           do it2 = irSA(1,1), irSA(1,2)
                xpt(1)   = x0(1) + dx(1) * dble(it2 - 1)
                do it3 = irSA(2,1), irSA(2,2), -1
                        xpt(2)   = x0(2) + dx(2) * dble(it3 - 1)
```

---

RF 3/30/00

RF

**Re-Test 6**

I then set the environment variable to find this new tpa.e [setenv TPA_TEST /vscr1/rfedors/TPA-Compile/; as noted above, the next day Ron Janetzke straightened out this problem and correctly recompiled the tpa40betaO version]. The data directories have to be kept separate, so I created ./TPA/dataK/ and ./TPA4/dataO/ directories and copied the appropriate external files for the version of *tpa.e* I was running (you cannot mix all external files between code versions because of small changes in the external files and the code).

The table below was created from *uzflow.rlt* files in:
./TPA4/RUNS/Real1000/
./TPA4/RUNS/re-Real1000/
where the tpa40betaO version was used with the uzflow parameters (*tpa.inp*) set to constant values so that a direct comparison could be made and the *maidtbl.dat* file created using 1000 realizations (./TPA4/ITYM/*maidtbl.dat.real1000*).

The following table shows that the subarea values for infiltration flux are reasonable with respect to western subareas having greater fluxes than the eastern subareas. As a reasonableness check, this shows that the subarea averaging is working properly.

Re-testing of UZFLOW after bug fixes were put in; indexing problem for subarea averaging.
volumetric flux from *uzflow.rlt* output file; infiltration flux is q/area*1000

| | Old UZFLOW at time=0 | | New UZFLOW, t=0 yr | | Old at t=10,000 yr | | New UZFLOW, t=10,000yr | |
|---|---|---|---|---|---|---|---|---|
| Subarea | q(m3/yr) | infilt (mm/yr) | q(m3/yr) | infilt (mm/yr) | q(m3/yr) | infilt (mm/yr) | q(m3/yr) | infil,mm/yr |
| 1 | 3843.4 | 5.31 | 4859.1 | 6.72 | 7149.1 | 9.88 | 8728.5 | 12.06 |
| 2 | 4923.8 | 6.27 | 3870.3 | 4.93 | 9034.5 | 11.51 | 7096 | 9.04 |
| 3 | 2085.3 | 5.34 | 2364.2 | 6.06 | 3889.4 | 9.96 | 4280.4 | 10.96 |
| 4 | 1025.2 | 4.94 | 831.61 | 4.01 | 1925.8 | 9.28 | 1562.4 | 7.53 |
| 5 | 2129.9 | 5.62 | 2137.2 | 5.64 | 3916.8 | 10.34 | 3894 | 10.28 |
| 6 | 2284.6 | 5.38 | 1912.8 | 4.50 | 4255.5 | 10.02 | 3544.6 | 8.34 |
| 7 | 928.08 | 5.66 | 710.97 | 4.34 | 1718.3 | 10.48 | 1323.5 | 8.07 |
| 8 | 1834.7 | 4.66 | 2282.9 | 5.80 | 3497 | 8.89 | 4140.8 | 10.52 |

**Recommendations for Changes to UZFLOW and ITYM:**

1. Change tab-delimited ascii text *itym.dat* input file to space-delimited, or change the read format in ITYM to be flexible to handle either space- or tab-delimited *itym.dat* format.
2. Add the standard deviation of infiltration estimates from ITYM as a separate DEM file for UZFLOW to use for LHS sampling. This brings a consistency of sampling distributions of parameters completely into the TPA realm.

**Archiving of Work**

All work was archived to a 250 Mbyte zip diskette. Unfortunately, Microsoft likes to remove case dependency when transferring files and directories between UNIX and WinNT and back to UNIX (scratch disks are deleted each Sunday night by IMS staff, thus necessitating the transfer back and forth). Therefore, the directory names and occasionally a file name are archived lower case, instead of the original and reported mixed case (directory names were often capitalized).

pages 26-45 taped into notebook on 4/4/03 KF

RF **10/14/02**

Primary computer running WindowsNT 4.00.1381 is called bubo (Acer, x86 Family 6 Model 4 Stepping 2; AT compatible with 512 MBytes RAM).

WinNT Software: ArcView version 3.2a; Lahey/Fujitsu Fortran 95 version 5.0; Excel 97 SR-2; WORD 97 SR-2. Spock is a SUN sparc Ultra 4 (4 cpu), 64-bit, running SunOS version (Kernel ID) Generic_108528-17 release 5.8 SUN Software: fortran 77 version 5.0 (SUN Workshop Compiler FORTRAN 77 version 5.0).

## TPA Modifications and Testing

Collaborators: Stuart Stothoff, David Woolhiser, George Adams, and Carol Schirer (testing only).

Objective is to modify UZFLOW and ITYM for TPA 5.0 to address the following:

1. Utilize variance estimated in ITYM for Latin Hypercube sampling in TPA code; also fix some known bugs.
2. Add effect of runon to ITYM.
3. Software Change Report (SCR) testing

### Runon/Runoff for ITYM

Dave Woolhiser (sci ntbk #444) developed the following relationship from the Split Wash KINEROS2 modeling results for storms from 1985 to 1995. The overall basis is being documented in an update of the Split Wash report with Roger Smith. The approach given to Stothoff for code changes to ITYM (TPA 5.0) is:

1. Read external files (DEMs are created once and used for all simulations; to be read by ITYM during execution)
   - estimate of number of contributing upslope pixels (Ar), estimate is for each pixel
   - estimate of mean depth of contributing pixels (hav), estimate is for each pixel

2. Calculate E = excess precipitation, which should be added to the existing precipitation applied to the pixel:

For soil depth i > 400 mm and Ar > 0 then
    $E = 4.097 + 0.300\ Ar - 0.0104\ hav$
else  $E = 0$

where Ar and hav are drawn from the external file created in item 1 above.

The channels are more difficult to address, though based on Woolhiser's analyses they are a small effect. It should be noted that the deep infiltration is very concentrated in channels, however, the channels occupy a small area of the watershed and will not contribute much to the watershed average. Think in terms of a 1- or 2-meter-wide channel crossing a 30-m pixel. So for now, I intend to omit their effect. This whole approach focuses on getting the reasonable values for the repository area. Strange results may occur in areas off the mountain. Hence, for now, I am inclined to mask-off the runon effect for areas around the mountain. Since there are some problem areas in the current implementation of ITYM for non-YM mountain/repository area, this deferment becomes more palatable.

Stothoff made the initial changes to the ITYM code. Below are the analyses of the testing results by George Adams and myself once we checked and revised Stothoff's code changes to ITYM. See George's TPA scientific notebook for these revisions.

Check of Output for Runon Abstraction

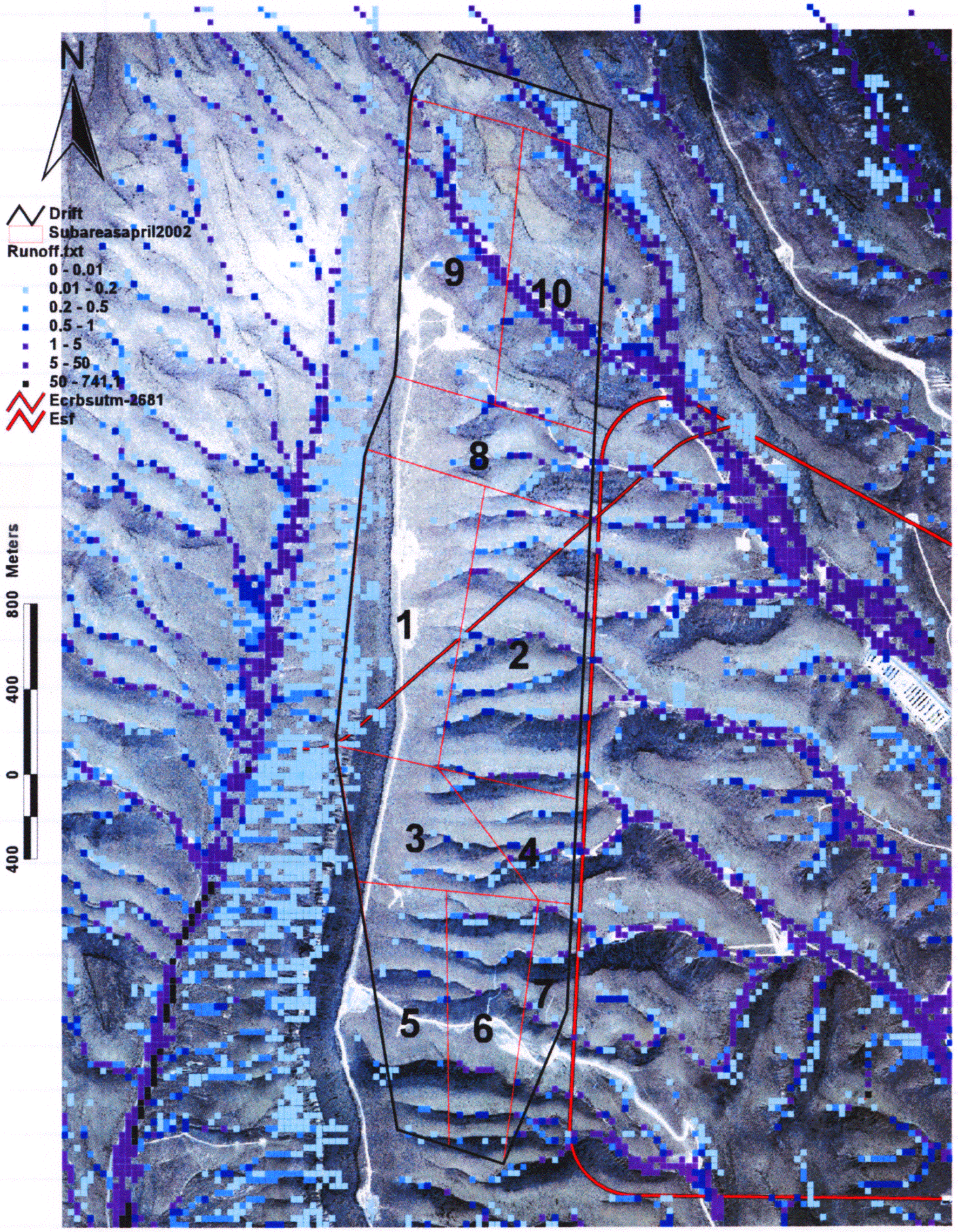
George Adams ran ITYM with and without the runoff abstraction, then subtracted the two results.
I reformatted the data to import into ArcView version 3.2 for plotting using the following script, compiled and executed on spock (SUN OS). Then I imported the data as a table and plotted the results by overlaying known features (e.g., repository outline, subareas, air photo all in UTM NAD27 coordinates). I plotted up the results; and stored them in:
spock ~/TPA_2002/RunoffCheck/*  extraction of point/cell data from infiltration map files
bubo: E:\AVData\TPA\testingTPA_April2002.apr  [and supporting ArcView files]
bubo: E:\ AVData\TPA \Runoff*

The script, a fortran code named arcread.f, was compiled using f77 (fortran 77 on spock). The output of this script is the ascii text file called "runoff.txt" that can be read into ArcView 3.2a.

```
         program arcread
c script for reading in infiltration maps from ITYM and reformatting them
c   in a file that ArcView can read in as a table. Run on spock (SUN OS, UNIX).
c RFedors  Oct 14, 2002
c  spock: ~/ITYM-Usage/arcread.f   or copied to bubo: J:\Itym-Usage\arcread.f
c23456789 123456789 123456789 123456789 123456789 123456789 123456789 12
      integer  ioread, iowrit, mx, i, j, k, ncols, nrows
      parameter (mx=100000)
      real*8  array(mx,3)
      real*8  xllcorner, yllcorner, cellsize, xpos, ypos
      character*9  junk
      character*60  header

c set input and output unit numbers
      ioread = 7
      iowrit = 8
c read in DEM of infiltration; note that the coordinates of the
c southwest corner of the domain are given in the header, but the
c ordering of data is row-major starting from the northwest corner.
c     open(unit = ioread, file = 'maidtbl.dat', form = 'formatted')
      open(unit = ioread, file = 'maidtbl-diff.dat', form = 'formatted')

      do i = 1, 4
        read(ioread,'(a60)') header
      enddo
      read(ioread,'(a9,i10)') junk, ncols
      read(ioread,'(a9,i10)') junk, nrows
      read(ioread,'(a9,f16.5)') junk, xllcorner
      read(ioread,'(a9,f16.5)') junk, yllcorner
      read(ioread,'(a9,f15.5)') junk, cellsize
      do i = 1, 3
        read(ioread,'(a60)') header
      enddo
      print*, ncols, nrows, cellsize, xllcorner, yllcorner
      ypos = yllcorner + cellsize * dfloat(nrows-1)
      xpos = xllcorner
      k = 1
      do i = 1, nrows
        do j = 1, ncols
          read(ioread,'(e15.8)') array(k,3)
          array(k,1) = xpos
          array(k,2) = ypos
          xpos = xpos + cellsize
          k = k + 1
        enddo
        ypos = ypos - cellsize
        xpos = xllcorner
      enddo
      close(ioread)
c writing out the array() matrix for digestion in arcinfo, which needs 3 columns
      open(unit = iowrit, file = 'runoff.txt', form = 'formatted')
      write(iowrit,*) 'Easting m, Northing m, Infilt-runon mm '
      do i = 1, ncols*nrows
         write(iowrit,100)  ( array(i,k), k = 1,3 )
      enddo
 100  format(2(f11.2,','),f10.5)
      stop
      end
```

The conclusion that the runon results are acceptable is made by qualitative judgement that the magnitudes and spatial patterns of increased net infiltration from runon are reasonable. The pattern of elevated net infiltration values from runon are reasonable based on the figure plotted below (Figure on page 28). The primary area of concern is in the repository footprint (in deep soils the abstraction may be way off). The magnitudes patterns are reasonable, and are grossly similar to DOE results. Note directory change on bubo, the old J: is now E:

Net Infiltration (mm/yr) from Runoff/Runon by ITYM Oct 2002; plotted ArcView, bubo: J:\AVData\TPA\Runoff



RF

**Testing PA-SCR-346**

Dec 26, 2002

**PL-3 Test**

Work saved in
bubo: E:\TPA_FY2002\Dec2002\Scr-346\PL-3_test\

Email from George:

Please find the attached archive containing the data for test pl-3 of PA-SCR-346. I'm asking for you to plot the data in maidtbl-acurrentclimate.dat.

PA-SCR-346, PL-3 (contained in ascii file pl-3.txt)

The files were generated as follows:
1) maidtbl-acurrentclimate.dat: Generated over 500 realizations with the current climate extracted from the resulting maidtbl.dat file.
2) PA-SCR-346_PL3a.out: Screen output from running the itym preprocessor. The itym.dat file was setup with the following parameters:
   A) 500 realizations
   B) 9 tables (3 MAP, 3 MAT)
   C) MAP range: 152.8 to 172.8
   D) MAT range: 15.38 to 19.38
   E) 30 m pixels
3) pl3.xls: Mean Annual Infiltration values were extracted from PA-SCR-346_PL3a.out.

The test calls for the following:
1) Plot the information contained in maidtbl-acurrentclimate.dat. Compare the resulting plot to DOE plots in terms of MAI magnitude and spatial variability. Compare the MAI magnitude to DOE tabulated values. These tabulated values were extracted from document: ANL-NBS-HS-000032 REV 00, Table 6-9 and are as follows:

| Modern Climate Scenaria Mean Average Annual Net Infiltration (mm/yr) | Lower Bound | Mean | Upper Bound |
|---|---|---|---|
| | 1.3 | 4.6 | 11.1 |

2) Verify the screen output values (PA-SCR-346_PL3a.out and pl3.xls) are reasonable for the climate conditions. The MAI values were extracted from PA-SCR-346_PL3a.out and placed in pl3.xls. It may not be possible to determine if the other values generated to the screen are reasonable.

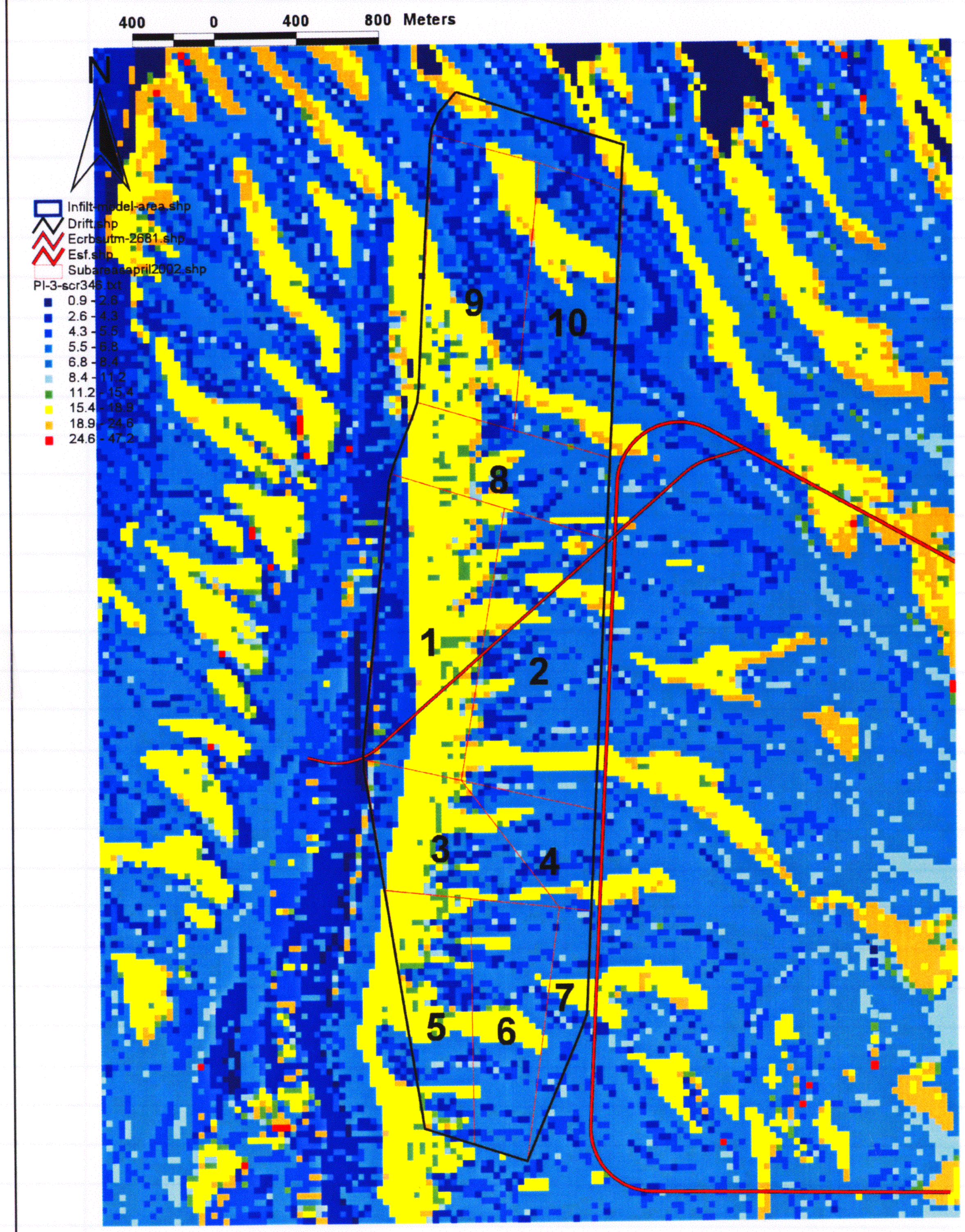
I recompiled arcread.f after changing the “open file” statement to instead read in “maidtbl-acurrentclimate.dat” and changed the output file name to “pl-3-scr346.txt.”

Again, the output from arcread.exe was imported into ArcView 3.2 and plotted, see next figure (page 30, next page).
bubo: E:\AVData\TPA\testingTPA_April2002.apr
See output file from ArcView as an Illustrator pdf file,
bubo: E:\TPA_FY2002\Dec2002\Scr-346\PL-3_test\pl3-scr346.pdf

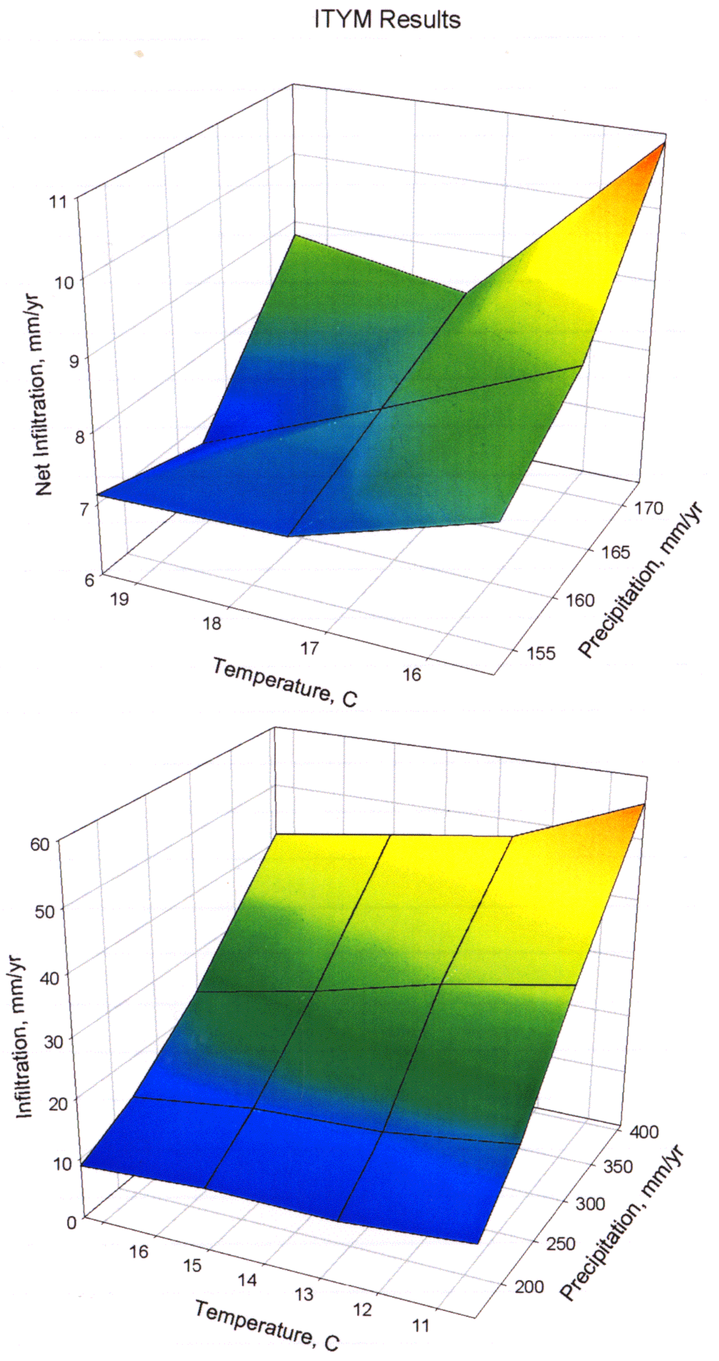
The values from ITYM are reasonable:

- the spatial distribution is similar to that of the DOE (ANL-NBS-HS-000032 REV 00);
- the average for ITYM results is within the bounds of the DOE table 6-9 averages (DOE UZ flow and transport model domain) for lower, mean, and upper bound cases;
- the ITYM model results remain slightly higher than the DOE mean case as expected and as maintained by CNWRA staff based on supporting information (temperature data and chloride data in perched water).

Figure for PA-SCR-346 PL-3 test, net infiltration at current climate



A plot of the variation of net infiltration as a function of climate (precipitation and temperature) is include on this page. There was some worry about the inflection points on the uppermost figure, but it was decided that this was just noise (note the small range in temperature and precipitation). The lowermost figure on page 31illustrates what was expected over periods of climate change (modern to monsoonal to glacial transition). This figure was created in Sigma Plot 2000 version 6.00 using the data collected by George Adams. (see file pl3.JNB in the PL-3_test directory).



## PA-SCR-346 SL-2 Test

Response to George Adams' email for PA-SCR-346 SL-2 test:

From: George R. Adams [mailto:george.adams@swri.org]
Sent: Thursday, January 02, 2003 3:44 PM
To: Randy Fedors
Subject: PA-SCR-346, SL-2

Randy,

Please find attached an updated archive containing the SL-2 test results. I updated the Excel spreadsheet to show the correct TPA4 values. The subarea rankings for the first 8 subareas are comparable to the new results except subareas 5 and 8 are reversed in the rankings. Since subareas 5 and 8 have MAIs that are relatively close together, it seems like the change in ranking is not significant.

The test calls for verifying the average infiltration values for each subarea are reasonable and change as expected from time = 0 to time = 10000. Would you comment on this?

Thanks,
George

Comment:

In the TPA 5.0 testing, the subarea averages are constrained to an average of 12.51 in the realization reported. The effect of future climates is also constrained by tpa.inp entries. The average net infiltration for modern and future climates (10,000 yrs) are reasonable given the current understanding of infiltration and percolation at Yucca Mountain of NRC and CNWRA hydrologists and considering DOE estimates.

TPA 5.0 appears to be working correctly since the rankings of net infiltration are similar to those of previous TPA versions (3.2 and 4.0), particularly when the new subareas are factored out. Subareas 5 and 8 have reversed their rankings between the different TPA versions (4.0 and 5.0). However, their (subarea 5 and 8) net infiltration rates are not significantly different, so the switch in rankings is not considered important. The net infiltration rankings of the 10 subareas is consistent with our understanding of net infiltration processes and projected zones of elevated net infiltration at Yucca Mountain, particularly the high infiltration zones on and near Yucca Mountain crest and the east-trending ridges where the caprock unit occurs at the ground surface.

see bubo: E:\TPA_FY2002\Dec2002\SCR-346\SL-2_test\sl-2.xls from George
A printout of the spreadsheet is provided here as reference (see table on page 33).

---

**Test Results for Test SL-2, October 15, 2002**

**ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] = 12.153**

**Results from file uzflow.rlt**

**Infiltration output q (m3/yr/sa)**

| | **TPA 4.0 (TPA3 option)** | | **TPA 4.0 (TPA4 option)** | | **Test SL-2** | **(TPA 5.0Beta)** | **% increase** |
|---|---|---|---|---|---|---|---|
| Subarea | Time 0 | Time 10000 | Time 0 | Time 10000 | Time 0 | Time 10000 | |
| 1 | 3867.6 | 9476.9 | 4859.10 | 8728.5 | 12527.0 | 29017.0 | 132% |
| 2 | 4667.5 | 11180.0 | 3870.30 | 7096.0 | 7646.3 | 17374.0 | 127% |
| 3 | 2133.3 | 5078.9 | 2364.20 | 4280.4 | 5677.5 | 13086.0 | 130% |
| 4 | 1246.8 | 3029.2 | 831.61 | 1562.4 | 1555.6 | 3523.2 | 126% |
| 5 | 2159.5 | 5172.8 | 2137.20 | 3894.0 | 5356.4 | 12365.0 | 131% |
| 6 | 2400.9 | 5563.4 | 1912.80 | 3544.6 | 3476.9 | 7883.0 | 127% |
| 7 | 768.9 | 1709.3 | 710.97 | 1323.5 | 1306.0 | 2972.4 | 128% |
| 8 | 1826.9 | 4659.5 | 2282.90 | 4140.8 | 5474.5 | 12573.0 | 130% |
| 9 | | | | | 8355.5 | 19376.0 | 132% |
| 10 | | | | | 5932.3 | 13634.0 | 130% |

**Results from file uzflow.rlt**

**Dividing out subarea size**

**Infiltration output divided by subarea size (mm/yr)**

| | **TPA 4.0 (TPA3 option)** | | **TPA 4.0 (TPA4 option)** | | | | **Subarea Size** | **Test SL-2** | |
|---|---|---|---|---|---|---|---|---|---|
| Subarea | Time 0 | Time 10000 | Time 0 | Rank | Time 10000 | Rank | | Time 0 | Rank (Time=0) |
| 1 | 5.35 | 13.10 | 6.72 | 1 | 12.06 | 1 | 723591.30 | 17.31 | 1 |
| 2 | 5.95 | 14.25 | 4.93 | 5 | 9.04 | 5 | 784763.00 | 9.74 | 7 |
| 3 | 5.46 | 13.01 | 6.06 | 2 | 10.96 | 2 | 390372.00 | 14.54 | 2 |
| 4 | 6.01 | 14.59 | 4.01 | 8 | 7.53 | 8 | 207581.30 | 7.49 | 10 |
| 5 | 5.70 | 13.65 | 5.64 | 4 | 10.28 | 4 | 378972.80 | 14.13 | 3 |
| 6 | 5.65 | 13.09 | 4.50 | 6 | 8.34 | 6 | 424872.50 | 8.18 | 8 |
| 7 | 4.69 | 10.43 | 4.34 | 7 | 8.07 | 7 | 163938.30 | 7.97 | 9 |
| 8 | 4.64 | 11.84 | 5.80 | 3 | 10.52 | 3 | 393468.90 | 13.91 | 4 |
| 9 | | | | | | | 660785.50 | 12.64 | 5 |
| 10 | | | | | | | 589497.10 | 10.06 | 6 |
| **MAI** | **5.50** | **13.23** | **5.47** | | **9.97** | | | **12.15** | |

**Results from file uzflow.rlt**

**Infiltration output divided by subarea size (mm/yr)**

| **Subarea Size** | **Test SL-2** | | |
|---|---|---|---|
| Rank {1-8} | Time 10000 | Rank (Time=10000) | Rank {1-8} |
| 1 | 40.10 | 1 | 1 |
| 5 | 22.14 | 7 | 5 |
| 2 | 33.52 | 2 | 2 |
| 8 | 16.97 | 10 | 8 |
| 3 | 32.63 | 3 | 3 |
| 6 | 18.55 | 8 | 6 |
| 7 | 18.13 | 9 | 7 |
| 4 | 31.95 | 4 | 4 |
| | 29.32 | 5 | |
| | 23.13 | 6 | |
| | **27.94** | | |

## SCR-346 SL-1 Test

RF **1/2/03**

bubo: E:\TPA_FY2002\Dec2002\SCR-346\SL-1_test\sl-1.xls from George

Email from George:
From: George R. Adams [mailto:george.adams@swri.org]
Sent: Monday, December 30, 2002 5:09 PM
To: Randy Fedors
Cc: Scherer Carol
Subject: PA-SCR-390, SL-1

Randy,
Please find the attached archive for test SL-1. This test verifies that mean annual infiltration increases in areas of the repository where runon occurs and that mean annual infiltration is reasonable at the end of the analysis period.

From the excel spreadsheet, sl-1.xls, for the three times (0, 10,000 years, and 100,000 years) the MAI in subareas 9 and 10 increases as expected with runon; however, at 10,000 years, the MAI in subarea 7 is also higher. Also, the rankings among all subareas remains unchanged with and without runon and at the three time values.

Would you comment on the output results?
Thanks,
George

These files are part of the SL-1 system level test.

The UZFLOW-A.rlt and UZFLOW-B.rlt files were generated as follows:
1) UZFLOW-A.rlt was generated from a baseline mean data case tpa run using maydtbl.dat and smaydtbl.dat files generated with runon.
2) UZFLOW-B.rlt was generated from a baseline mean data case tpa run using maydtbl.dat and smaydtbl.dat files generated without runon.

The test calls for the following (Results are summarized in sl-1.xls, see printout in table on page 35):
1) Compare the resulting mean annual infiltration with and without runon. Verify that mean annual infiltration increases as expected due to runon in the different subareas for the current climate.
2) Verify the end of simulation mean annual infiltration is reasonable across the repository.

Comments:
Subareas 9 & 10 do show the greatest increase in runon-based net infiltration of all the subareas. This was expected because Drill Hole Wash and Tea Cup Wash both cross subareas 9 & 10. These washes area prominent areas of runon because of their large upslope contributions of runoff.

Subarea 7 has less prominent increase in net infiltration as caused by runon compared to the other subareas. This also seems reasonable because subarea 7 is located to the east; i.e., it's area is dominated by lower portions of east-flanking washes, other subareas have a mixture of Yucca crest and lower and upper wash portions. Note that the small east-flank washes have less upslope contribution as compared to Drill Hole and Tea Cup Washes.

Subareas 2, 4, & 6 have the next highest portion of lower wash, and accordingly have the next least amount of change when runoff and runon are considered.

**TEST SL-1, 12-30-02**

**Test Parameters:** UZFLOW Sample Mode 1(Sample MAI0 and ignore stdev(MAI) from ITYM)
MAI0 Constant {8.50}; Mean Data Set, 1 Realization; Precip Multiplier Constant {2.0}; Temperature Increase Constant {-7.5}

**Test Case A (With Runon)** **Test Case B (Without Runon)**

**Time = 0 years**

| | Extracted from uzflow-A.rlt | | | | Extracted from uzflow-B.rlt | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | diff |
| Subarea 1 | 8627.70 | 723591.3 | 11.9234 | 1 | 8761.60 | 723591.3 | 12.1085 | 1 | -0.1850 |
| Subarea 2 | 5326.70 | 784763.0 | 6.7877 | 7 | 5348.10 | 784763.0 | 6.8149 | 7 | -0.0273 |
| Subarea 3 | 3908.50 | 390372.0 | 10.0122 | 2 | 3971.00 | 390372.0 | 10.1723 | 2 | -0.1601 |
| Subarea 4 | 1081.10 | 207581.3 | 5.2081 | 10 | 1088.00 | 207581.3 | 5.2413 | 10 | -0.0332 |
| Subarea 5 | 3687.20 | 378972.8 | 9.7295 | 3 | 3746.40 | 378972.8 | 9.8857 | 3 | -0.1562 |
| Subarea 6 | 2411.20 | 424872.5 | 5.6751 | 8 | 2431.90 | 424872.5 | 5.7238 | 8 | -0.0487 |
| Subarea 7 | 912.80 | 163938.3 | 5.5679 | 9 | 913.49 | 163938.3 | 5.5722 | 9 | -0.0042 |
| Subarea 8 | 3793.60 | 393468.9 | 9.6414 | 4 | 3829.00 | 393468.9 | 9.7314 | 4 | -0.0900 |
| Subarea 9 | 5988.00 | 660785.5 | 9.0619 | 5 | 5844.10 | 660785.5 | 8.8442 | 5 | 0.2178 |
| Subarea 10 | 4347.40 | 589497.1 | 7.3748 | 6 | 4149.20 | 589497.1 | 7.0385 | 6 | 0.3362 |
| **sum** | **40084.20** | **4717842.7** | | | **40082.79** | **4717843** | | | |
| **MAI** | **8.496** | | | | **8.496** | | | | |

**Time = 10,000 years**

| | Extracted from uzflow-A.rlt | | | | Extracted from uzflow-B.rlt | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | |
| Subarea 1 | 20855.00 | 723591.3 | 28.8215 | 1 | 21168.00 | 723591.3 | 29.2541 | 1 | -0.4326 |
| Subarea 2 | 12578.00 | 784763.0 | 16.0278 | 7 | 12617.00 | 784763.0 | 16.0775 | 7 | -0.0497 |
| Subarea 3 | 9385.80 | 390372.0 | 24.0432 | 2 | 9533.50 | 390372.0 | 24.4216 | 2 | -0.3784 |
| Subarea 4 | 2542.20 | 207581.3 | 12.2468 | 10 | 2556.40 | 207581.3 | 12.3152 | 10 | -0.0684 |
| Subarea 5 | 8867.40 | 378972.8 | 23.3985 | 3 | 9007.70 | 378972.8 | 23.7687 | 3 | -0.3702 |
| Subarea 6 | 5677.00 | 424872.5 | 13.3617 | 8 | 5721.90 | 424872.5 | 13.4673 | 8 | -0.1057 |
| Subarea 7 | 2157.30 | 163938.3 | 13.1592 | 9 | 2156.30 | 163938.3 | 13.1531 | 9 | 0.0061 |
| Subarea 8 | 9070.30 | 393468.9 | 23.0521 | 4 | 9148.80 | 393468.9 | 23.2516 | 4 | -0.1995 |
| Subarea 9 | 14488.00 | 660785.5 | 21.9254 | 5 | 14084.00 | 660785.5 | 21.3140 | 5 | 0.6114 |
| Subarea 10 | 10411.00 | 589497.1 | 17.6608 | 6 | 9887.40 | 589497.1 | 16.7726 | 6 | 0.8882 |
| **sum** | **96032.00** | **4717842.7** | | | **95881.00** | **4717843** | | | |
| **MAI** | **20.355** | | | | **20.323** | | | | |

**Time = 100,000 years**

| | Extracted from uzflow-A.rlt | | | | Extracted from uzflow-B.rlt | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | |
| Subarea 1 | 8352.50 | 723591.3 | 11.5431 | 1 | 8482.30 | 723591.3 | 11.7225 | 1 | -0.1794 |
| Subarea 2 | 5169.10 | 784763.0 | 6.5868 | 7 | 5190.20 | 784763.0 | 6.6137 | 7 | -0.0269 |
| Subarea 3 | 3786.30 | 390372.0 | 9.6992 | 2 | 3847.00 | 390372.0 | 9.8547 | 2 | -0.1555 |
| Subarea 4 | 1049.90 | 207581.3 | 5.0578 | 10 | 1056.70 | 207581.3 | 5.0905 | 10 | -0.0328 |
| Subarea 5 | 3571.90 | 378972.8 | 9.4252 | 3 | 3629.30 | 378972.8 | 9.5767 | 3 | -0.1515 |
| Subarea 6 | 2340.90 | 424872.5 | 5.5097 | 8 | 2361.10 | 424872.5 | 5.5572 | 8 | -0.0475 |
| Subarea 7 | 886.19 | 163938.3 | 5.4056 | 9 | 886.91 | 163938.3 | 5.4100 | 9 | -0.0044 |
| Subarea 8 | 3676.20 | 393468.9 | 9.3431 | 4 | 3710.60 | 393468.9 | 9.4305 | 4 | -0.0874 |
| Subarea 9 | 5800.00 | 660785.5 | 8.7774 | 5 | 5661.60 | 660785.5 | 8.5680 | 5 | 0.2094 |
| Subarea 10 | 4215.00 | 589497.1 | 7.1502 | 6 | 4023.70 | 589497.1 | 6.8256 | 6 | 0.3245 |
| **sum** | **38847.99** | **4717842.7** | | | **38849.41** | **4717843** | | | |
| **MAI** | **8.234** | | | | **8.235** | | | | |

RF 2/6/03

**PA-SCR-346 PL-2 Test**

E:\AVData\Tpa\testingTPA_April2002.apr was again used to display data in ArcView 3.2 on bubo (NTbox).
E:\TPA_FY2002\Dec2002\SCR-346\PL-2_test\* for the input files to be plotted and the arcread.f program.

Again, arcread.f (see page 27) was used, though minor changes to input file name and ouput file name were made in the code. The log10 values in maytbl* used the code executable arcread10.exe. I hand calculated the first entry in the maytbl* file to make sure that the fortran code correctly accounted for the log10 to natural space conversion.

pl-2-scr346_41j.txt from maidtbl_41jp200t147.dat
pl-2-scr346_mai.txt from maidtbl_Cp200t147.dat
pl-2-scr346_may.txt from maydtbl_Cp200t147.dat (also modified code to account for log10 values)

This code was run three times to create the ascii files needed for importing into ArcView; the output file was renamed after each execution.

Message from George on what was needed (pl2.txt):

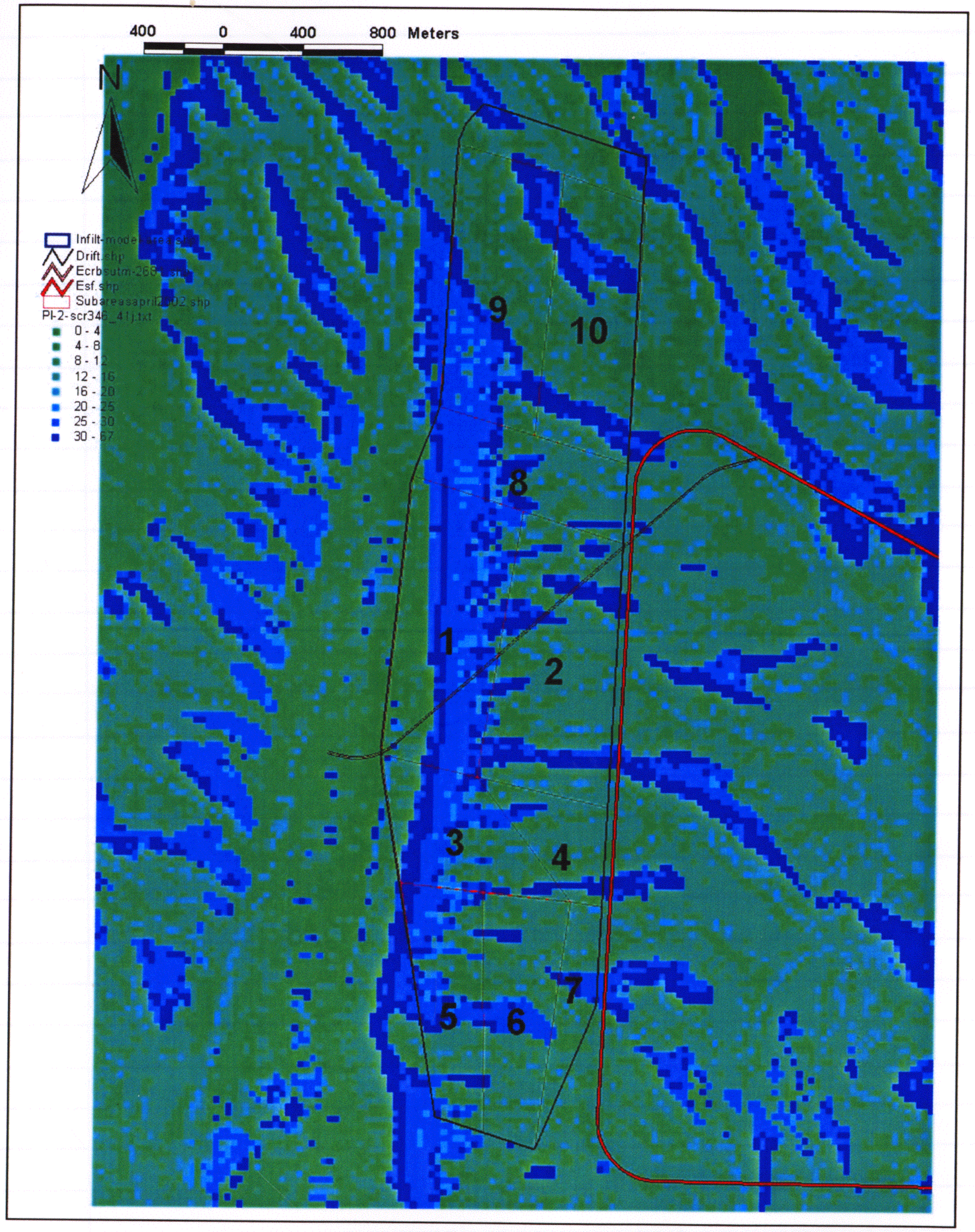
```
PA-SCR-346, PL-2
The output files generated as part of process level test pl-2 are included in this
directory.

The files were generated as follows:
   Mean annual infiltration generated over 500 realizations.
   Table extracted for climate at MAP = 200, MAT = 14.7.

1) maidtbl_41jp200t147.dat  Build 4.1j of the TPA code.
2) maidtbl-Cp200t147.dat    Build 5.0Beta of the TPA code.
3) maydtbl-Cp200t147.dat    Build 5.0Beta of the TPA code.

The test calls for the following:
1) Plot the first two files (maidtbl_41jp200t147.dat and maidtbl-Cp200t147.dat) and
   compare the resulting plots in terms of MAI magnitude and spatial variability.
2) Plot the last two files (maidtbl-Cp200t147.dat and maydtbl-Cp200t147.dat{converted
   from log10[MAI] to MAI}) and compare the resulting plots.
```

RFedors Comments (see figures on page 37, 38, 39):

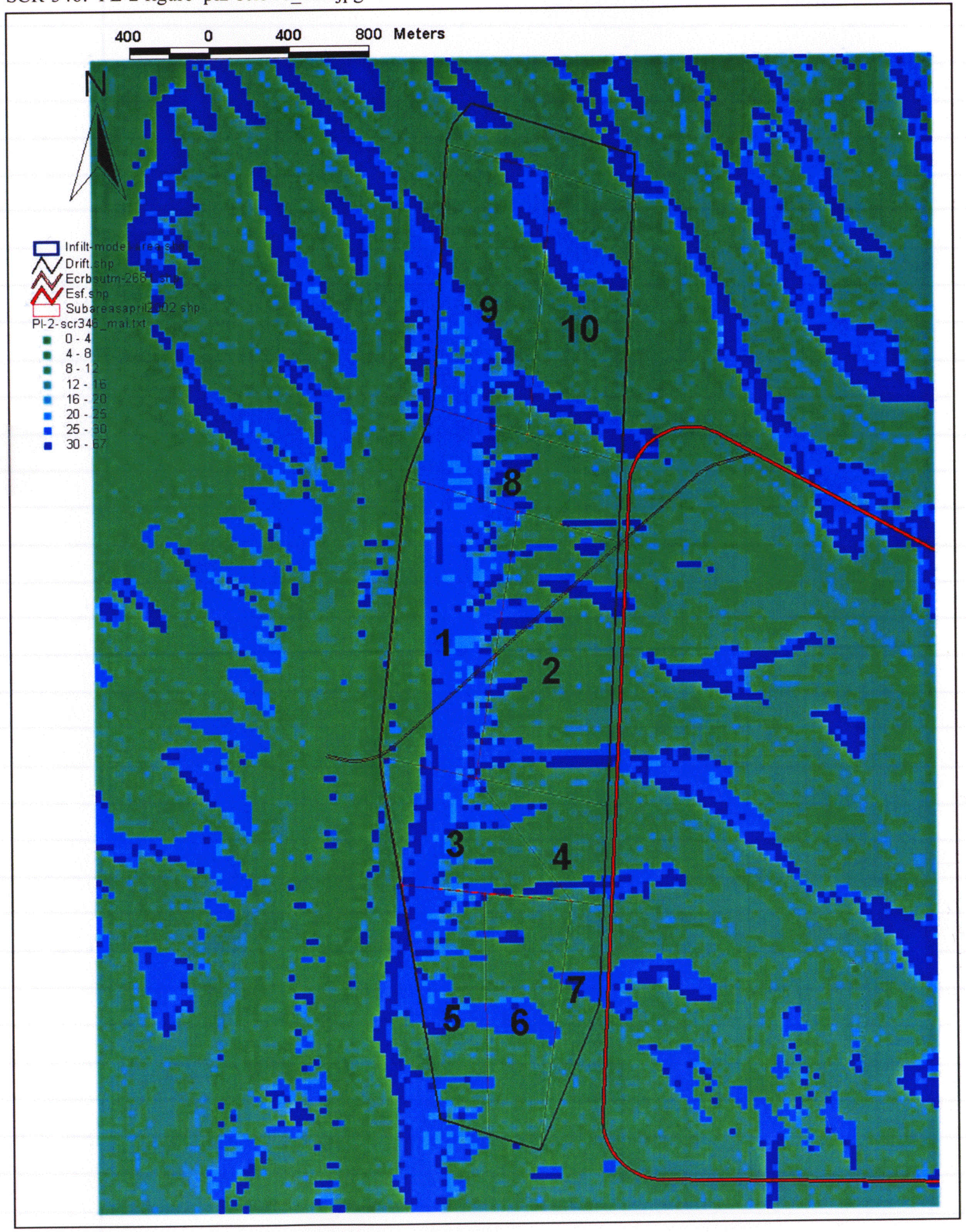
1. Plots of data from the maidtbl_41jp200t147.dat and maidtbl-Cp200t147.dat files with the repository and ESF overlay were used to visually compare magnitude and distribution of net infiltration. These plots are included on pages 37, 38 and 39 (jpegs are stored in .\AVData\Tpa\Pl-2files* with the same base name as the *.txt files near the top of this page). The patterns are virtually identical and the magnitudes appear to be the same. Slight differences of specific pixels are not significant, where significance is judged in the context of overall uncertainty in net infiltration estimates. The overall distribution of net infiltration is consistent with our understanding of the physical processes; i.e., we expect higher values in areas where the caprock is exposed and soils are thin (on ridgetops and Yucca Mountain crest), higher values where the PTn is exposed on the west flank of Yucca Mountain, and lowest values where the soils are thick (alluvial valleys). There are areas outside of the repository footprint (e.g., to the north on the ridgetops) where errors have continued for both TPA 4.1j and TPA 5.0. These errors do not affect the results of TPA since all emplacement/subareas are within the repository. If the repository footprint were to change, then the errors would have to be fixed.
2. Plots of data from the maidtbl-Cp200t147.dat and maydtbl-Cp200t147.dat files (log10) showed similar distribution of net infiltration across Yucca Mountain. The magnitudes of the log10 estimates of net infiltration, however, are much lower those for the natural space (maidtbl-Cp200t147.dat). This was previously noted when ITYM was implemented, and should be expected since a number of the important parameters are lognormally distributed. Net infiltration itself is expected to be lognormally distributed (spatially), thus supporting the log10 approach. The natural space mean annual infiltration map is output

from ITYM to better link current results with early TPA results (the comparison of maidtbl_41jp200t147.dat and maidtbl-Cp200t147.dat makes illustrates this connection).

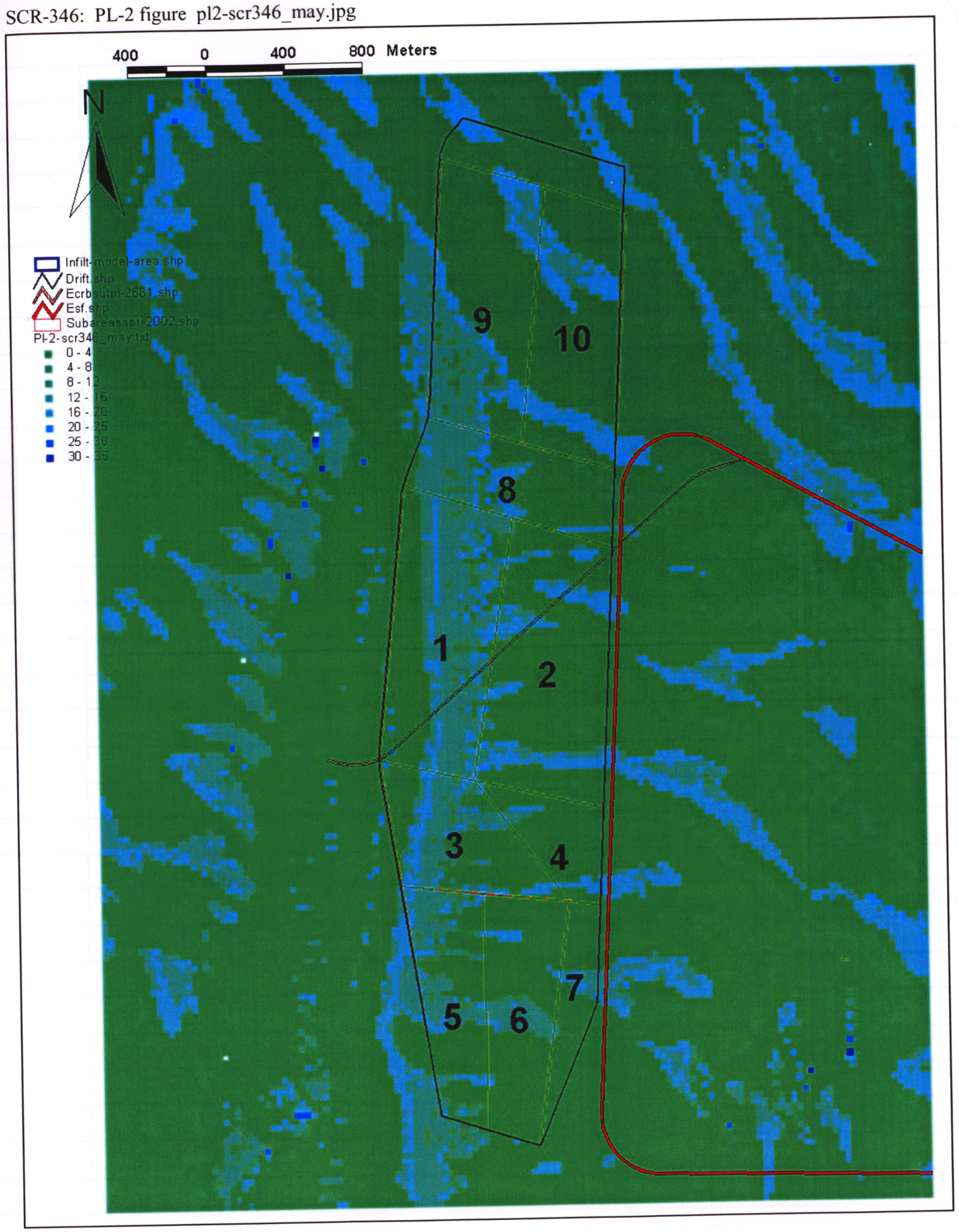
SCR-346: PL-2 figure pl2-scr346_41j.jpg



SCR-346: PL-2 figure pl2-scr346_mai.jpg



SCR-346: PL-2 figure pl2-scr346_may.jpg



**Final Testing of SCR-390 (Runoff Abstraction)** RF 2/7/03

Per George Adams email:

```
From: George R. Adams [george.adams@swri.org]
Sent: Thursday, December 19, 2002 1:09 PM
To: Randy Fedors
Cc: Scherer Carol
Subject: PA-SCR-390, PROCESS LEVEL TEST PL-1

Randy,

Please find the data for process level test PL-1 included in the archive with an
explanation in the text file.  The section of the text file titled, "The test calls
for the following:" is what we're verifying.  I'm asking you to plot the data, and if
possible, return to Carol and I in electronic format.

There's a system level test, SL-1 for this SCR that I'll forward separately.

Thanks,
George
```

The contents of text file in zipped file: Pl-1.zip

The output file generated as part of process level test pl-1 is included in this directory:
(bubo E:\TPA_FY2002\Dec2002\Scr-390\.

The maidtbl-diff.dat file was generated as follows:

1) The ITYM Preprocessor was run two separate times. It was run first with runon and second without runon.
2) The current climate was extracted from the maidtbl.dat files for the two runs.
3) The difference between the values in the two maidtbl.dat files was generated.
4) The difference between the two maidtbl.dat files for the current climate was then output to maidtbl-diff.dat.

The test calls for the following:

1) Plot the data in maidtbl-diff.dat overlaid on a map of the repository. There was a previous plot with this informatio identified as follows: Net Infiltration (mm/yr) from Runoff/Runon by ITYM Oct 2002; plotted ArcView, bubo: J:\AVData\TPA\Runoff.
2) Verify that runon occurs in low-lying areas of the repository.
3) In these low-lying areas, infiltration increases as expected.

Using arcread.f fortran script as described on page 26, I reformatted the data for ArcView 3.2a input and re-created the ArcView figure below (page 41). Again, "arcread.f" was recompiled using the Lahey/Fujitsu Fortran 95 version 5.00b compiler.

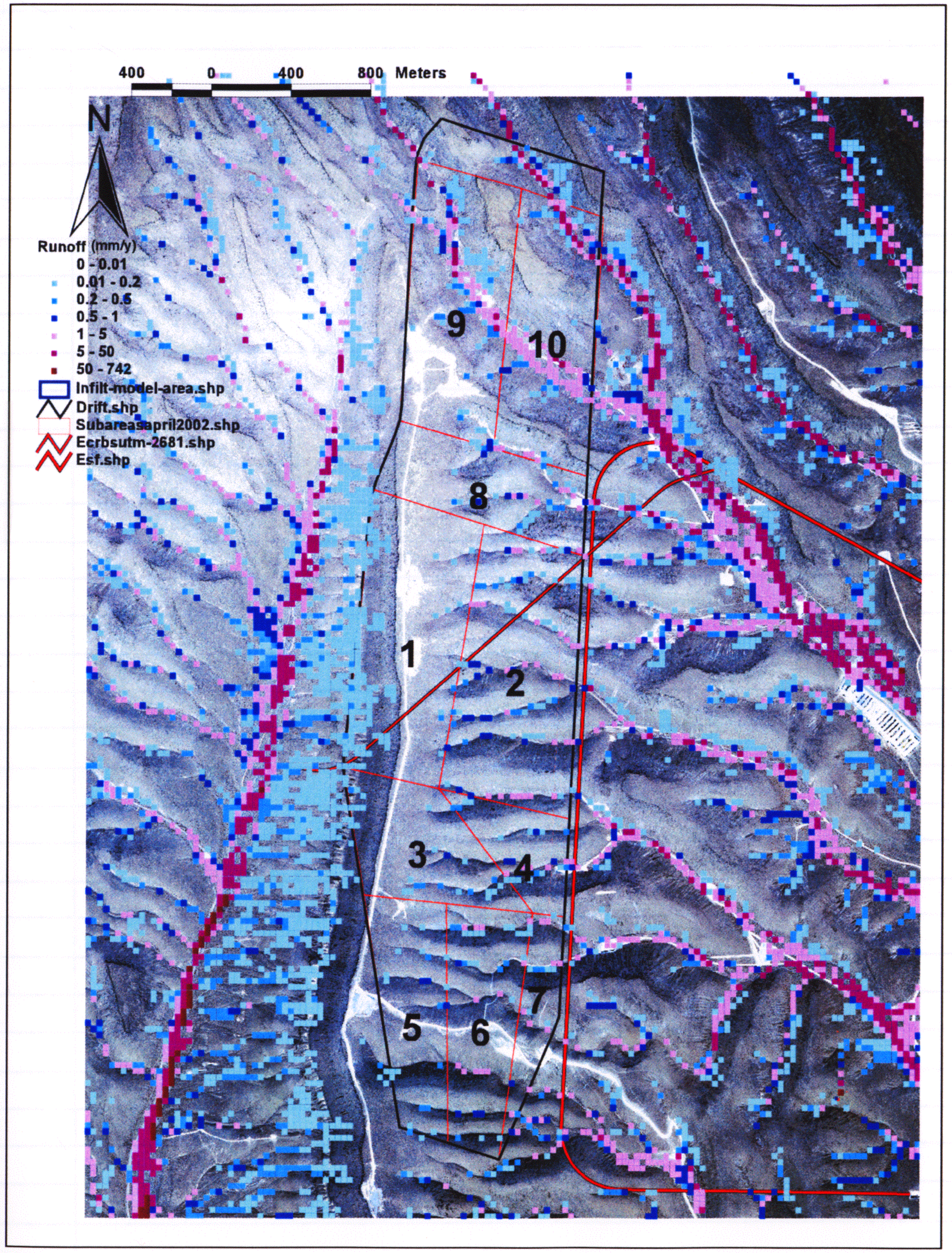
See directory bubo: E:\TPA_FY2002\Dec2002\Scr390\ for fortran code and executable and output "runoff.txt"

"runoff.txt" was created using arcread.f and copied as "runoff-2.txt" to:
bubo: E:\AVData\TPA\Runoff\runoff-2.txt

ArcView 3.2a imported this table, I used the same project file as before
(Project -> Add Table; then View-> Add Event Theme)
bubo: E:\AVData\TPA\testingTPA_April2002.apr

runoff-2.txt data was imported as theme called "Runoff-2.txt" in the ArcView project file.

Output from ArcView saved as eps, imported into Illustrator 8.0, modified text, then saved as jpeg to send to George and Carol. It is included here as the figure on page 41:



## SCR-346 SL-3 Test

Files stored in: bubo: E:\TPA_FY2002\Dec2002\SCR-346\SL-3_test\*
E:\AVData\Tpa\testingTPA_April2002.apr

The output files generated as part of test SL-3 are included in the directory noted above.

The purpose of this test is to perform a check between the itym results for the current climate and the TPA results for the current climate.

1) A FORTRAN program was run to extract the log10[MAI] for the current climate from maydtbl.dat. The log10[MAI] values were averaged for each subarea. This average log10[MAI] value for each subarea was converted to an MAI value (10**(average{log10[MAI]}) and placed in the Excel spreadsheet.

2) Three TPA test cases were run:

Test Case A was run with sample mode 1
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] is sampled from {uniform, 4.0 to 13}
UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] is ignored

Test Case B was run with sample mode 2
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] is a constant 8.5
UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] is sampled from {normal, -3.0857 to 3.0857}

Test Case C was run with sample mode 3
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] is ignored
UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] is sampled from {normal, -3.0857 to 3.0857}

The spreadsheet, sl-3.xls, contains a summary for the three test cases. The sl-3.xls spreadsheet is included here for reference
(Test case A is table on page 43).
(Test case A is table on page 44).
(Test case A is table on page 45).

The test calls for the following: Verify the average infiltration values for each subarea are comparable between execution of the itym code and the TPA code.

The Excel spreadsheet shows that the rankings among subareas remains unchanged between the itym results and all three TPA test cases. The MAI magnitudes vary quite a bit in Test Case B and Test Case C; however, they vary in the expected direction for changes in the uncertainty parameter.

Mode 2 was found to be disjointed, conceptually-speaking. The data suggests that the conceptualization is formulated in an inconsistent manner and should not be used at all. Henceforth, mode 2 was eliminated from UZFLOW, and mode 3 was shifted to mode 2 designation.

Mode 1: Use mean and uncertainty form tpa.inp inputs for modern climate mean annual infiltration at start

Mode 2: Use mean and uncertainty from itym results

---

**10-23-02 results** 100000 Years

**Test Case A**

**Test Parameters:** UZFLOW Sample Mode 1(Sample MAI0 and ignore stdev(MAI) from ITYM)

MAI0 Uniform Distribution {4.0, 13.0}
50 Realizations
Precipitation Multiplier = 1.0
Temperature Increase = 0.0

Realization 50, Time = 0,
AAIO = 11.642

| | Extracted from uzflow-A.rlt | | | | | Environment of 162.5, 17.38 (Taken from File summary.dat) Extracted from maydtbl.dat | | |
|---|---|---|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference | q(m3/yr) | MAI(mm/yr) | Rank |
| Subarea 1 | 12073.00 | 723591.3 | 16.6848 | 1 | 4.283 | 2285.32 | 3.1583 | 1 |
| Subarea 2 | 7229.30 | 784763.0 | 9.2121 | 7 | 4.282 | 1368.76 | 1.7442 | 7 |
| Subarea 3 | 5423.20 | 390372.0 | 13.8924 | 2 | 4.283 | 1026.49 | 2.6295 | 2 |
| Subarea 4 | 1460.40 | 207581.3 | 7.0353 | 10 | 4.281 | 276.55 | 1.3323 | 10 |
| Subarea 5 | 5121.70 | 378972.8 | 13.5147 | 3 | 4.283 | 969.45 | 2.5581 | 3 |
| Subarea 6 | 3256.60 | 424872.5 | 7.6649 | 8 | 4.282 | 616.56 | 1.4512 | 8 |
| Subarea 7 | 1226.90 | 163938.3 | 7.4839 | 9 | 4.282 | 232.29 | 1.4169 | 9 |
| Subarea 8 | 5221.40 | 393468.9 | 13.2702 | 4 | 4.283 | 988.26 | 2.5117 | 4 |
| Subarea 9 | 8135.60 | 660785.5 | 12.3120 | 5 | 4.284 | 1539.53 | 2.3299 | 5 |
| Subarea 10 | 5749.60 | 589497.1 | 9.7534 | 6 | 4.284 | 1088.18 | 1.8460 | 6 |
| **sum** | **54897.70** | **4717842.7** | | | | **10391.40** | | |
| **MAI** | **11.636** | | | | | **2.203** | | |

Realization 45, Tim= 0,
AAIO=8.7158

| | Extracted from uzflow-A.rlt | | | | |
|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference |
| Subarea 1 | 9039.10 | 723591.3 | 12.4920 | 1 | 2.955 |
| Subarea 2 | 5412.40 | 784763.0 | 6.8969 | 7 | 2.954 |
| Subarea 3 | 4060.20 | 390372.0 | 10.4008 | 2 | 2.955 |
| Subarea 4 | 1093.40 | 207581.3 | 5.2673 | 10 | 2.954 |
| Subarea 5 | 3834.50 | 378972.8 | 10.1181 | 3 | 2.955 |
| Subarea 6 | 2438.20 | 424872.5 | 5.7387 | 8 | 2.955 |
| Subarea 7 | 918.56 | 163938.3 | 5.6031 | 9 | 2.954 |
| Subarea 8 | 3909.10 | 393468.9 | 9.9350 | 4 | 2.956 |
| Subarea 9 | 6090.90 | 660785.5 | 9.2177 | 5 | 2.956 |
| Subarea 10 | 4304.60 | 589497.1 | 7.3022 | 6 | 2.956 |
| **sum** | **41100.96** | **4717842.7** | | | |
| **MAI** | **8.712** | | | | |

**10-23-02 results, Test Case B** 10000 Years

**Test Parameters:** UZFLOW Sample Mode 2(Sample MAI0 (constant for mean) and use stdev(MAI) from ITYM)

MAI0 constant {8.5} 50 Realizations Precipitation Multiplier = 1.0 Temperature Increase = 0.0

Realization 50, Time = 0, MAI0 = 8.5, Uncertainty Parameter = -1.4941 Environment of 162.5, 17.38 (Taken from File summary.dat)

| | Extracted from uzflow-B.rlt | | | | | Extracted from maydtbl.dat | | |
|---|---|---|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference | q(m3/yr) | MAI(mm/yr) | Rank |
| Subarea 1 | 531.00 | 723591.3 | 0.7338 | 1 | -0.768 | 2285.32 | 3.1583 | 1 |
| Subarea 2 | 266.97 | 784763.0 | 0.3402 | 7 | -0.805 | 1368.76 | 1.7442 | 7 |
| Subarea 3 | 222.50 | 390372.0 | 0.5700 | 2 | -0.783 | 1026.49 | 2.6295 | 2 |
| Subarea 4 | 50.17 | 207581.3 | 0.2417 | 10 | -0.819 | 276.55 | 1.3323 | 10 |
| Subarea 5 | 210.22 | 378972.8 | 0.5547 | 3 | -0.783 | 969.45 | 2.5581 | 3 |
| Subarea 6 | 114.03 | 424872.5 | 0.2684 | 8 | -0.815 | 616.56 | 1.4512 | 8 |
| Subarea 7 | 41.89 | 163938.3 | 0.2555 | 9 | -0.820 | 232.29 | 1.4169 | 9 |
| Subarea 8 | 209.43 | 393468.9 | 0.5323 | 4 | -0.788 | 988.26 | 2.5117 | 4 |
| Subarea 9 | 341.57 | 660785.5 | 0.5169 | 5 | -0.778 | 1539.53 | 2.3299 | 5 |
| Subarea 10 | 223.92 | 589497.1 | 0.3798 | 6 | -0.794 | 1088.18 | 1.8460 | 6 |
| **sum** | **2211.71** | **4717842.7** | | | | **10391.40** | | |
| **MAI** | **0.469** | | | | | **2.203** | | |

Realization 47, Time = 0, MAI0 = 8.5, Uncertainty Parameter = 0.33103

Extracted from uzflow-B.rlt

| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference |
|---|---|---|---|---|---|
| Subarea 1 | 16427.00 | 723591.3 | 22.7020 | 1 | 6.188 |
| Subarea 2 | 10225.00 | 784763.0 | 13.0294 | 7 | 6.470 |
| Subarea 3 | 7493.30 | 390372.0 | 19.1953 | 2 | 6.300 |
| Subarea 4 | 2098.90 | 207581.3 | 10.1112 | 10 | 6.589 |
| Subarea 5 | 7076.10 | 378972.8 | 18.6718 | 3 | 6.299 |
| Subarea 6 | 4660.60 | 424872.5 | 10.9694 | 8 | 6.559 |
| Subarea 7 | 1765.60 | 163938.3 | 10.7699 | 9 | 6.601 |
| Subarea 8 | 7250.80 | 393468.9 | 18.4279 | 4 | 6.337 |
| Subarea 9 | 11184.00 | 660785.5 | 16.9253 | 5 | 6.265 |
| Subarea 10 | 8036.60 | 589497.1 | 13.6330 | 6 | 6.385 |
| **sum** | **76217.90** | **4717842.7** | | | |
| **MAI** | **16.155** | | | | |

Realization 45, Time = 0, MAI0 = 8.5, Uncertainty Parameter = -1.0776

Extracted from uzflow-B.rlt

| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference |
|---|---|---|---|---|---|
| Subarea 1 | 1162.20 | 723591.3 | 1.6062 | 1 | -0.491 |
| Subarea 2 | 613.46 | 784763.0 | 0.7817 | 7 | -0.552 |
| Subarea 3 | 496.50 | 390372.0 | 1.2719 | 2 | -0.516 |
| Subarea 4 | 117.63 | 207581.3 | 0.5667 | 10 | -0.575 |
| Subarea 5 | 469.04 | 378972.8 | 1.2377 | 3 | -0.516 |
| Subarea 6 | 265.95 | 424872.5 | 0.6260 | 8 | -0.569 |
| Subarea 7 | 98.39 | 163938.3 | 0.6002 | 9 | -0.576 |
| Subarea 8 | 470.29 | 393468.9 | 1.1952 | 4 | -0.524 |
| Subarea 9 | 757.31 | 660785.5 | 1.1461 | 5 | -0.508 |
| Subarea 10 | 506.97 | 589497.1 | 0.8600 | 6 | -0.534 |
| **sum** | **4957.74** | **4717842.7** | | | |
| **MAI** | **1.051** | | | | |

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pages 26-45 taped into notebook 4/4/03 KF

**TEST SL-3, 10-23-02** 100000 Years

**Test Case C**

**Test Parameters:** UZFLOW Sample Mode 3(Ignore MAI0 and use stdev(MAI) from ITYM) MAI0 {Ignored

50 Realizations Precipitation Multiplier = 1.0 Temperature Increase = 0.0

Realization 50, Time = 0, Uncertainty Parameter = -1.4941 Environment of 162.5, 17.38 (Taken from summary.dat)

| | Extracted from uzflow-C.rlt | | | | | Extracted from maydtbl.dat | | |
|---|---|---|---|---|---|---|---|---|
| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference | q(m3/yr) | MAI(mm/yr) | Rank |
| Subarea 1 | 184.00 | 723591.3 | 0.2543 | 1 | -0.919 | 2285.32 | 3.1583 | 1 |
| Subarea 2 | 86.74 | 784763.0 | 0.1105 | 7 | -0.937 | 1368.76 | 1.7442 | 7 |
| Subarea 3 | 75.64 | 390372.0 | 0.1938 | 2 | -0.926 | 1026.49 | 2.6295 | 2 |
| Subarea 4 | 16.04 | 207581.3 | 0.0773 | 10 | -0.942 | 276.55 | 1.3323 | 10 |
| Subarea 5 | 71.55 | 378972.8 | 0.1888 | 3 | -0.926 | 969.45 | 2.5581 | 3 |
| Subarea 6 | 36.84 | 424872.5 | 0.0867 | 8 | -0.940 | 616.56 | 1.4512 | 8 |
| Subarea 7 | 13.46 | 163938.3 | 0.0821 | 9 | -0.942 | 232.29 | 1.4169 | 9 |
| Subarea 8 | 70.81 | 393468.9 | 0.1800 | 4 | -0.928 | 988.26 | 2.5117 | 4 |
| Subarea 9 | 112.51 | 660785.5 | 0.1703 | 5 | -0.927 | 1539.53 | 2.3299 | 5 |
| Subarea 10 | 71.46 | 589497.1 | 0.1212 | 6 | -0.934 | 1088.18 | 1.8460 | 6 |
| **sum** | **739.04** | **4717842.7** | | | | **10391.40** | | |
| **MAI** | **0.157** | | | | | **2.203** | | |

Realization 47, Time = 0, Uncertainty Parameter = 0.33103

Extracted from uzflow-C.rlt

| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference |
|---|---|---|---|---|---|
| Subarea 1 | 4715.50 | 723591.3 | 6.5168 | 1 | 1.063 |
| Subarea 2 | 3047.90 | 784763.0 | 3.8838 | 7 | 1.227 |
| Subarea 3 | 2184.00 | 390372.0 | 5.5947 | 2 | 1.128 |
| Subarea 4 | 633.34 | 207581.3 | 3.0510 | 10 | 1.290 |
| Subarea 5 | 2059.20 | 378972.8 | 5.4336 | 3 | 1.124 |
| Subarea 6 | 1407.10 | 424872.5 | 3.3118 | 8 | 1.282 |
| Subarea 7 | 531.81 | 163938.3 | 3.2440 | 9 | 1.289 |
| Subarea 8 | 2119.70 | 393468.9 | 5.3872 | 4 | 1.145 |
| Subarea 9 | 3206.50 | 660785.5 | 4.8526 | 5 | 1.083 |
| Subarea 10 | 2333.40 | 589497.1 | 3.9583 | 6 | 1.144 |
| **sum** | **22238.45** | **4717842.7** | | | |
| **MAI** | **4.714** | | | | |

Realization 45, Time = 0, Uncertainty Parameter = -1.0776

Extracted from uzflow-C.rlt

| | q(m3/yr) | size(m2) | MAI(mm/yr) | Rank | Fractional Difference |
|---|---|---|---|---|---|
| Subarea 1 | 385.77 | 723591.3 | 0.5331 | 1 | -0.831 |
| Subarea 2 | 195.44 | 784763.0 | 0.2490 | 7 | -0.857 |
| Subarea 3 | 162.95 | 390372.0 | 0.4174 | 2 | -0.841 |
| Subarea 4 | 37.12 | 207581.3 | 0.1788 | 10 | -0.866 |
| Subarea 5 | 154.03 | 378972.8 | 0.4064 | 3 | -0.841 |
| Subarea 6 | 84.60 | 424872.5 | 0.1991 | 8 | -0.863 |
| Subarea 7 | 31.15 | 163938.3 | 0.1900 | 9 | -0.866 |
| Subarea 8 | 153.82 | 393468.9 | 0.3909 | 4 | -0.844 |
| Subarea 9 | 241.67 | 660785.5 | 0.3657 | 5 | -0.843 |
| Subarea 10 | 158.34 | 589497.1 | 0.2686 | 6 | -0.854 |
| **sum** | **1604.88** | **4717842.7** | | | |
| **MAI** | **0.340** | | | | |

RF **6/12/03**

Primary computer running WindowsNT 4.00.1381 is called bubo (Acer, x86 Family 6 Model 4 Stepping 2; AT compatible with 512 MBytes RAM).

WinNT Software:
ArcView version 3.2a;
Lahey/Fujitsu Fortran 95 version 5.0;
Excel 97 SR-2;
WORD 97 SR-2.
Spock is a SUN sparc Ultra 4 (4 cpu), 64-bit, running SunOS version (Kernel ID) Generic_108528-17 release 5.8
SUN Software:
fortran 77 version 5.0 (SUN Workshop Compiler FORTRAN 77 version 5.0).

**TPA Modifications and Testing**

Software validation tests for TPA 5.0, formal tests for TSPAI intermediate milestone. For UZFLOW. There were 4 tests:

| | |
|---|---|
| CI-1 | |
| CI-2 | BREATH |
| CI-3 | Pixel resolution, subarea averaging |
| CI-4 | 3-Springs Watershed comparison |

Collaborators: Roland Benke is ensuring that the work gets done, and is doing some of the testing (CI-4) at mine and George Adams' direction and help. I am doing CI-2 and helping George with CI-1 and CI-3.

All I needed to do for the CI-4 test was interpret the McKinley and Oliver (1994) report for Roland; i.e., tell Roland the relevant recharge values to compare with the TPA 5.0 output.

McKinley, P.W. and T.A. Oliver. Meteorological, Stream-Discharge, and Water-Quality Data for 1986 through 1991 from Two Small Basins in Central Nevada. USGS Open-File Report 93-651. Denver, CO: U.S. Geological Survey. 1994.

**Plotting for CI-3**

bubo E:\SoftwareValidation\TPA-June2003\
bubo E:\AVData\TPA\TPA50-test-June2003\

George asked that I plot 3 files of ITYM output created at different resolutions
maydtbl_120m_current.dat
maydtbl_60m_current.dat
maydtbl_30m_current.dat

1. Use maid.for script to reformat ITYM output to ArcView input
   create a *.txt file (required by ArcView)

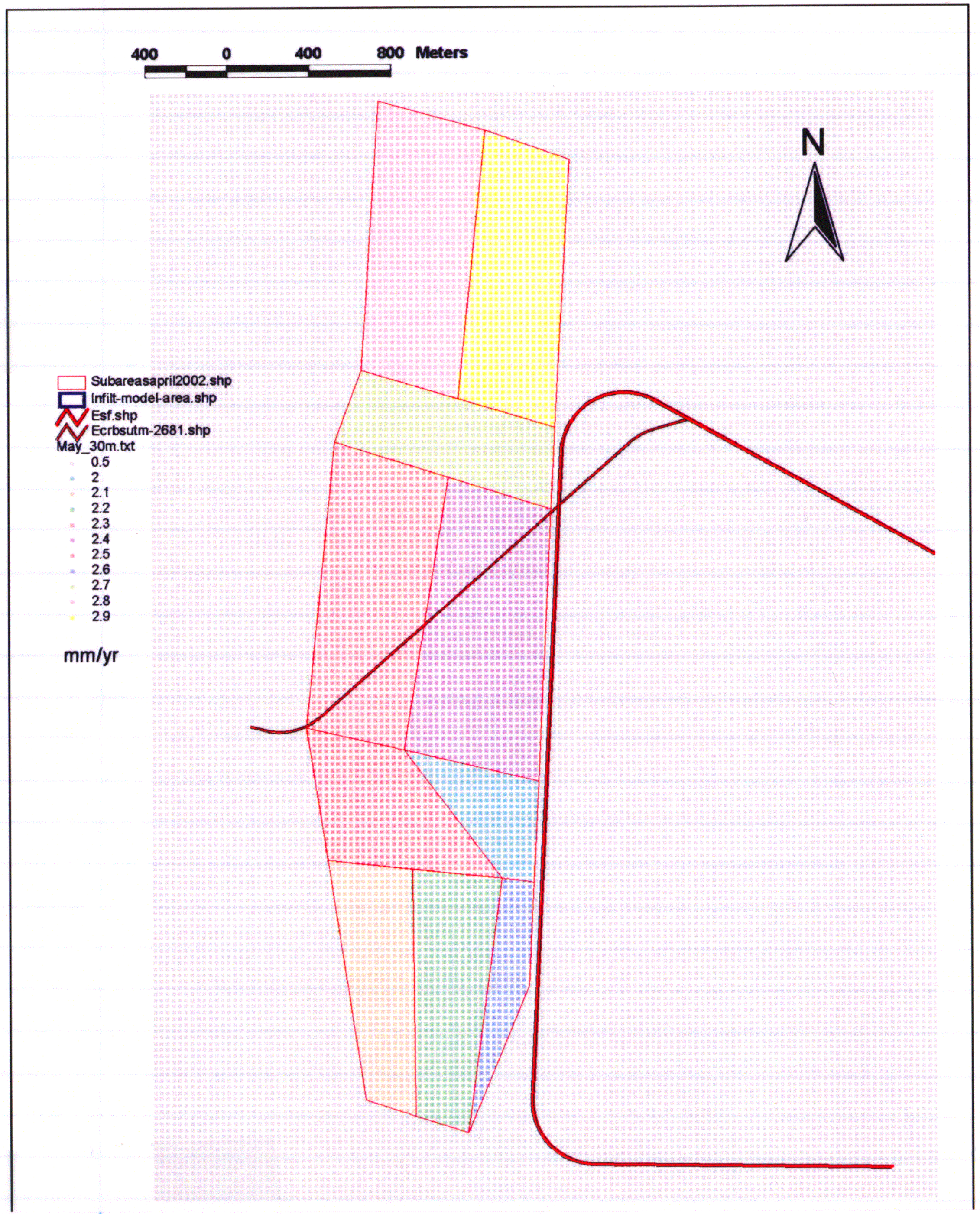
2. Plotted in ArcView 3.2a using the specified project file (*.apr)
   Open project file
   Project--> Add Table (*.txt table)
   Make View active, then View-->Add Event Theme
   - set easting & northing
   - set theme properties (unique colors for infiltration)

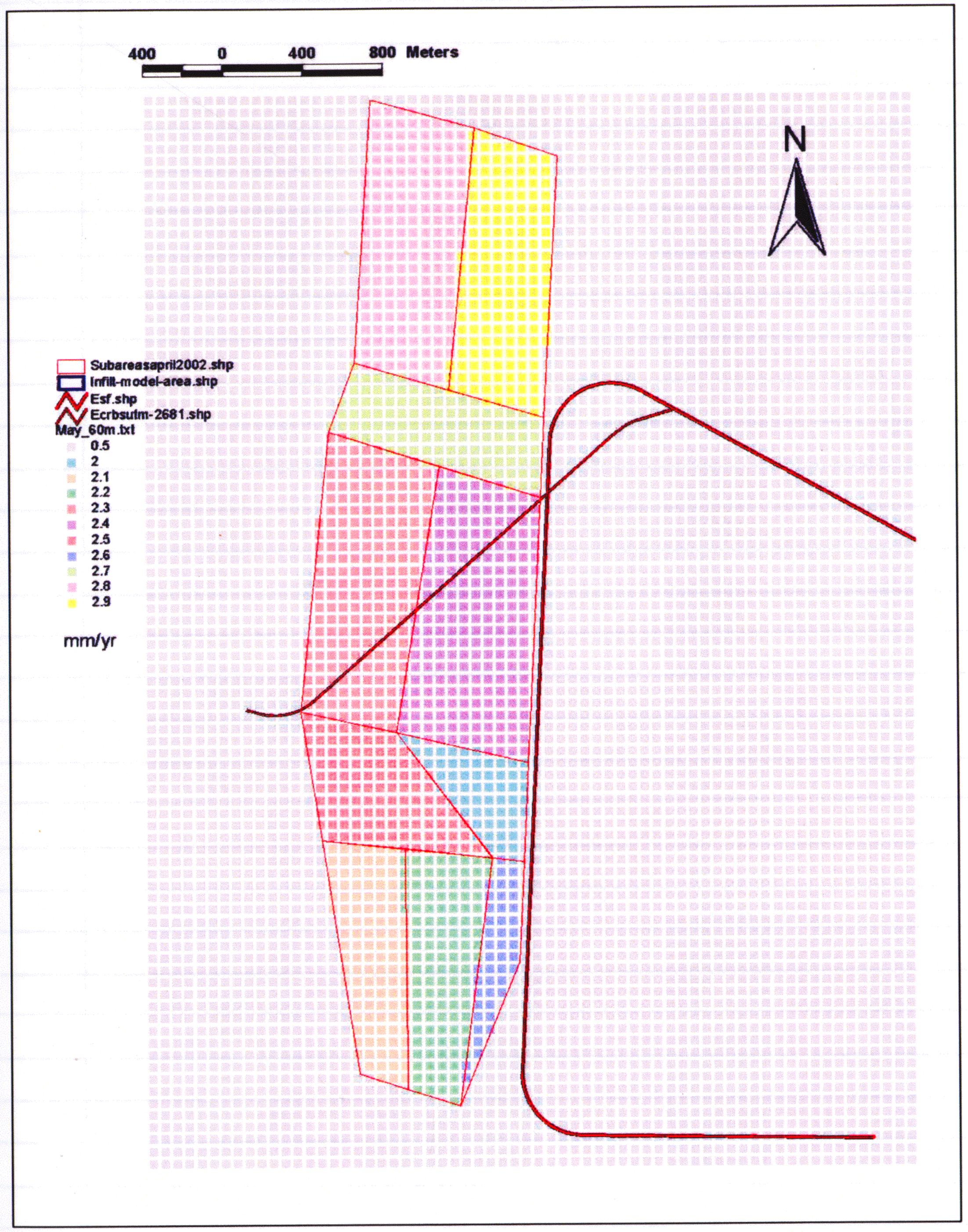
Files needed to plot ITYM output:
bubo E:\AVData\TPA\TPA-test-June2003\testingtpa_june2003.apr
bubo E:\AVData\TPA\TPA-test-June2003\ShapeFiles\* (associated files)
bubo E:\SoftwareValidation\TPA-June2003\CodeExtractionArcView\maid.for which is included below:

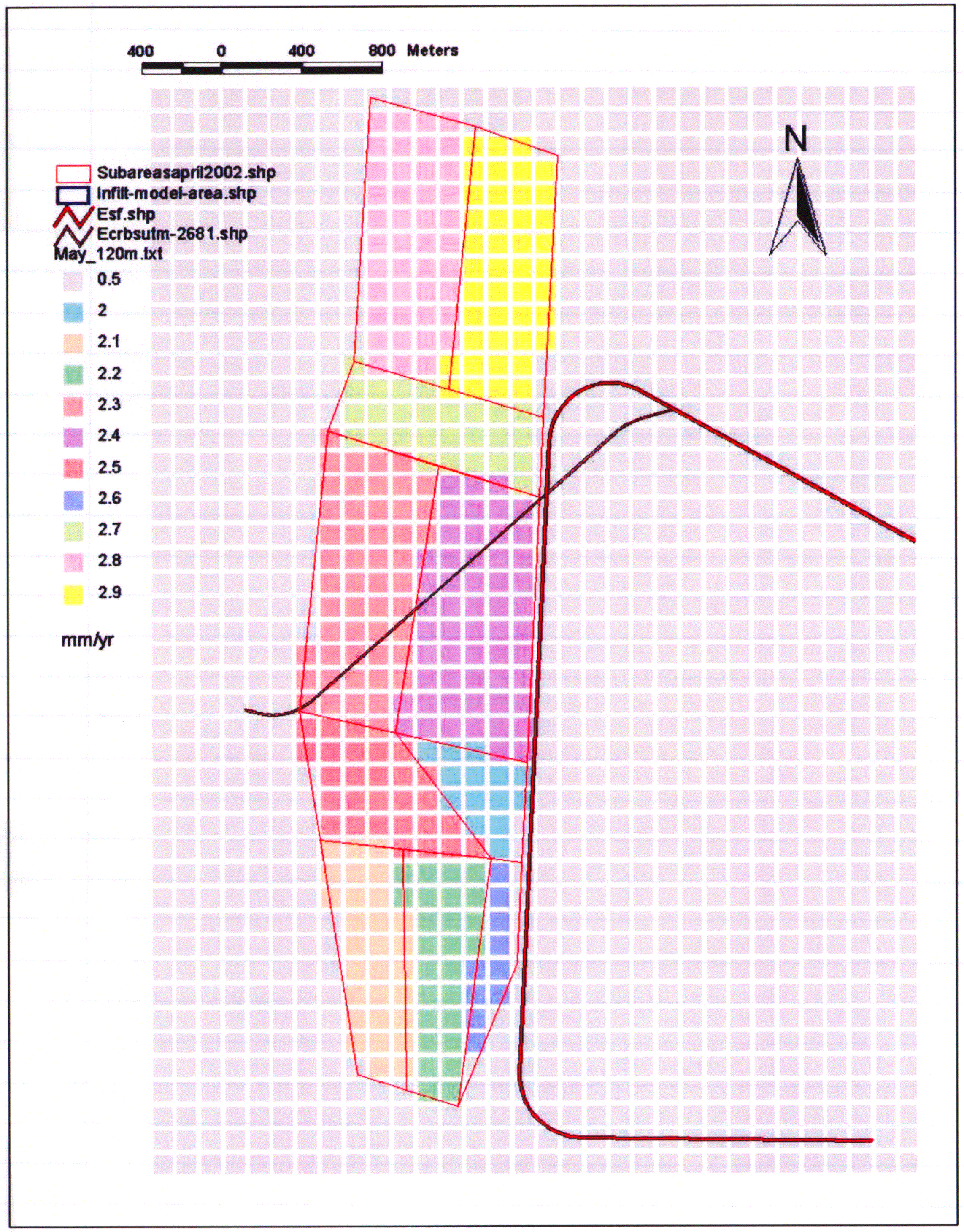
```
================
program maid
c Script reformats data for input to ArcView in grid format
c RFedors  June 4, 2002; revised June 12, 2003
c23456789 123456789 123456789 123456789 123456789 123456789 123456789 12
      integer ioread, iowrit, mx, mxx, i, j, k
      parameter (mx=1000,mxx=100000)
      real*8 array(mxx,3)
      real*8 xllcorner, yllcorner, cellsize, xpos, ypos
      character*25 file1, file2, junk
      character*60 header
c set input and output unit numbers
      ioread = 7
      iowrit = 8
c read in DEM of infiltration; note that the coordinates of the
c southwest corner of the domain are given in the header, but the
c ordering of data is row-major starting from the northwest corner.
      write(*,10)
 10   format(' enter input filename ')
      read(*,'(a25)') file1
      write(*,20)
 20   format(' enter output filename ')
      read(*,'(a12)') file2
      open(unit = ioread, file = file1, status = 'unknown')
      do i = 1, 4
        read(ioread,'(a60)') header
      enddo
      read(ioread,'(a9,i10)') junk, ncols
      read(ioread,'(a9,i10)') junk, nrows
      read(ioread,'(a9,f16.5)') junk, xllcorner
      read(ioread,'(a9,f16.5)') junk, yllcorner
      read(ioread,'(a9,f15.5)') junk, cellsize
      do i = 1, 3
        read(ioread,'(a60)') header
      enddo
      print*, ncols, nrows, cellsize, xllcorner, yllcorner
      ypos = yllcorner + cellsize * dfloat(nrows-1)
      xpos = xllcorner
      k = 1
      do i = 1, nrows
        do j = 1, ncols
          read(ioread,'(e15.8)') array(k,3)
          array(k,1) = xpos
          array(k,2) = ypos
          xpos = xpos + cellsize
          k = k + 1
        enddo
        ypos = ypos - cellsize
        xpos = xllcorner
      enddo
      close(ioread)
c write out reformatted data including easting and northing locations
      open(unit=iowrit, file=file2, status='unknown', form='formatted')
      write(iowrit,*) 'easting-m, northing-m, infilt-mmyr'
      do k = 1, nrows*ncols
         write(iowrit,'(e14.7,",",e14.7,",",e14.7)')
     &                    array(k,1), array(k,2), 10**array(k,3)
```

```
      enddo
      close(iowrit)
      stop
      end
===================
```

Output of maid.for (maid.exe) : may_120m.txt, may_60m.txt, may_30m.txt
Plots of these files (*.txt) using existing shapefiles for subareas, ESF, ECRB, etc…
On the following 3 pages: 30-m pixels on page 48, 60-m pixels on page 49, and 120-m pixels on page 50.







RF 7/21/03

**CL-2 Test Original**

The original suggested test was to compare results from BREATH to those from the ITYM response surface in TPA 5.0. Test is defined in TSPAI plan for validation report as:

"Estimates produced by the infiltration response surface function, which is constructed and evaluated by the ITYM stand-alone pre-processor, will be compared to simulation results from the BREATH computer code for several specific cases, including the base case modern climate. For specified values of MAP and MAT, the infiltration response surface, when evaluated at a specific spatial location and time, should provide an estimate of MAI that is within 10 percent of that estimated by the BREATH code using long-term average climate values."

Validation of TPA 5.0 UZFLOW module for TSPAI major milestone report includes a comparison of BREATH simulation results and ITYM results. To do this, I simplified the itym.dat input file so that a reasonable BREATH model could be created. A number of pixels were chosen for the comparison. One itym.dat input file could be used for all pixels. Separate BREATH models had to be created, one for each pixel.

**Recompile of BREATH v1.2 and Installation Check**

BREATH version 1.2 was used for the testing. To recompile BREATH so that an executable could be created for the current SUN architecture (Spock and Texas are the SUNs used to run the simulations; Texas uses the same SunOS and fundamentally same hardware type as Spock). Difficulty in compiling the brcatch.c module of BREATH (the only C coded module) on the current SUN operating system and c-code compiler caused me to use the old brcatch.o object file (compiled on previous SunOs of Spock), then link it with the rest of the fortran modules using the current fortran compiler. All the other fortran modules of BREATH v1.2 compiled correctly using the makefile supplied with the BREATH v1.2 code (only minor modifications were needed to get the make file to work, e.g., setting the correct paths for the current Spock setup). BREATH v1.2 was compiled and saved in the directory noted in the alias command below. The alias for BREATH allowed it to be run from any directory.

```
alias breath '~/TPA50d/TPA50-Validation/V1.2/Src/breath
```

To check the compiled code, I re-ran one test case from the BREATH validation report. The test case for couple heat and mass was chosen as a relevant problem to the comparison test for TPA ITYM.

```
Spock:  ~/TPA50d/TPA50-Validation/BREATH_Check/*
```

Two output files were created, the same ones as used in the BREATH validation testing using the following command

```
% breath < coupled.brt > /dev/null
```

The input file coupled.brt calls for coupled.mtr and coupled.out to be created. The file coupled.met is needed for the simulation (it's the meteorological data file).

1. coupled.out contains all the input echos and the initialized parameters (water pressure, saturation, vapor density in porous media, and temperature. All the entries visually checked in the original coupled.out were the same as the re-simulated values in coupled.out.17July2003.

2. coupled.mtr contains a mass tracing of 15 different variables (e.g., cumulative fluxes) retained during the simulation. The original coupled.mtr entries visually checked were exactly the same as the re-simulated entry values in the file coupled.mtr.17July2003.

Therefore, the recompiled breath executable works exactly as intended by the code author.

**ITYM Input File**

The changes to the itym.dat input file were done to simplify the problem that BREATH would have to solve. BREATH is a single continuum, 1-dimensional model that does not include the effect of vegetation, and runoff/runon.

1. One realization was needed, mean values would be used throughout the itym.dat file.
2. Pixel size was set to 30 m (no aggregation)
3. Precipitation and Temperature set to 162.9 mm/yr and 17.38 C (create a map for YM that has these values at the 1400 m elevation).
4. Turn runoff/runon off by commenting-out the two runon external file names (careadem.dat and cdepdem.dat).
5. Set all standard deviation table (e.g., UncertaintyTableSdev) entries (ignore correlation tables) and all sdev columns in mean tables (e.g., UncertaintyTableMean) to zero. Retain values in columns of mean values of mean tables.
6. Set all Vegetation parameters to mean values of 0; this removes effect of vegetation.
7. Set Soil VolFrac Table entries for means to zero for soil and –20 for rockfrac. Since these are log(Fraction) values, this sets rockfragment fraction to essentially zero for the soil. Doing the same for Lithology VolFrac Tables, sets the fracture porosity to zero. However, I want fracture flow for soil-filled fractures to occur, so set these to the desired values (log(frac)=-2, and frac=0.01), and the open and carbonate-filled fractures to log10(frac)=-20. Options are:
   Use the "All" pathway option in itym.inp and the arithmetically weighted flow properties in BREATH.
   Use the "MaxOnly" pathway option in itym.inp with only the filled fractures modeled in BREATH.

The modified ITYM input file is saved as
spock: ~rfedors/TPA50d/TPA50-Validation/itym_sdev0.dat.9July2003

During the course of this testing, some errors were found in the estimator.f subroutine of ITYM in TPA5.0. These errors led to software change report SCR-468. The three errors were (only the first error was significant):

1. Units of elevations for values incorporated in a data statement were inconsistent with elevdem.dat units (meters) in subroutine calc_DEM_props.

Change the following for consistency:
2. Values of elevation and average temperature for central Nevada site are slightly different than reported in cited USGS Open-File Report 93-651. Minor impact expected, recommend changing the values for the sake of consistency.
3. Cited document had both 1992 and 1994 for year of publication in subroutine calc_DEM_props. Should be 1994.

To fix these 3 items:
Change elevation of Central Nevada station (variable ECN) from 7200 ft to 7070 ft and then convert to meters; should be 2155 m.
Change Central Nevada station average temperature (variable dAAT) from -10.d0 to -9.65d0
Convert Desert Rock elevation (variable EDR) from 3298 ft to 1005 m.

---

**BREATH v1.2 Input Files**

To create an input file to approximate the production run by Stothoff, I used the same settings for many parameters. An input file had to be separately constructed because Stothoff used scripts to construct input files on the fly (changing "met" commands, options, and settings and changing flow parameter values). It was not prudent to use his MatLab scripts to generate input files.

The primary variables in the BREATH input file that have to be changed are the flow properties, initial conditions, grid, and meteorological data options.

The Desert Rock meteorological data file used by Stothoff was also used here. This is a 10-yr record. To remove the bias of initial conditions on flux estimates, the Desert Rock 10-year data record is rewound and cycled through additional times. Short versions of the meteorological data record were used with abundant tracing of parameter values to make sure that the simulations were set up in the proper manner. An example of this was retained the directory
~/TPA50d/TPA50-Validation/Breath-July2003/Check/*

The Desert Rock data was obtained from a cdrom obtained previously from Stothoff, and presumed linked to his Scientific Notebook #163. The meteorological file was used for the production runs that were used to generate the response surface for net infiltration. Extra records were added by Stothoff to ensure constant precipitation flux over the 1-hr time periods (early versions of Breath linearly interpolated meteorological data between times).

To determine the inputs for BREATH for the selected pixels, values from the appropriate positions in the ITYM external files were extracted and recorded in the Excel spreadsheet:

spock: ~rfedors/TPA50d/TPA50-Validation/Properties.xls see "Properties" worksheet
The element number in the list of each external ITYM file is the key for obtaining the properties. In searching the following external files, note that the header lines are not included in finding the element number (i.e., using vi, don't just go to line number such and such; one must subtract the number of header lines).

| | |
|---|---|
| bunitdem.dat | bedrock type |
| careadem.dat | not used, this is used for runoff component |
| cdepdem.dat | not used, this is used for runoff component |
| elevdem.dat | elevation data |
| maswtbl.dat | mean annual solar radiation table, interpolate value by calculating slope aspect using elevation data |
| soildem.dat | soil depth |
| sunitdem.dat | soil type |
| winddem.dat | average wind speed |

parameter values for hydraulic properties of the soil type and bedrock type were obtained from the itym.inp file that comes with TPA 5.0.

| **PARAMETER INPUTS TABLE**<br>Parameters to input into BREATH simulations for selected pixel locations | | | | | |
|---|---|---|---|---|---|
| | | | | | Too similar to YM crest pixel |
| | header lines in DEM | Middle Subarea 9, Drill Hole Wash | West central Subarea 8, YM crest | Subarea 4 moderate soil thickness over TCw | NW corner Subarea 1, PTn & thin soil |

| | | | | | |
|---|---|---|---|---|---|
| element # in list | | 18209 | 23375 | 35925 | 25952 |
| UTM NAD m Easting | | 547980 | 547740 | 548130 | 547440 |
| UTM NAD m Northing | | 4080240 | 4079460 | 4077570 | 4079070 |
| | | | | | |
| elev, m | 8 | 1353 | 1469 | 1389 | 1364 |
| soildem, m | 8 | 6.46695 | 0.147292 | 0.407757 | 0.116986 |
| winddem, m/s | 8 | 3.56354 | 4.24366 | 3.62138 | 3.74522 |
| Carea, m$^2$ | 6 | 3290.62 | 541.849 | | 2185.7 |
| Cdep, m | 6 | 0.43479 | 0.472819 | | 0.232319 |
| sunit | 10 | 9 | 5 | 9 | 5 |
| unit name | | TypicCalciargids | LithicHaplocambids | TypicCalciargids | LithicHaplocambids |
| log10(k), cm$^2$ | | -8.235 | -8.165 | -8.235 | -8.165 |
| log10(f) | | -0.4921 | -0.4815 | -0.4921 | -0.4815 |
| log10(a), kPa | | 0.2596 | 0.2518 | 0.2596 | 0.2518 |
| van Gen m | | 0.2308 | 0.4382 | 0.2308 | 0.4382 |
| bunit | 10 | 7 | 9 | 7 | 12 |
| unit name | | tcw | cuc | tcw | bt3 |
| log10(k), cm$^2$ | | -13.23 | -10.41 | -13.23 | -9.272 |
| log10(f) | | -1.143 | -0.6144 | -1.143 | -0.4737 |
| log10(a), kPa | | 2.907 | 2.082 | 2.907 | 0.3815 |
| van Gen m | | 0.4083 | 0.4565 | 0.4083 | 0.1896 |
| | | | | | |
| sunit | 10 | 9 | 5 | 9 | 5 |
| unit name | | TypicCalciargids | LithicHaplocambids | TypicCalciargids | LithicHaplocambids |
| k, cm$^2$ | | 5.821E-09 | 6.839E-09 | 5.821E-09 | 6.839E-09 |
| f | | 0.3220 | 0.3300 | 0.3220 | 0.3300 |
| a, Pa | | 1818.0 | 1785.7 | 1818.0 | 1785.7 |
| van Gen m | | 0.2308 | 0.4382 | 0.2308 | 0.4382 |
| | | | | | |
| 1% soil-filled fracture | 0.01 | scale permeability and porosity | | scale only permeability | |
| Properties are always the | | k, cm$^2$ | 6.839E-11 | 6.839E-11 | |
| same in itym; hence, use | | f | 0.0033 | 0.010 | |
| LithicHaplocambids here. | | a, Pa | 1785.7 | 1.786E+03 | |
| | | van Gen m | 0.4382 | 4.382E-01 | |
| | | | | | |
| ITYM basecase soil-filled fracture properties | | | | scale only k | scale k and porosity |
| log10(k), cm$^2$ | | -7.903 | k, cm$^2$ | 1.25026E-10 | 1.25026E-10 |
| log10(f) | | -0.3279 | f | 0.01 | 0.004700023 |
| log10(a), kPa | | 0.1139 | a, Pa | 1299.9 | 1299.9 |
| van Gen m | | 0.345 | van Gen m | 0.345 | 0.3 |

---

Note that the fracture properties have to be scaled by the fracture porosity. One could also scale the matrix properties, but the adjustment is minor because the matrix component of the total porosity dominates the fracture component of total porosity. A value of 0.01 (1%) was chosen for fracture porosity.

| | | ITYM code, itym.dat basecase input instructions | | | |
|---|---|---|---|---|---|
| | | Middle Subarea 9, Drill Hole Wash, Soil | West central Subarea 8, YM crest, CUC | Subarea 4 moderate soil thickness over TCw | NW corner Subarea 1, PTn & thin soil |
| | New itym approach | 1 | 2 | 3 | 4 |
| | elev | 1353 | 1469 | 1389 | 1364 |
| | MAP | 157.4169523 | 169.4374864 | 161.0532525 | 158.5192468 |
| | MAT | 17.3055 | 16.5515 | 17.0715 | 17.234 |
| | MAV | 4.97737E-06 | 3.81066E-06 | 4.58142E-06 | 4.85289E-06 |
| Desert Rock Avg | | | | | |
| 162.8 | MAP ratio DS->YM | 0.9669 | 1.0408 | 0.9893 | 0.9737 |
| 17.38 | MAT shift DS->YM | -0.0745 | -0.8285 | -0.3085 | -0.1460 |
| 4.52E-06 | MAV ratio DS->YM | 1.1007 | 0.8427 | 1.0131 | 1.0732 |

For each selected pixel case, separate BREATH simulations were run using the appropriate parameter value inputs (see Parameter Inputs table on page 53-54) and meteorological shifts and scaling of the Desert Rock data (see Meteorological table on page 54 for shifting and scaling). Separate directories were created for the 3 chosen pixel (I dropped the 4th pixel because the results were too similar to one of the other pixels for both ITYM and BREATH). The directories names are linked to the column headings, i.e.,

pixel 18209 → spock: ~rfedors/TPA50d-TPA50-Validation/Breath-July2003/Soil/*
pixel 23375 → spock: ~rfedors/TPA50d-TPA50-Validation/Breath-July2003/CUC/*
pixel 35925 → spock: ~rfedors/TPA50d-TPA50-Validation/Breath-July2003/TCw/*

The following table contains a summary of the testing:

## SOFTWARE VALIDATION TEST REPORT (SVTR)

| | |
|---|---|
| **SVTR#:** | **Project#:** 20.060002.01.113 |
| **Software Name:** TPA | **Version:** 5.0h |
| **Test ID:** C1-2 | **Test Series Name:** UZFLOW |

**Test Method**

☐ code inspection
☒ output inspection
☐ hand calculation

☐ spreadsheet
☐ graphical
☒ comparison with external code results

**Test Objective:** Estimates produced by the infiltration response surface function, which is constructed and evaluated by the ITYM stand-alone pre-processor, will be compared to simulation results from the BREATH computer code for several specific cases, including the base case modern climate. For specified values of MAP and MAT, the infiltration response surface, when evaluated at a specific spatial location and time, should provide an estimate of MAI that is within 10 percent of that estimated by the BREATH code using long-term average climate values.

Note: The constraint of 10-percent error was too stringent. To be within 10 percent for small values of net infilration is not practical and the difference would not be important. For small values of net infiltration, such as 1 mm/yr, 10 percent of the net infiltration does not affect subarea averages of net infiltration when subarea averages are on the order of 8.5 mm/yr). For larger values of net infiltration, the 10-percent errors are more precise than warranted by estimates of net infiltration supported by measurements at Yucca Mountain.

Also, the response surface created from the 500 BREATH simulations was expected to have errors at individual locations, but ensemble spatial averages have been shown to be reasonable (Stothoff, 1999). As with all GIS (Geographic Information System) approaches, local differences may be prominent, but subarea averages should be reasonable. BREATH cannot simulate ensemble averages. An environment known to be problematic was extremely thin soils over fractured bedrock. The polynomial equations used in ITYM to represent the response surface of net infiltration to flow and climatic factors does poorly for the extremely thin soils. This environment occurs over the repository, so it should not be ignored. Also, since BREATH does not include the effect of vegetation, large errors may occur when vegetation is excluded.

A reasonable constraint is to be within a factor of 2, except for extremely thin soils where the effect of vegetation in ITYM compensates for errors in the response surface.

**Test Environment Setup**

**Hardware (platform, peripherals):** SUNW, Ultra-4, "TEXAS" and "SPOCK"

**Software (OS, compiler, libraries, auxiliary codes or scripts):** SUN-OS 5.8; f77 version 5.0

**Input Data (files, data base, mode settings):** Compare the results of the ITYM module to simulation results from BREATH Version 1.2. Three markedly different net infiltration terrains that occur over the repository are assessed: deep soil (Test A), thin soil over fractured bedrock (Test B), and moderately thick soil over fractured bedrock (Test C). For locations of Test A and Test B, the fractured bedrock beneath the soil layer contains multiple flow pathways in ITYM. The pathway chosen for the comparison with BREATH was the soil-filled fracture pathway.

ITYM: The base case input file (itym.dat) was modified to create a scenario that BREATH could mimic. This entailed the following:

**1.** Change itym.dat to run one realization (*num_realize_per_table*) and set all standard deviation values to zero to

get mean case ($2^{nd}$ column in *UncertaintyMeanTables* throughout itym.dat).

**2.** Set *PathwaySum* to *"MaxOnly."* This is base case value; setting *PathwaySum* to *"All"* results in slight increase in net infiltration due to matrix contribution. Note that we cannot run ITYM module with matrix volume fractions (*VolFrac*) set to nearly zero, hence simulations with *MaxOnly* setting and *All* setting were used to show that maximum contribution comes from flow in the filled fracture. See Spock:~/TPA50d/TPA50-Validation/ITYM/All/maytbl.dat and ~/TPA50d/TPA-Validation/Properties.xls, "Infilt Summary" worksheet for numerical results.

**3.** Comment-out the runoff external files (careadem.dat and cdepdem.dat); this causes runon to be zero for all pixels.

**4.** Set pixel size to 30 m (*num_pixel_merge* set to 1), number of tables to 1 (*num_MAP_table* and *num_MAT_table* both set to 1) and precipitation and temperature set to 162.8 mm/yr and 17.38 °C (*MAP_min* and *MAP_max* set to 162.8 and *MAT_min* and *MAT_max* set to 17.38).

**5.** Set means and standard deviations of vegetation parameters to zero to eliminate effect of vegetation on net infiltration (6 records in *UncertaintyTableMean* for *UncertaintyTableID*=Vegetation).

**6.** Set all volumes of rock fragments in soil to nearly zero (*Soil VolFrac Tables*, set log10 mean of *rockfrag* entries for each soil type to -20), thus allowing for flow properties of soils to be used directly.

**7.** Set all fracture volumes of open and carbonate filled fractures to nearly zero (log10 mean values for *unfilled* and *carbfill* records in *Lithology VolFrac Tables* set to -20).

**BREATH Inputs:**

Inputs for BREATH V1.2 were determined from the itym.dat file for unsaturated flow properties and climatic conditions. Initial conditions were determined by cycling through the Desert Rock meteorological data set multiple times before obtaining quantitative estimates of net infiltration. The locations and entry number (in external files, exclude header lines) are:

| | Test A | Test B | Test C | Soil in Filled Fracture (from itym.dat) |
|---|---|---|---|---|
| element # in list | 18209 | 23375 | 35925 | |
| UTM NAD m Easting | 547980 | 547740 | 548130 | |
| UTM NAD m Northing | 4080240 | 4079460 | 4077570 | |

The external files for ITYM were the source of the following data for each Test location:

| | | | | |
|---|---|---|---|---|
| soil thickness, m | 6.46695 | 0.147292 | 0.407757 | |
| wind speed, m/s | 3.56354 | 4.24366 | 3.62138 | |
| soil unit | 5 | 9 | 5 | |

The itym.dat file was the source of the following data for each Test location:

| | | | | |
|---|---|---|---|---|
| log10(k), $cm^2$ | -8.235 | -8.165 | -8.235 | -7.903 |
| log10(f) | -0.4921 | -0.4815 | -0.4921 | -0.3279 |
| log10(a), kPa | 0.2596 | 0.2518 | 0.2596 | 0.1139 |
| van Gen m | 0.2308 | 0.4382 | 0.2308 | 0.345 |

For soil unit names 5=TypicCalciargids 9=LithicHaplocambids

To determine unsaturated zone properties for modeling soil-filled fractures in BREATH, the permeability and the porosity of the soil in the fractures were scaled by the fracture porosity (0.01).

For climatic conditions, the mean annual precipitation, temperature, and vapor density of air above soil were derived using the same equations as used in ITYM and the same coefficients for these equations as in the base case itym.dat file. Elevations for locations A, B and C were taken from external file. BREATH simulations were done using the 10-yr Desert Rock meteorological data set. The input file for BREATH allows for scaling of the meteorological data set to retain the desired mean annual precipitation, temperature, and vapor density.

Desert Rock Averages: MAP=162.8 mm/yr, MAT=17.38 °C, MAV=4.522e-06 g/$cm^3$.

| | Test A | Test B | Test C |
|---|---|---|---|
| elev, m | 1353 | 1469 | 1389 |
| MAP, mm/yr | 157.42 | 169.44 | 161.05 |
| MAT, degree C | 17.31 | 16.55 | 17.07 |
| MAV, g/cm3 | 4.97E-06 | 3.81E-06 | 4.58E-06 |

Ratios for Desert Rock to Yucca Mountain

| | | | |
|---|---|---|---|
| MAP ratio | 0.9669 | 1.0408 | 0.9893 |
| MAT shift | -0.0745 | -0.8285 | -0.3085 |
| MAV ratio | 1.1007 | 0.8427 | 1.0131 |
| MASW ratio | 0.5809 | 0.6536 | 0.6999 |

Mean Annual Precipitation (MAP), Temperture (MAT), and Vapor Density (MAV) for Test A, B, and C were scaled or shifted based on the Desert Rock averages. Mean Annual Solar radiation (MASW) was scaled to account for ground surface aspect (angle of surface plane to sun position). The external file maswtab.dat used by the ITYM module provides solar radiation as a function of north-south and east-west angles relative to the horizontal plane. Slope angles were calculated from the elevdem.dat file for Test A, B, and C locations. The angles are (i) north-facing 5.7° and east-facing 18° for Test A, (ii) south-facing -5.7° and east-facing -15.8° for Test B, (iii) south-facing -1° and west-facing 18° for Test C. The maximum value of solar radiation in the maswtab.dat file was used to estimate the ratio noted above.

**Assumptions, constraints, and/or scope of test:** The ITYM module includes all the prominent processes that significantly affect estimates of net infiltration over a small area (~ 30-m pixel). The BREATH Version 1.2 codes does not include the affect of vegetation, which prominently affects net infiltration. BREATH Versiosn 1.2 does not include the affect of runoff and runon. Also, the ITYM module includes multiple net infiltration pathways (through bedrock matrix or fractures filled with different materials), different types of fracture filling material (soil, carbonate, open), rock fragments in the soil of varying percentages. Therefore, the input file itym.dat was modified to greatly simplify the net infiltration scenario so that BREATH Version 1.2 could approximately mimic the scenario. The assumption of Desert Rock meteorological data (elevation 1005 m) representing environmental conditions at the base elevation of 1400 m for Yucca Mountain requires further analysis. Also the use of the maximum value of solar radiation in the maswtab.dat file to scale the solar radiation of any pixel on Yucca Mountain also requires further analysis; the measurement device at Desert Rock used to record net solar radiation may reflect a value representing a horizontal surface rather than a surface that is, on the average, closer to being perpendicular to the sun.

**Test Procedure:**

ITYM:

Base directory: spock:~rfedors/TPA50d/TPA50-Validation/ITYM/

1. Recompile the current version of ITYM module (matches TPA version), rename itym.e to itym50?, where the ? refers to the current version being tested.
2. Run itym50? to create the maytbl.dat file, which contains log10 values of net infiltration. The ITYM module is executed by the following command (e.g., using version TPA5.0m: itym50m). The default input file for ITYM is itym.dat.
3. Input and output files copied to appropriate subdirectory for archival. Compare the ITYM result extracted from the appropriate record in the ITYM output file "maytbl.dat" to the BREATH result.

BREATH Simulations

Base directory where ITYM executable and external files reside:: spock:~rfedors/TPA50d/TPA50-Validation/Breath-July2003/

The t.met file (Desert Rock data) and BREATH input files must be in the same directory command execution. The BREATH executable is used via an alias:

```
alias breath '/TPA50d/TPA50-Validation/V1.2/Src/breath'
```

1. Create input files
   - Test A: ./Soil/soil.dat
   - Test B: ./CUC/cuc-kf0047.dat
   - Test C: ./TCw/tcw-kf0047.dat
2. Run BREATH using the command (see shell script in appropriate directory)
   `breath < input.filename > /dev/null`
3. The BREATH input file calls for the creation of following files of cumulative mass flux:
   - Test A ./Soil/cumflx_Soil.out.SW.5809
   - Test B ./CUC/cumflx_CUC_kf0047.out
   - Test C ./TCw/cumflx_tcw_kf00047.out

---

The "met" command in these input file cause the Desert Rock meteorological data (10-yr record) to be cycled through 11 times (nmetcyc=10) to remove bias of initial conditions. The cumulative flux for simulated years 100 to 110 are extracted from the output files. The cumulative fluxes are subtracted and an annual average is calculated.

**Test Results**

**Location:** ITYM results are in spock:~rfedors/TPA50d/TPA50-Validation/ITYM/
BREATH v1.2 results are in spock:~rfedors/TPA50d/TPA50-Validation/Breath-July2003/

**Test Criterion or Expected Results:**
Test A: ITYM 14.2 mm/yr; BREATH 9.1 mm/yr.
Test B: ITYM 18.2 mm/yr; BREATH 3.5 mm/yr.
Test C: ITYM 2.4 mm/yr; BREATH 1.4 mm/yr.

**Qualifications:**
The Test B location is off by a factor of 5. This particular environment was known to problematic in the response surface generated from the 500 BREATH realizations (Stothoff, 1999). The equations in the ITYM module represent the response surface. When vegetation is heuristically included in the ITYM simulation, the net infiltration value for Test B is 4.4 mm/yr. While this lower value should not be directly compared with the BREATH results, it does indicate that the vegetation model compensates for the error in the response surface. The value of 4.4 mm/yr errs to the conservative side, and thus is considered acceptable.

**Test Evaluation (Pass/Fail):** PASS, with realistic constraints of a factor of 2.

**Notes:** References
Stothoff S.A. Infiltration Abstractions for Shallow Soil Over Fractured Bedrock in a Semiarid Climate. CNWRA Letter Report. San Antonio, TS: Center for Nuclear Waste Regulatory Analyses. 1999.

| | |
|---|---|
| **Tester:** Randy Fedors | **Date:** 7-21-03 |

This version of the validation test report was not satisfactory to TSPAI staff, and a new approach for validation was devised that focused more on validation in terms of implementation (see next section).

RF 7/30/03

**CL-2 Test Revised**

Since the original test plan to compare BREATH results to the ITYM results was dropped because of too stringent of criteria for passing (Gordon set the criteria without our knowledge), here is the revise CL-2 test and results. This version checked that the response surface was implemented correctly.

When discrepancies were found, discussions via a number of emails with Stu Stothoff led to the realization that the correct equations were included in his tmai.xls Excel spreadsheet. The Stothoff 1999 report, previously cited as the source of the equations, had equations that were not consistent with the coding in the ITYM source code files. Apparently, the equations were revised slightly when the ITYM module was created (which occurred after the Stothoff 1999 report was created (this was the journal article that was to be submitted to Water Resources Research, but was rejected because it was too big).

# SOFTWARE VALIDATION TEST REPORT (SVTR)

**SVTR#:**

**Project#:** 20.060002.01.113

**Software Name:** TPA

**Version:** 5.0m

**Test ID:** C1-2

**Test Series Name:** UZFLOW

**Test Method**

☐ code inspection
☒ output inspection
☐ hand calculation
☒ spreadsheet
☐ graphical
☐ comparison with external code results

**Test Objective:** [Original Objective] Estimates produced by the infiltration response surface function, which is constructed and evaluated by the ITYM stand-alone pre-processor, will be compared to simulation results from the BREATH computer code for several specific cases, including the base case modern climate. For specified values of MAP and MAT, the infiltration response surface, when evaluated at a specific spatial location and time, should provide an estimate of MAI that is within 10 percent of that estimated by the BREATH code using long-term average climate values.

Note: The constraint of 10-percent error was too stringent. To be within 10 percent for small values of net infilration is not practical and the difference would not be important. For example, small values of net infiltration, such as 1 mm/yr, and 10 percent errors in net infiltration does not affect subarea averages of net infiltration when subarea averages are on the order of 8.5 mm/yr). Also, the response surface created from the 500 BREATH bare-soil simulations was expected to have errors at individual locations, but ensemble spatial averages have been shown to be reasonable (Stothoff, 1999). An environment known to be problematic was extremely thin soils over fractured bedrock. The response surface of net infiltration to flow and climatic factors implemented in ITYM is represented by a complex set of polynomial equations that performs poorly for the extremely thin soils. The complex interplay between the unsaturated properties of both layers and flow between the layers make the response surface difficult to match with specific simulations. For example, a capillary barrier situation between two layers can readily change to a permeability barrier or a capillary attractor situation with small changes to some of the unsaturated zone flow properties or different precipitation patterns. Since the thin-soil environment occurs over the repository, it should not be ignored. Also, since BREATH does not include the effect of vegetation, large errors may occur when vegetation is excluded.

Therefore, the test plan was modified to better reflect the objective of confirming that code segments are functioning as intended; i.e., an implementation check. The specific aspect of ITYM that will be checked is the implementation of the bare-soil response surface. Factors reflecting soil thickness, soil properties, bedrock properties, and weather will be used as input in spreadsheet calculations. Mean annual net infiltration will be calculated for matrix and soil-filled fracture flow pathways at 4 test locations in the repository footprint. For the locations tested, the spreadsheet calculations should provide an estimate of net infiltration that is within 10 percent of that estimated by the ITYM module.

**Test Environment Setup**

**Hardware (platform, peripherals):** ITYM run on SUNW, Ultra-4, "TEXAS" and "SPOCK,"
and Excel 97 SR-2 run on WinNT 4.00.1381 called "bubo."

**Software (OS, compiler, libraries, auxiliary codes or scripts):** recompile of ITYM module used SUN-OS 5.8; f77 version 5.0

**Input Data (files, data base, mode settings):** The revised test for C1-2 checked the implementation of the 2nd tier of equations that lead directly to the net infiltration (bare-soil) value. The calculation check starts with inputs

for the soil thickness factor (pCov), soil properties factor (S), bedrock properties factor (B), and weather factor (W). Coefficients for the 2nd tier equations were obtained from Stothoff's tmai.xls spreadsheet; which was where the response surface was developed. Values for the pCov, S, B, and W factors were obtained from selected output of intermediate calculations in the ITYM module. For reference, the 2nd tier of equations for the response surface is

H= ao + [a1+S*(1+as*H)+W*(1+aw*H)]*pCov+B*(1+ab*B*H)
where H= log10(MAI/MAP)
This can be rearranged into the form:
H = A1 / (1 - A2)
where MAI is mean net infiltration, MAP is mean annual precipitation and
A1 = ao + [a1 + S + W]*pCov + S + B + W
A2 = [as*S + aw*W]*pCov + as2*S + ab*B+ aw2*W

Four markedly different net infiltration terrains that occur over the repository are assessed: deep soil (Test A), thin soil over fractured bedrock (Test B), and moderately thick soil over fractured bedrock (Test C), and thin soil over highly permeable nonwelded bedrock . For locations of Test A and Test B, the fractured bedrock beneath the soil layer contains multiple flow pathways in ITYM. The pathways chosen for the comparison were the matrix and the soil-filled fracture pathways. The locations and entry number (in external files, exclude header lines) are:

| | Test A | Test B | Test C | Test D |
|---|---|---|---|---|
| element # in list | 18209 | 23375 | 35925 | 25952 |
| UTM NAD m Easting | 547980 | 547740 | 548130 | 547440 |
| UTM NAD m Northing | 4080240 | 4079460 | 4077570 | 4079070 |
| elev, m | 1353 | 1469 | 1389 | 1364 |
| MAP, mm/yr | 157.42 | 169.44 | 161.05 | 158.5 |

Using values for the coefficients directly from Stothoff (1999) resulted in test failure (errors ranged from 9.6 to 18.4 percent); the coefficient values used 4 to 5 significant figures (less than 32-bit precision). Using the values of coefficients with 64-bit precision (12-14 significant figures), the maximum error was 0.02 percent. This change in error illustrates the sensitivity of the response surface to precision of inputs. The calculations were done in the Excel spreadsheet C1-2_TPA50.xls.

ITYM Inputs Description: The base case input file (itym.dat) was modified to create a scenario that spreadsheet calculations could directly check the implementation of the response surface equations. This entailed the following:

**1.** Change itym.dat to run one realization (*num_realize_per_table*) and set all standard deviation values to zero to get mean case (2$^{nd}$ column in *UncertaintyMeanTables* throughout itym.dat).

**2.** Set *PathwaySum* to *"MaxOnly"* and to *"All"* depending on the desired output; both will be used for the validation test. This base case entry is *"MaxOnly;"* setting *PathwaySum* to *"All"* results in slight increase in net infiltration due to the soil-filled contribution. Note that we cannot run ITYM module with matrix volume fractions (*VolFrac*) set to nearly zero, but the fractions of carbonate-filled and open fractures are set to essentially zero(see item 7). Hence, simulations with *MaxOnly* setting and *All* setting could be used to show the contributions of flow coming from the matrix and the soil-filled fracture.
See Spock:~/TPA50d/TPA50-Validation/ITYM/All/maytbl.dat and ~/TPA50d/TPA-Validation/Properties.xls, "Infilt Summary" worksheet for numerical results.

**3.** Comment-out the runoff external files (careadem.dat and cdepdem.dat); this causes runon to be zero for all pixels.

**4.** Set pixel size to 30 m (*num_pixel_merge* set to 1), number of tables to 1 (*num_MAP_table* and *num_MAT_table* both set to 1) and precipitation and temperature set to 162.8 mm/yr and 17.38 °C (*MAP_min* and *MAP_max* set to 162.8 and *MAT_min* and *MAT_max* set to 17.38).

**5.** Set means and standard deviations of vegetation parameters to zero to eliminate effect of vegetation on net infiltration (6 records in *UncertaintyTableMean* for *UncertaintyTableID*=Vegetation).

**6.** Set all volumes of rock fragments in soil to nearly zero (*Soil VolFrac Tables*, set log10 mean of *rockfrag* entries for each soil type to -20), thus allowing for flow properties of soils to be used directly.

**7.** Set all fracture volumes of open and carbonate-filled fractures to nearly zero (log10 mean values for *unfilled* and *carbfill* records in *Lithology VolFrac Tables* set to -20).

**Assumptions, constraints, and/or scope of test:** The scope of the test is described here. There are two tiers of equations that form the net infiltration response surface in ITYM. The response surface accounts for bare-soil net infiltration and was based on approximately 500 BREATH v1.2 simulations. Also, there are two options for selecting net infiltration pathways to use in the ITYM calculation. Both the *MaxOnly* and *All* pathways options were checked as part of this test. The *MaxOnly* option uses the maximum value of net infiltration from one of the following pathways; (i) soil layer over bedrock matrix, (ii) soil layer over carbonate-filled fractures, (iii) soil layer over soil-filled fractures, and (iv) soil layer over open fractures. The *All* option sums the contributions from the four pathways. The four sites (pixel locations on Yucca Mountain) selected for checking the calculation fall into the category of the capillary attractor response surface. There is also a capillary barrier response surface. The base case ITYM scenario for estimating net infiltration is dominated by capillary attractors. The capillary barrier and attractor are distinguished by the behavior flow in the fractures below the soil layer and is dependent on the properties of both the soil layer and the fractures.

**Test Procedure:**

ITYM Estimate of Net Infiltration:

Base directory: spock:~rfedors/TPA50d/TPA50-Validation/ITYM/*

**1.** Recompile the current version of ITYM module (matches TPA version), rename itym.e to itym50?, where the ? refers to the current version being tested. The recompile is performed by running the unix make command in the directory above the ./src/ directory for ITYM (default to official release directory of ./codes/itym/ and run the unix *make* command.

**2.** Run itym50? to create the maytbl.dat file, which contains log10 values of net infiltration. The ITYM module is executed by the following command "itym5.0m" (using the compiled version ITYM from TPA5.0m). The default input file for ITYM is itym.dat must be in the same directory; the required external files must also be in the directory.

**3.** Input and output files copied to appropriate subdirectory for archival. Compare the ITYM result extracted from the appropriate record in the ITYM output file "maytbl.dat" to the spreadsheet calculation.

Excel 97 SR-2 Calculation

**1.** Implement the response surface equations described previously (see C1-2_TPA50.xls).

**2.** Enter the values for the factors from intermediate calculations by running appropriate versions of ITYM that are recompiled to print out data for the appropriate element location corresponding to Test A (element 18209), Test B (element 23375), Test C (element 35925), and Test D (element 25952). The appropriate ITYM (TPA5.0m) executables are itym.18209, itym.23375, itym.35925, and itym.25952. The screen output identifies the pCov, S, B, and W factors along with other intermediate outputs. The commands to capture the screen output for each Test location is :

```
    itym.18209 > test.18209
    itym.23375 > test.23375
    itym.35925 > test.35925
    itym.25952 > test.25952
```

The screen output files and specified ITYM executables are located in
spock:~rfedors/TPA50d/TPA50-Validation/ITYM/Test/*

**3.** When the ITYM executable needs to be recompiled, the following inserts to estimator.f will print the appropriate intermediate results to the screen:

a.) In subroutine calc_MAI_tpa4, after the line with "do it1 = 1,nDEM", add

```
        if(it1.eq.18209) then
        print*, it1, ' the pixel number'
```

b.) Complete the if-endif combination by adding the following lines just before the "enddo" line at the end of the subroutine;

```
        else
```

```
        endif
```

c.) Add the following line in the subroutine calc_pixMAI, immediately before the "return" statement at the end of the subroutine:

```
        print*, 'pCov pSoil pBed pWea ', pCov, pSoil, pBed, pWea
```

These screen outputs are the factors that are used as input to the spreadsheet calculation.

### Test Results

**Location:** ITYM results are in spock:~rfedors/TPA50d/TPA50-Validation/ITYM/
Excel 97 SR-2 spreadsheets are in spock:~rfedors/TPA50d/TPA50-Validation/*.xls

**Test Criterion or Expected Results:** Results are in units of mm/yr except where stated. Error calculated using the ITYM result as "truth;" i.e., 100*(ITYM-Excel)/ITYM. Errors were to be less than 10 percent.

| | ITYM Matrix | ITYM Soil-Filled Fracture | Percent Error | Excel Matrix | Excel Soil-Filled Fracture | Percent Error |
|---|---|---|---|---|---|---|
| Test A: | 14.22138 | 0.025676 | 8.8e-3 | 14.22013 | 0.025670 | 2.3e-3 |
| Test B: | 18.15228 | 3.592509 | 7.1e-3 | 18.15099 | 3.592157 | 9.8e-3 |
| Test C: | 2.35936 | 1.846279 | 1.2e-2 | 2.35909 | 1.846032 | 1.3e-2 |
| Test D: | 19.32607 | 4.525618 | 6.8e-3 | 19.32474 | 4.525080 | 1.2e-2 |

**Test Evaluation (Pass/Fail):** PASS

**Notes:** References

Stothoff S.A. Infiltration Abstractions for Shallow Soil Over Fractured Bedrock in a Semiarid Climate. CNWRA Letter Report. San Antonio, TS: Center for Nuclear Waste Regulatory Analyses. 1999.

**Tester:** Randy Fedors **Date:** 7-30-03

RF 7/30/03

Last Entry, notebook will be closed-out.

RF. 9/21/04

I have reviewed this SN and determined that it complies with QAP-001. An earth scientist with expertise in near-surface hydrologic process should be able to replicate the work described herein.

Gordon Wittmeyer
9/24/2004

## ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 227

| | |
|---|---|
| **Document Date:** | 09/19/1997 |
| **Availability:** | Southwest Research Institute®<br>Center for Nuclear Waste Regulatory Analyses<br>6220 Culebra Road<br>San Antonio, Texas 78228 |
| **Contact:** | Southwest Research Institute®<br>Center for Nuclear Waste Regulatory Analyses<br>6220 Culebra Road<br>San Antonio, TX 78228-5166<br>Attn.: Director of Administration<br>210.522.5054 |
| **Data Sensitivity:** | ■"Non-Sensitive" ☐ Sensitive<br>☐"Non-Sensitive - Copyright" ☐ Sensitive - Copyright |
| **Date Generated:** | 09/22/2004 |
| **Operating System:** (including version number) | Windows NT, Sun OS, UNIX |
| **Application Used:** (including version number) | WordPerfect 8.0; Word 97, SR–2, PowerPoint 97, SR–2; Kodak Photo Images; Excel 97, SR-2; Adobe Illustrator 8.0; ArcView 7.2a; Fortran 77 |
| **Media Type:** (CDs, 3 1/2, 5 1/4 disks, etc.) | 2 - CDs |
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