

SCIENTIFIC NOTEBOOK

451 E

BY ALBERT LOZANO

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SCIENTIFIC NOTEBOOK No. 451E INITIALS: A. L.

SCIENTIFIC NOTEBOOK

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SCIENTIFIC NOTEBOOK No.

451E INITIALS: A. L.

INITIAL ENTRIES

Scientific Notebook: #451E

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Title: Metric Measure & Other Exploratory Work

Participants: Albert Lozano

Statement of Purpose:

The work to be performed is exploratory in nature. At this time we do not know whether any of the information in this notebook will be incorporated into any deliverable item. The software that was developed was strictly to achieve our exploratory goals. At this time we do not believe that any of this software will be delivered or used in any formal reports.

The first section of the notebook is for work performed on the evaluation of an article describing an uncertainty importance measure.

Starting Date Prior to Feb. 5, 2001

This work started with the evaluation of an article from a publication
RELIABILITY ENGINEERING & SAFETY SYSTEM 70 (2000) 313-321.

The title of the article is *An uncertainty importance measure using a distance metric for the change in a cumulative distribution function*.

The distance metric described in the article is computed from two cumulative distribution functions produced from a change in distribution of one of the input parameters.

The method is being implemented for Case 3 in the article, empirical distribution. The equation being implemented is equation (14) in the article.

Other work done in this time was the development of several MATLAB programs to help us determine beta distribution equivalents for the uniform and normal, and logbeta distribution equivalents for loguniform and lognormal distributions.

The MatLab programs are located in ../Moose/gdrive/mohanty/Alozano/MatLab.

» **betafixed run results;**

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This function `betafixed()` plots the normal distribution, the beta equivalent distribution, and the 10% shifted mean beta distribution. The distributions are determined for $x=0$ to $x=1$. The beta equivalent parameters are $p=5$ and $q=5$. The 10% shifted parameters are $p=7.5$, $q=5$.

beta equivalent to normal distribution

median1 = 0.5000

mean1 = 0.5000

ypeak1 = 2.4609

ypeak1pos = 501

10% mean shift beta distribution

median2 = 0.6050

mean2 = 0.6000

ypeak2 = 2.8416

ypeak2pos = 620

Matlab Code

This code is exploratory code to help us determine input parameters for the `tpa.inp` file used by the `tpa` code. This code is not deliverable.

```
function z=betafixed()

x=0:.001:1.0;
nloops=1001;
median = 0;
pasthalf = 0;
p=5;
q=5;
ypeak1=0;
ypeak1pos=0;
mean1 = 0.0;
for i=1:nloops,
    betaout= (gamma(p+q)/(gamma(p)*gamma(q)))*(x(i)^(p-1))*((1-x(i))^(q-1));
    y(i) = betaout;
    if i == 1
        z(i) = y(i);
        mean1 = x(i)*y(i)+mean1;
        ypeak1=y(i);
        ypeak1pos = i;
    else
        z(i) = z(i-1) + y(i);
        mean1 = x(i)*y(i)+mean1;
        if ypeak1 < y(i)
            ypeak1 = y(i);
            ypeak1pos = i;
        end;
        if pasthalf == 0
            if z(i) >= 500.0
                median = x(i);
                pasthalf = 1;
            end;
        end;
    end;
end;
median1 = median
mean1 = mean1/1000
ypeak1
ypeak1pos
median = 0;
pasthalf = 0;
p=7.5;
q=5;
ypeak2=0;
ypeak2pos=0;
mean2=0.0;
for i=1:nloops,
    betaout= (gamma(p+q)/(gamma(p)*gamma(q)))*(x(i)^(p-1))*((1-x(i))^(q-1));
    y1(i) = betaout;
    if i == 1
        z1(i) = y1(i);
        mean2 = x(i)*y1(i) + mean2;
```

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```

        ypeak2=y1(i);
        ypeak2pos = i;
    else
        z1(i) = z1(i-1) + y1(i);
        mean2 = x(i)*y1(i) + mean2;
        if ypeak2 < y1(i)
            ypeak2 = y1(i);
            ypeak2pos = i;
        end;
        if pasthalf == 0
            if z1(i) >= 500.0
                median = x(i);
                pasthalf = 1;
            end;
        end;
    end;
end;
median2 = median
mean2 = mean2/1000
ypeak2
ypeak2pos
mean = .5;
stddev = 1.0/6.180465
pasthalf = 0;
median = 0;
for i=1:nloops,
    betaout= (1/(stddev*sqrt(2*pi)))*(exp(-1.0*(x(i)-mean)^2/(2.0*stddev^2)));
    y2(i) = betaout;
    if i == 1
        z3(i) = y2(i);
    else
        z3(i) = z3(i-1) + y2(i);
        if pasthalf == 0
            if z3(i) >= 500.0
                median = x(i);
                pasthalf = 1;
            end;
        end;
    end;
end;
z2 = (z3+(1000.0-z3(nloops))/2)/1000.0;
median3 = median
figure(1); % pdf
%plot(x,z/1000.0,'-',x,z1/1000.0,'--',x,z2,':');
plot(x,z/1000.0,'-',x,z1/1000.0,'--');
%AXIS([5 15 0 20])
xlabel('Variable 1 ')
ylabel('CDF')
title('Mean Varied by 10% of the Range')

figure(2); %cdf
%plot(x,y,'-',x,y1,'--',x,y2,':');
plot(x,y,'-',x,y1,'--');
%AXIS([5 15 0 20])
xlabel('Variable 1 ')
ylabel('Frequency')
title('Mean Varied by 10% of the Range')

```

» **betafixeduniform run results;**

This function betafixeduniform() plots the uniform distribution, the beta equivalent distribution, and the 10% shifted mean beta distribution. The distributions are determined for $x=0$ to $x=1$. The beta equivalent parameters are $p=1$ and $q=1$. The 10% shifted parameters are $p=1.5$, $q=1$.

beta equivalent to normal distribution
median1 = 0.4990

10% mean shift beta distribution
median2 = 0.6300

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mean1 = 0.5005
 ypeak1 = 1
 ypeak1pos = 1

mean2 = 0.6008
 ypeak2 = 1.5000
 ypeak2pos = 1001

The MatLab code for betafixeduniform is the same as betafixed with the exception of the p and q values.

Feb. 05-07, 2001 – Developed code related to determining the metric measure.

The peak dose values obtained from a TPA run are contained in a file named *gwpkdos.res*. The values are located in the third column (pktede), one row per realization, and are not in numerical order. The calculation for the distance metric requires that the values be in ascending order. I wrote *ordersort.f* and *sort.f* to extract the peak dose values from *gwpkdos.res* and write the sorted results in *gwpkdos.sorted*. The executable program, *orderdose*, must be run in the directory containing the *gwpkdos.res* file. The source code for this software is located in `.../vulcan/home/alozano/tpa4leMean/tpaOrderDose`.

Fortran Code

This code is exploratory code to produce a sorted file, *gwpkdos.sorted*, from the Ground Water Peak Dose File, *gwpkdos.res*. The produced file is used only in the code that calculates distance metric and is not a deliverable code.

```

      Program SortDose
      implicit none

C      This program reads the gwpkdos.res file and creates a
C      new file gwpkdos.sorted.

C      Albert Lozano ext 2718      05 Feb 2001

      real*4 peakdosraw(500), peakdossorted(500)

C      inputline - Buffer for an input string
      character*800 inputline

C      release - Buffer used to search for word "Release" in file
      character*8 release

C      stayinloop - Used to stay in while loop while value is not zero
      integer*2 stayinloop

C      readdata -Used to switch from reading text strings (value = 0)
C      to reading data records(value=1)
      integer*2 readdata

C      index - Array index
      integer*2 index, ii

C      rvalue - temporary value
      real*4 rvalue

      print *, "This program Reads the gwpkdos.res file and generates"
      print *, "the gwpkdos.sorted file"
C      print *, "Make sure that the file gwpkdos.res exists in current directory"

      stayinloop = 0
C      stayinloop = 1
      do while (stayinloop .eq. 1)
C      print *,
C      1  "Type ""exit"" to exit the program now, or ""go"" to continue"
C      read(' (A)') inputline
C      if ((inputline(1:2) .eq. "EX").or.(inputline(1:2) .eq. "Ex")
C      1  .or. (inputline(1:2) .eq. "eX")
C      2  .or. (inputline(1:2) .eq. "ex")) then
C      stayinloop = 2

```

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```

C      elseif ((inputline(1:2) .eq. "GO")
C 1      .or.(inputline(1:2) .eq. "Go")
C 2      .or. (inputline(1:2) .eq. "gO")
C 3      .or.(inputline(1:2) .eq. "go")) then
C          stayinloop = 0
C      endif
C  end do

C      If stayinloop = 0 then the program will attempt to convert the file
C      If stayinloop = 2 then the program will stop
C      if (stayinloop .eq. 0) then
C          print *, "\n***** Reading gwpkdos.res *****"

          open(111, FILE='./gwpkdos.res', STATUS='old',
1          ACCESS='sequential', ERR=95)
          stayinloop=1
          readdata = 0
          do while (stayinloop .eq. 1)

C              Read a record from the file. On end of file goto 90
              read(111, '(A)', END=90) inputline

              release = inputline(5:12)

C              Initially readdata = 0. When readdata = 1 the read data
              if (readdata .eq. 1) then
C                  ***** Read Data *****
                  read(inputline, *) index, rvalue, peakdosraw(index)
                  peakdossorted(index) = peakdosraw(index)
C                  print *, index, rvalue, peakdosraw(index)
              else
C                  ***** Look for Word Release *****
                  if (release .eq. "unitless") then
                      readdata = 1
                  endif
              endif

C          end do
90      close (111)
          call sort(index, peakdossorted)
          open(111, FILE='./gwpkdos.sorted', STATUS='unknown',
1          ACCESS='sequential', ERR=98)
          do ii=1, index
              write(111, *, ERR=99) peakdossorted(ii), peakdosraw(ii)
          enddo
          close(111)
      else
C          ***** Early Exit path *****
          print *, "Good bye"
          endif
          stop
95      print *, "Problem opening ""./gwpkdos.res"" ."
          stop
98      print *, "Problem opening ""./gwpkdos.sorted"" ."
          stop
99      print *, "Problem writing to ""./gwpkdos.sorted"" ."
          end

      subroutine sort( NumberOfEntries, EntryArray)
      implicit none

      integer*2 NumberOfEntries
      real*4 EntryArray(NumberOfEntries)

      real*4 rtemp
      integer*2 gap, ii, jj

      rtemp = 0.0

```

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```

gap = (NumberOfEntries-1) / 2
do while (gap .gt. 0)
  ii = gap
  do while (ii .le. (NumberOfEntries-1))
    jj = ii - gap
    do while ( jj .ge. 0 )
      if ( EntryArray(jj+1) .gt. EntryArray(jj+1+gap)) then
        rtemp = EntryArray(jj+1)
        EntryArray(jj+1) = EntryArray(jj+1+gap)
        EntryArray(jj+1+gap) = rtemp
      endif
      jj = jj - gap
    end do
    ii = ii + 1
  end do
  gap = gap / 2
end do
do ii=1,NumberOfEntries
  print *,EntryArray(ii)
end do
return
end

```

Two TPA runs must be performed to determine the distance metric. One run is considered the base case and the other is considered the sensitivity case. For our purposes, the base case is considered to be the case most closely related to the standard tpa.inp file. The sensitivity case is the case where the distribution has been shifted such that the mean of the selected parameter is increased by 10% of the range. The source code for the metric distance calculation is located in `.../vulcan/home/alozano/tpa4leMean/tpaMeasure`. The names of the source files are *measure.f* and *getmetricdistance.f* and the name of the executable file is called *measure*. The program requires two subdirectories named *basecase* and *sensitivitycase*, and the program must be run with the current directory set to the parent of the two subdirectories. Before running the program copy the *basecase gwpkdos.sorted* file into the *basecase* subdirectory and the sensitivity case *gwpkdos.sorted* file into the *sensitivitycase* subdirectory. Set the current directory to the parent directory and run *measure*. The results are written to file *measure.res* in the current directory.

Fortran Code

This code is exploratory code to determine the distance metric as described in the aforementioned article. At this time, we do not foresee that this code is deliverable.

```

Program Measure
  implicit none

C      This program is based on the paper
C      "An uncertainty importance measure using a distance metric
C      for the change in a cumulative distribution function"
C      Moon-Hyun Chun, Seok-Jung Han, Nam-IL Tak

C      Reliability Engineering and System Safety 70 (2000) 313-321

C      Albert Lozano ext 2718          17 Jan 2001

C      baseprob - base case probability array
C      basevalue - base case y value array
C      sensitivityprob - sensitivity case probability array
C      sensitivityvalue - sensitivity case y value array
C      real*4 basevalue(500)
C      real*4 sensitivityValue(500)

C      inputline - Buffer for an input string
C      character*80 inputline

C      stayinloop - Used to stay in while loop while value is not zero

```


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```

integer*2 stayinloop

C      basecounter, sensitivitycounter - Used to count the number of
C      datapoints in the basecase and the sensitivity case
integer*2 basecounter, sensitivitycounter

C      index - Array index
integer*2 index

C      metricdistance, GetMetricDistance - The value and function
C      described in the referenced paper
real*4 metricdistance, GetMetricDistance

C      Program Start

print *, "This program calculates the Metric Distance"
print *, "between two "gwpcdos.sorted" files."
print *, "This program expects one"
print *, "file to be located in the "basecase" subdirectory"
print *, "and the other file to be located in the"
print *, ""sensitivitycase"" subdirectory.\n\n"
print *, "The results are presented in current directory"
print *, " "measure.res" file."

      stayinloop = 0
      stayinloop = 1
      do while (stayinloop .eq. 1)
      C      print *,
C      1 "Type "exit" to exit the program now, or "go" to continue"
      read('A') inputline
      C      if ((inputline(1:2) .eq. "EX").or.(inputline(1:2) .eq. "Ex")
C      1 .or. (inputline(1:2) .eq. "eX")
C      2 .or. (inputline(1:2) .eq. "ex")) then
      C      stayinloop = 2
      C      elseif ((inputline(1:2) .eq. "GO")
C      1 .or. (inputline(1:2) .eq. "Go")
C      2 .or. (inputline(1:2) .eq. "gO")
C      3 .or. (inputline(1:2) .eq. "go")) then
      C      stayinloop = 0
      C      endif
      C      end do

C      If stayinloop = 0 then the program will attempt to determine
C      the metric distance. If stayinloop = 2 then the program will stop
      if (stayinloop .eq. 0) then
      C      print *, "\n***** BASE CASE *****"

      open(111, FILE='./basecase/gwpcdos.sorted', STATUS='old',
      1 ACCESS='sequential', ERR=95)
      stayinloop=1
      basecounter=1
      do while (stayinloop .eq. 1)
      read(111, *, END=90) basevalue(basecounter)
      basecounter = basecounter+1
      end do
      90 close (111)
      basecounter = basecounter-1
      C      print *, "\n***** SENSITIVITY CASE *****"
      open(111, FILE='./sensitivitycase/gwpcdos.sorted', STATUS='old',
      1 ACCESS='sequential', ERR=98)

      stayinloop=1
      sensitivitycounter=1
      do while (stayinloop .eq. 1)
      read(111, *, END=92) sensitivityvalue(sensitivitycounter)
      sensitivitycounter = sensitivitycounter+1
      end do
      92 close (111)

```

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```

sensitivitycounter = sensitivitycounter-1
C   Test to see if number of points for both cases are the same
C   and that there is at least one data point
    if ((basecounter .eq. sensitivitycounter) .and.
1   (basecounter .gt. 0 )) then
        print *, "NumberOfPoints = ", sensitivity counter
        open(111, FILE='./measure.res', STATUS='unknown',
1   ACCESS='sequential', ERR=100)

C   ***** Print header *****
        write(111,*,ERR=99)"\n\n Index", "          BaseValue",
1   "   SensitivityValue"

C   ***** Print Data *****
        do index=1,basecounter
            write(111, '(i6,3x,i6,2(3x,e15.4))', ERR=99)
1   basecounter-index, index, basevalue(index),
2   sensitivityvalue(index)
        end do

C   ***** Calculate the Metric Distance *****
1   metricdistance = GetMetricDistance(basecounter,
        basevalue, sensitivityvalue)

C   If metric distance is < 0.0, this indicates error.
    if ( metricdistance .ge. 0.0) then
        write(111,*,ERR=99)"\n\nMetric Distance = ",metricdistance
    else
        write(111,*,ERR=99)"GetMetricDistanceFailed - No Data"
    endif
    close(111)
else
C   ***** Error condition *****
    print *, "basecounter ", basecounter,
1   "   sensitivitycounter = ", sensitivitycounter
    print *, "The two data arrays are different lengths"
    print *, "or basecounter is zero."
    endif
else
C   ***** Early Exit path *****
    print *, "Good bye"
endif
stop
95 print *, "Problem opening ""./basecase/gwpcdos.sorted"" ."
stop
98 print *, "Problem opening ""./sensitivitycase/gwpcdos.sorted"" ."
stop
99 print *, "Problem writing ""./measure.res"" ."
stop
100 print *, "Problem opening ""./measure.res"" ."
end

real*4 function
1   GetMetricDistance( npts, basedata, sensdata)

    implicit none

C   npts - Number of data points in both arrays
    integer*2 npts

C   basedata - Base case data array
    real*4 basedata(1)

C   sensdata - sensitivity case data array
    real*4 sensdata(1)

C   numeratorsum, denominatorsum - Summation variables
C   diff - Difference between a sensitivity and base case
C   data point

```

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```

real*4 numeratorsun, denominatorsun, diff
C      index - Array Index
integer*2 index

      if (npts .gt. 0) then

C          Initialize the summation variables to zero
          numeratorsun = 0.0
          denominatorsun = 0.0

C          Determine the numerator and denominator values
          do index=1,npts
C              Determine the square of the diff between two data points
              diff = sensdata(index)-basedata(index)

C              Sum the diff values
              numeratorsun = numeratorsun + diff*diff

C              Sum the denominator values
              denominatorsun = denominatorsun+basedata(index)
          end do

C          Take the squareroot of the numeratorsun / number of data points
          numeratorsun = sqrt( numeratorsun/npts )

C          Take the denominatorsun / number of data points
          denominatorsun = denominatorsun/npts

C          Calculate the metric distance
          GetMetricDistance = numeratorsun/denominatorsun
      else

C          Error Condition
          GetMetricDistance = -1.0
      endif
      return
      end

```

Feb. 08-09, 2001 – Determine tpa.inp input parameters for TPA runs.

The input distributions that will be varied are for the 10 most sensitive parameters in peak dose. The mean of the input distributions will be changed by 10% of the range. The peak dose cumulative distribution function, CDF, is determined for a base case and a sensitivity case as described in the article. The table parameters below were determined as follows. For the normal and uniform distributions, the MatLab functions were used. For the triangular, lognormal, and loguniform distributions a tpa.inp file was generated to vary only the selected parameter. All other parameters were held constant. The tpa code was run only long enough to produce an *lhs.out* file. The following program, *calcmean.f*, was written to calculate the mean from the *lhs.out* file. The source code is located in *.../vulcan/home/alozano/tpa41eLHS/logbetaX_5*.

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This code is exploratory code to calculate the mean from the lhs.out file and to writelhs.txt. This code is not a deliverable.

```
Program CalcMean
  implicit none
```

```
C      Albert Lozano ext 2718      17 Jan 2001
```

```
      real*4 rdummy, basevalue(500)
      real*4 rmean, rsum
```

```
C      stayinloop - Used to stay in while loop while value is not zero
      integer*2 stayinloop
```

```
C      counter - Used to count the number of datapoints
      integer*2 counter
```

```
C      Program Start
```

```
      open(112,FILE='lhs.txt', STATUS='unknown',
1       ACCESS='sequential', ERR=100)
      open(111,FILE='lhs.out', STATUS='old',
1       ACCESS='sequential',ERR=95)
      stayinloop=1
      counter=1
      rsum = 0.0
      do while (stayinloop .eq. 1)
        read(111,*,END=90)rdummy
        read(111,*,END=90)basevalue(counter)
        write(112,*,ERR=101)basevalue(counter)
        rsum = rsum+basevalue(counter)
        counter = counter+1
      end do
90     close (111)
      close (112)
      counter = counter-1
      rmean = rsum / counter
      print *, 'The mean, rsum, count is ', rmean, rsum, counter
      stop
95     print *, "Problem opening " "lhs.out" " ."
      stop
100    print *, "Problem opening " "lhs.txt" " ."
      stop
101    print *, "Problem writing " "lhs.out" " ."
      stop
      end
```

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The following table shows the values that were used in the tpa.inp files for each of the tested parameters.

Resultant Distribution Table

Parameters	Original Distribution	Base beta	Sensitivity beta
AA_1_1[C/m ² /yr]	normal 1.6e3, 1.7e4	1.6e3, 1.7e4, 5.0, 5.0	1.6e3, 1.7e4, 7.5, 5.0
SubAreaWetFraction	uniform 0.0, 1.0	beta 0.0, 1.0, 1.0, 1.0	beta 0.0, 1.0, 1.5, 1.0
Preexponential_ SFDissolutionModel2	loguniform 1.2e3, 1.2e6	logbeta 1.2e3, 1.2e6, 1.0, 1.0	logbeta 1.2e3, 1.2e6, 1.97, 1.0
ArealAverageMeanAnnual- InfiltrationAtStart [mm/yr]	uniform 4.0, 13.0	beta 4.0, 13.0, 1.0, 1.0	beta 4.0, 13.0, 1.5, 1.0
InterceptionFraction/ Irrigate	triangular 0.06, 0.4, 1.0	triangular 0.06, 0.4, 1.0	triangular 0.06, 0.7, 1.0
MeanAveragePrecipitation_ MultiplierAtGlacialMaximum	uniform 1.5, 2.5	beta 1.5, 2.5, 1.0, 1.0	beta 1.5, 2.5, 1.5, 1.0
KD_Soil_Tc[cm ³ /g]	lognormal 2.7e-4, 3.7e1	logbeta 2.7e-4, 3.7e1, 5.0, 5.0	logbeta 2.7e-4, 3.7e1, 8.2, 2.8
SFWettedFraction_Corrosion_1	uniform 0.0, 1.0	beta 0.0, 1.0, 1.0, 1.0	beta 0.0, 1.0, 1.5, 1.0
SFWettedFraction_Corrosion_9	Not Applicable for one subarea run.		
SFWettedFraction_Corrosion_2	Not Applicable for one subarea run.		

Feb. 12-14, 2001 – File Preparation and Mean runs. (tpa.inp with constant values)

The first set of TPA runs were run in .../vulcan/home/alozano/tpa41eMean. This required the creation of subdirectories and the appropriate tpa.inp files as well as run time scripts.

Subdirectories

(Note: Every subdirectory contains a slightly different tpa.inp file. Only the selected parameter is sampled)

tpa41eMean/dirAA_1_Base
 tpa41eMean/dirAA_1_Sens
 tpa41eMean/dirArealAvg_Base
 tpa41eMean/dirArealAvg_Sens
 tpa41eMean/dirInterception_Base
 tpa41eMean/dirInterception_Sens
 tpa41eMean/dirKD_Soil_Tc_Base
 tpa41eMean/dirKD_Soil_Tc_Sens
 tpa41eMean/dirMeanAverage_Base
 tpa41eMean/dirMeanAverage_Sens
 tpa41eMean/dirPreexpo_Base
 tpa41eMean/dirPreexpo_Sens

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tpa41eMean/dirSFWettedCorr1_Base
tpa41eMean/dirSFWettedCorr1_Sens
tpa41eMean/dirSFWettedCorr2_Base
tpa41eMean/dirSFWettedCorr2_Sens
tpa41eMean/dirSFWettedCorr9_Base
tpa41eMean/dirSFWettedCorr9_Sens
tpa41eMean/dirSubArea_Base
tpa41eMean/dirSubArea_Sens

Run Time Scripts

tpa41eMean/cshrunAA_1
tpa41eMean/cshrunArealAverage
tpa41eMean/cshrunInterception
tpa41eMean/cshrunKD_Soil_Tc
tpa41eMean/cshrunMeanAverage
tpa41eMean/cshrunPreexpo
tpa41eMean/cshrunSFWetFrCor1
tpa41eMean/cshrunSFWetFrCor2
tpa41eMean/cshrunSFWetFrCor9
tpa41eMean/cshrunSubAreaFraction

Example Script *tpa41eMean/cshrunAA_1*

```

cp dirAA_1_Base/tpa.inp tpa.inp
$TPA_TEST/tpa.e
cp lhs.out dirAA_1_Base/lhs.out
cp gwpkdos.res dirAA_1_Base/gwpkdos.res
cp gwccdf.res dirAA_1_Base/gwccdf.res
./tpaOrderDose/orderdose
cp gwpkdos.sorted dirAA_1_Base/gwpkdos.sorted
cp gwpkdos.sorted tpaMeasure/basecase/gwpkdos.sorted
cp dirAA_1_Sens/tpa.inp tpa.inp
$TPA_TEST/tpa.e
cp lhs.out dirAA_1_Sens/lhs.out
cp gwpkdos.res dirAA_1_Sens/gwpkdos.res
cp gwccdf.res dirAA_1_Sens/gwccdf.res
./tpaOrderDose/orderdose
cp gwpkdos.sorted dirAA_1_Sens/gwpkdos.sorted
cp gwpkdos.sorted tpaMeasure/sensitivitycase/gwpkdos.sorted
cd tpaMeasure
measure
cp measure.res ../dirAA_1_Sens/measure.res
cd ../

```

Feb. 15-16, 2001 – File Preparation and Base runs. (Base tpa.inp file with standard distributions)

These set of TPA runs were run in two directories *.../vulcan/home/alozano/tpa41eBase* and *.../vulcan/home/alozano/tpa41eBase2*. This also required the creation of subdirectories and the appropriate tpa.inp files as well as run time scripts.

Subdirectories

(Note: Every subdirectory contains a slightly different *tpa.inp* file. Only the selected parameter is sampled)

tpa41eBase/dirAA_1_Base
tpa41eBase/dirAA_1_Sens
tpa41eBase/dirMeanAverage_Base
tpa41eBase/dirMeanAverage_Sens
tpa41eBase/dirPreexpo_Base

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tpa41eBase/dirPreexpo_Sens
tpa41eBase/dirSFWettedCorr1_Base
tpa41eBase/dirSFWettedCorr1_Sens
tpa41eBase/dirSubArea_Base
tpa41eBase/dirSubArea_Sens

tpa41eBase2/dirArealAvg_Base
tpa41eBase2/dirArealAvg_Sens
tpa41eBase2/dirInterception_Base
tpa41eBase2/dirInterception_Sens
tpa41eBase2/dirKD_Soil_Tc_Base
tpa41eBase2/dirKD_Soil_Tc_Sens

Run Time Scripts

tpa41eBase/cshrunAA_1
tpa41eBase/cshrunMeanAverage
tpa41eBase/cshrunPreexpo
tpa41eBase/cshrunSFWetFrCor
tpa41eBase/cshrunSubAreaFraction
tpa41eBase2/cshrunArealAverage
tpa41eBase2/cshrunInterception
tpa41eBase2/cshrunKD_Soil_Tc

Example Script *tpa41eBase/cshrunAA_1*

```

cp dirAA_1_Base/tpa.inp tpa.inp
$TPA_TEST/tpa.e | tee dirAA_1_Base/screen.txt
cp *.out dirAA_1_Base
cp *.res dirAA_1_Base
./tpaOrderDose/orderdose
cp gwpkdos.sorted dirAA_1_Base/gwpkdos.sorted
cp gwpkdos.sorted tpaMeasure/basecase/gwpkdos.sorted
cp dirAA_1_Sens/tpa.inp tpa.inp
$TPA_TEST/tpa.e | tee dirAA_1_Sens/screen.txt
cp *.out dirAA_1_Sens
cp *.res dirAA_1_Sens
./tpaOrderDose/orderdose
cp gwpkdos.sorted dirAA_1_Sens/gwpkdos.sorted
cp gwpkdos.sorted tpaMeasure/sensitivitycase/gwpkdos.sorted
cd tpaMeasure
measure
cp measure.res ../dirAA_1_Sens/measure.res
cd ../

```

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451E INITIALS: A. L.**Feb. 19-20, 2001 – File Preparation and Base runs continued.**

This set of data was compiled from a run where the compliance period was set to 100,000 years. Data was compiled using the gwpkds.res files.

**Tabulation of results
for the metric distance.**

Parameter	tpa.inp.mean Only 1 parameter was varied 100 Realizations 1 Sub Area metric distance	tpa.inp.base Only 1 test parameter varied 330 Realizations 1 Sub Area metric distance
AA_1_1[C/m2/yr]	0.811379	1.44733
SubAreaWetFraction	0.218389	1.10344
Preexponential_ SFDissolutionModel2	0.706982	1.42306
ArealAverageMeanAnnual- InfiltrationAtStart [mm/yr]	0.111806	0.240756
InterceptionFraction/ Irrigate	0.097912	0.415865
MeanAveragePrecipitation_ MultiplierAtGlacialMaximum	0.070242	0.221675
KD_Soil_Tc[cm3/g]	0.009716	0.047372
SFWettedFraction_Corrosion_1	0.232558	0.408281
SFWettedFraction_Corrosion_9	Not applicable for one subarea.	
SFWettedFraction_Corrosion_2	Not applicable for one subarea.	

Feb. 21, 2001 – Prepared to run a new set of runs.

Today we decided to determine the metric distance values for the 10,000 year data. The peak dose data is supposed to be in the *gwpkds_c.res* file; however, this was not the case because I ran the TPA code with the compliance period set to 100,000 years. I copied *orderdose.f* into *orderdose10yr.f* to use the *gwpkds_c.res* file and generate *gwpkds_c.sorted* file. The source code is located in *.../vulcan/home/alozano/tpa41eMean/tpaOrderDose*.

This code is exploratory code to produce a sorted file, *gwpkds_c.sorted*, from the Ground Water Peak Dose File, *gwpkds_c.res*. The produced file is used only with the code that calculates distance metric and is not a deliverable code.

```

Program OrderDose10yr
  implicit none

C      This program reads the gwpkds_c.res file and creates a
C      new file gwpkds_c.sorted.

C      Albert Lozano ext 2718          05 Feb 2001

      real*4 peakdosraw(500), peakdossorted(500)

C      inputline - Buffer for an input string

```


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```

character*800 inputline

C      release - Buffer used to search for word "Release" in file
character*8 release

C      stayinloop - Used to stay in while loop while value is not zero
integer*2 stayinloop

C      readdata -Used to switch from reading text strings (value = 0)
C      to reading data records(value=1)
integer*2 readdata

C      index - Array index
integer*2 index, ii

C      rvalue - temporary value
real*4 rvalue

print *, "This program Reads the gwpkdos.res file and generates"
print *, "the gwpkdos.sorted file"
C      print *, "Make sure that the file gwpkdos.res exists in current directory"

      stayinloop = 0
C      stayinloop = 1
C      do while (stayinloop .eq. 1)
C          print *,
C      1  "Type "exit" to exit the program now, or "go" to continue"
C          read('A') inputline
C          if ((inputline(1:2) .eq. "EX").or.(inputline(1:2) .eq. "Ex")
C      1      .or. (inputline(1:2) .eq. "eX")
C      2      .or. (inputline(1:2) .eq. "ex")) then
C              stayinloop = 2
C          elseif ((inputline(1:2) .eq. "GO")
C      1      .or. (inputline(1:2) .eq. "Go")
C      2      .or. (inputline(1:2) .eq. "gO")
C      3      .or. (inputline(1:2) .eq. "go")) then
C              stayinloop = 0
C          endif
C      end do

C      If stayinloop = 0 then the program will attempt to convert the file
C      If stayinloop = 2 then the program will stop
      if (stayinloop .eq. 0) then
C          print *, "\n***** Reading gwpkdos.res *****"

          open(111, FILE='./gwpkds_c.res', STATUS='old',
      1      ACCESS='sequential', ERR=95)
          stayinloop=1
          readdata = 0
          do while (stayinloop .eq. 1)

C              Read a record from the file. On end of file goto 90
              read(111, '(A)', END=90) inputline

              release = inputline(5:12)

C              Initially readdata = 0. When readdata = 1 the read data
              if (readdata .eq. 1) then
C                  ***** Read Data *****
                  read(inputline, *) index, rvalue, peakdosraw(index)
                  peakdossorted(index) = peakdosraw(index)
C                  print *, index, rvalue, peakdosraw(index)
              else
C                  ***** Look for Word Release *****
                  if (release .eq. "unitless") then
                      readdata = 1
                  endif
              endif
C          end do

```

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```

end do
90  close (111)
    call sort(index,peakdossorted)
    open(111,FILE='./gwpkds_c.sorted', STATUS='unknown',
1    ACCESS='sequential',ERR=98)
    do ii=1,index
        write(111, *, ERR=99) peakdossorted(ii), peakdosraw(ii)
    enddo
    close(111)
    else
C    ***** Early Exit path *****
        print *, "Good bye"
    endif
    stop
95  print *, "Problem opening " "./gwpkds_c.res" " ."
    stop
98  print *, "Problem opening " "./gwpkds_c.sorted" " ."
    stop
99  print *, "Problem writing to " "./gwpkds_c.sorted" " ."
    end

```

Feb. 22, 2001 – Prepared to run a new set of runs.

Today I edited the appropriate *tpa.inp* files and set the compliance period to 10,000 years and started a new TPA run. I also copied *orderdose.f* into *orderdose10yr.f* to use the *gwpkds_c.res* file and generate *gwpkds_c.sorted* file. The source code is located in *.../vulcan/home/alozano/tpa41eMean/tpaOrderDose* . I started the the run .

Feb. 23, 2001 – Continued running the One Sub Area Runs.

The run output files are in */net/vulcan/home/alozano/tpa41eBase_1SubArea* and */net/vulcan/home/alozano/tpa41eBase2_1SubArea*

This set of data was compiled from a run where the compliance period was set to 10,000 years. Data was compiled using the *gwpkds_c.res* files for th 10,000 year compliance and the *gwpkds.res* files for the MAX (100,000 years)

Parameter	tpa.inp (Base) Only 1 parameter was varied 330 Realizations 1 Sub Area gwpkds_c.res 10,000 years metric distance	tpa.inp (Base) Only 1 test parameter varied 330 Realizations 1 Sub Area gwpkds.res 100,000 years metric distance
AA_1_1[C/m2/yr]	0.000000	1.88156
SubAreaWetFraction	0.457227	1.09192
Preexponential_ SFDissolutionModel2	1.940530	1.81598
ArealAverageMeanAnnual- InfiltrationAtStart [mm/yr]	1.046980	0.216068
InterceptionFraction/ Irrigate	0.556255	0.400783
MeanAveragePrecipitation_ MultiplierAtGlacialMaximum	0.740721	0.169630
KD_Soil_Tc[cm3/g]	2.63336	0.047754

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SFWettedFraction_Corrosion_1

0.000000

0.439667

SFWettedFraction_Corrosion_9

SFWettedFraction_Corrosion_2

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451E INITIALS: A, J,**Feb. 23, 2001 – Continued.**

Today I also edited the appropriate *tpa.inp* files and left the compliance period at 10,000 years, set the file up for 10 subareas, and started a new TPA run.

Feb. 26, 2001 – Continued running 10 subarea runs and experimented with new paramters.

The following table shows the new parameters and distributions used. These parameters are considered least sensitive by our current classification. The *tpa.inp* files were created using the information in this table.

Resultant DistributionTable

Parameters	Original Distribution	Base	Sensitivity
LeafyVegetableIrrigation RateCB[in/yr]	uniform 37.0, 53.0	beta 37.0, 53.0, 1.0, 1.0	beta 37.0, 53.0, 1.5, 1.0
LeafyVegetableIrrigation RatePB[in/yr]	triangular 23.0, 43.0, 43.0	triangular 23.0, 43.0, 43.0	triangular 29.5, 43.0, 43.0
DistanceToTuff AlluviumInterface[km]	uniform 10.0, 19.9	beta 10.0, 19.9, 1.0, 1.0	beta 10.0, 19.9, 1.5, 1.0

Feb. 27, 2001 – Continued running 10 subarea runs and compiled data for new parameters.

This set of data was compiled from a run where the compliance period was set to 10,000 years. Data was compiled using the *gwpkds_c.res* files for the 10,000 year compliance and the *gwpkdos.res* files for the MAX (100,000 year). These parameters are the 18th, 19th, and 20th parameters on the sensitivity list.

Parameter	tpa.inp (Base) Only 1 parameter was varied 330 Realizations 1 Sub Area gwpkds_c.res 10,000 years metric distance	tpa.inp (Base) Only 1 test parameter varied 330 Realizations 1 Sub Area gwpkdos.res 100,000 years metric distance
LeafyVegetableIrrigation RateCB[in/yr]	0.090219	0.040054
LeafyVegetableIrrigation RatePB[in/yr]	0.000000	0.002348
DistanceToTuffAlluvium Interface[km]	0.722369	0.653993

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Feb. 28, 2001 – Continued running 10 subarea runs. Prepared and started one for change in distribution type.

The following table shows the values that were used in the tpa.inp files for each of the tested parameters.

Resultant DistributionTable

Parameters	Original Distribution	Base	Sensitivity
AA_1_1[C/m2/yr]	normal 1.6e3, 1.7e4	normal 1.6e3,1.7e4,	uniform 1.6e3,1.7e4
SubAreaWetFraction	uniform 0.0, 1.0	uniform 0.0,1.0	normal 0.0,1.0
Preexponential_ SFDissolutionModel2	loguniform 1.2e3, 1.2e6	loguniform 1.2e3,1.2e6	lognormal 1.2e3,1.2e6
ArealAverageMeanAnnual- InfiltrationAtStart [mm/yr]	uniform 4.0,13.0	uniform 4.0,13.0	normal 4.0,13.0
MeanAveragePrecipitation_ MultiplierAtGlacialMaximum	uniform 1.5,2.5	uniform 1.5,2.5	normal 1.5,2.5
KD_Soil_Tc[cm3/g]	lognormal 2.7e-4,3.7e1	lognormal 2.7e-4,3.7e1	loguniform 2.7e-4,3.7e1
SFWettedFraction_Corrosion_1	uniform 0.0,1.0	uniform 0.0,1.0	normal 0.0,1.0,1.5,1.0
LeafyVegetableIrrigation RateCB[in/yr]	uniform 37.0, 53.0	uniform 37.0, 53.0	normal 37.0,53.0,1.5,1.0
DistanceToTuff AlluviumInterface[km]	uniform 10.0, 19.9	uniform 10.0, 19.9	normal 10.0, 19.9,1.5,1.0

The run output files are in */net/vulcan/home/alozano/tpa41eBase_1SubAreaChangeDistribution* and */net/vulcan/home/alozano/tpa41eBase2_1SubAreaChangeDistribution*

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Mar. 01-02, 2001 – Continued running 10 subarea runs. Continued running one subarea runs for change in distribution type.

This set of data was compiled from a run where the compliance period was set to 10,000 years. Data was compiled using the gwpkds_c.res files for the 10,000 year compliance and the gwpkdos.res files for the MAX (100,000 year) for 1 subarea. The distribution was changed from uniform to normal or from normal to uniform.

Parameter	tpa.inp (Base) Only 1 parameter was varied 330 Realizations 1 Sub Area gwpkds_c.res 10,000 years metric distance	tpa.inp (Base) Only 1 test parameter varied 330 Realizations 1 Sub Area gwpkdos.res 100,000 years metric distance
AA_1_1[C/m2/yr]	0.000000	0.451999
SubAreaWetFraction	0.732842	0.396241
Preexponential_ SFDissolutionModel2	2.00378	1.17827
ArealAverageMeanAnnual- InfiltrationAtStart [mm/yr]	0.695751	0.276860
InterceptionFraction/ Irrigate	N/A	N/A
MeanAveragePrecipitation_ MultiplierAtGlacialMaximum	0.336592	0.114659
KD_Soil_Tc[cm3/g]	1.36675	0.0462276
SFWettedFraction_Corrosion_1	0.000000	0.392761
LeafyVegetableIrrigation RateCB[in/yr]	0.090921	0.0462179
LeafyVegetableIrrigation RatePB[in/yr]	N/A	N/A
DistanceToTuffAlluvium Interface[km]	0.483467	0.243034

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Mar. 05, 2001 – Continued running 10 subarea runs. Completed running one subarea runs for change in distribution type.

Went over the results and completed table entry.

Status of 10 subarea runs.

AA_1_1[C/m2/yr]	Complete
SubAreaWetFraction	In Progress
Preexponential_	
SFDissolutionModel2	Complete
ArealAverageMeanAnnual-	
InfiltrationAtStart	
[mm/yr]	Complete
InterceptionFraction/	
Irrigate	In Progress
MeanAveragePrecipitation_	
MultiplierAtGlacialMaximum	Complete
KD_Soil_Tc[cm3/g]	In Progress
SFWettedFraction_Corrosion_1	In Progress

Mar. 06-09, 2001 – Continued running 10 subarea runs.

Mar. 12-16, 2001 – On Travel.

Mar. 19, 2001 – 10 subarea run completed.

The results for the 10 sub area run are as follows.

Parameter	tpa.inp (Base) Only 1 parameter was varied 330 Realizations 10 Sub Area gwpkds_c.res 10,000 years metric distance	tpa.inp (Base) Only 1 test parameter varied 330 Realizations 10 Sub Area gwpkds.res 100,000 years metric distance
AA_1_1[C/m2/yr]	0.000000	1.44368
SubAreaWetFraction	0.451687	0.886234
Preexponential_		
SFDissolutionModel2	1.33038	1.07276
ArealAverageMeanAnnual-		
InfiltrationAtStart		
[mm/yr]	0.501163	0.238467
InterceptionFraction/		
Irrigate	0.450826	0.368533
MeanAveragePrecipitation_		
MultiplierAtGlacialMaximum	0.376682	0.194447
KD_Soil_Tc[cm3/g]	2.94183	0.047304
SFWettedFraction_Corrosion_1	0.000000	0.102211

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The following is a list of all the tpa data directories

330 Realization 10 Subarea Runs – Shifted distribution mean value.

~alozano/tpa41eBase/

~alozano/tpa41eBase2/

330 Realization 1 Subarea Runs – Shifted distribution mean value.

~alozano/tpa41eBase_1SubArea/

~alozano/tpa41eBase2_1SubArea/

330 Realization 1 Subarea runs. – Changed normal distributions to uniform and vice versa

~alozano/tpa41eBase_1SubAreaChangeDistribution/

~alozano/tpa41eBase2_1SubAreaChangeDistribution/

330 Realization 1 Subarea runs. – Shifted distribution mean value.

The tpa compliance period was mistakenly set at 100,000 years.

~alozano/tpa41eBase100Kyr/

~alozano/tpa41eBase2_100Kyr/

~alozano/tpa41eLHS/

100 Realization 1 Subarea runs. – Mean values used.

~alozano/tpa41eMean/

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Mar. 29, 2001 – Apr. 04, 2001 New Section, New Work.

After a period of no action, work has begun again. Today I began documenting the file “supermodsign.f”. This task is being done to understand the code better as well as documenting the code.

Apr. 05, 2001 – Scanner

This work consisted of developing a program that determines the number of points in each of four quadrants as the x value is scanned. The data is presented in two columns representing an x and y.

First the median of all the y values is determined. From this we know that half the data points are above the median and half are at or below the median.

Then the xy data pairs are sorted in increasing order by the x value.

Four counters are defined as follows.

belowleft - Number of points that have x values \leq current x and y values at or below the y median.

aboveleft - Number of points that have x values \leq current x and y values above the y median.

belowright = Number of points that have x values $>$ current x and y values at or below the y median.

aboveright = Number of points that have x values \leq current x and y values above the y median

At the beginning we assume that x is set to below the minimum x value and four counters are initialized as follows.

belowleft = 0

aboveleft = 0

belowright = Total number of points at or below the y median.

aboveright = Total number of points above the y median

These counters are modified at every point as follows

For each point

 If $y > y_{\text{mean}}$ then

 aboveleft = aboveleft + 1

 aboveright = aboveright - 1

 else

 belowleft = belowleft + 1

 belowright = belowright - 1

 endif

 output the x value and all four counters

end the for loop

Apr. 06, 2001 – Scanner

The scanner program was modified to report the following.

x, belowleft, aboveleft, belowright, aboveright, belowleft+aboveright, aboveleft+belowright.

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451E INITIALS: A. L.**Apr. 10, 2001 – Scanner Modification**

I began to modify the scanner program to read a file, "output1.txt", and obtain results for each data column. The parameters are

```

ArealAverageMeanAnnualInfiltrationAtStar
MeanAveragePrecipitationMultiplierAtGlac
MeanAverageTemperatureIncreaseAtGlacialM
FractionOfCondensateRemoved[1
FractionOfCondensateTowardRepository[1
TemperatureGradientInVicinityOfBoilingIs
ThermalConductivityofYMRock[W
CriticalRelativeHumidityAqueousCorrosion
ThicknessOfWaterFilm[m]
AA_1_1[C
ChlorideMultFactor
DripShieldFailureTime[yr]
RockModulusOfElasticityforSEISMO[Pa]
RockPoissonRatioforSEISMO[]
SEISMOJointSpacing1[m]
SEISMOJointSpacing2[m]
SEISMOJointSpacing3[m]
SEISMOJointSpacing4[m]
SEISMOJointSpacing5[m]
VerticalExtentOfRockFall12_1[m]
,VerticalExtentOfRockFall12_2[m]
,VerticalExtentOfRockFall12_3[m]
,VerticalExtentOfRockFall12_4[m]
,VerticalExtentOfRockFall12_5[m]
,VerticalExtentOfRockFall12_6[m]
,VerticalExtentOfRockFall12_7[m]
,VerticalExtentOfRockFall12_8[m]
,VerticalExtentOfRockFall12_9[m]
,VerticalExtentOfRockFall12_10[m]
,VerticalExtentOfRockFall13_1[m]
,VerticalExtentOfRockFall13_2[m]
,VerticalExtentOfRockFall13_3[m]
,VerticalExtentOfRockFall13_4[m]
,VerticalExtentOfRockFall13_5[m]
,VerticalExtentOfRockFall13_6[m]
,VerticalExtentOfRockFall13_7[m]
,VerticalExtentOfRockFall13_8[m]
,VerticalExtentOfRockFall13_9[m]
,VerticalExtentOfRockFall13_10[m]
,VerticalExtentOfRockFall14_1[m]
,VerticalExtentOfRockFall14_2[m]
,VerticalExtentOfRockFall14_3[m]
,VerticalExtentOfRockFall14_4[m]
,VerticalExtentOfRockFall14_5[m]
,VerticalExtentOfRockFall14_6[m]
,VerticalExtentOfRockFall14_7[m]
,VerticalExtentOfRockFall14_8[m]
,VerticalExtentOfRockFall14_9[m]
,VerticalExtentOfRockFall14_10[m]
,VerticalExtentOfRockFall15_1[m]
,VerticalExtentOfRockFall15_2[m]

```

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```

,VerticalExtentOfRockFall15_3[m]
,VerticalExtentOfRockFall15_4[m]
,VerticalExtentOfRockFall15_5[m]
,VerticalExtentOfRockFall15_6[m]
,VerticalExtentOfRockFall15_7[m]
,VerticalExtentOfRockFall15_8[m]
,VerticalExtentOfRockFall15_9[m]
,VerticalExtentOfRockFall15_10[m]
,DefectiveFractionOfWPs
,Preexponential_SFDisolutionModel2
,SubGrainFragmentRadiusAfterTransFrac[m]
,SolubilityNp[kg
,SFWettedFraction_Initial_1
,SFWettedFraction_Initial_3
,SFWettedFraction_Initial_5
,SFWettedFraction_Initial_7
,SFWettedFraction_Initial_9
,SFWettedFraction_FAULTO
,SFWettedFraction_SEISMO1_1
,SFWettedFraction_SEISMO1_3
,SFWettedFraction_SEISMO1_5
,SFWettedFraction_SEISMO1_7
,SFWettedFraction_SEISMO1_9
,SFWettedFraction_SEISMO2_1
,SFWettedFraction_SEISMO2_3
,SFWettedFraction_SEISMO2_5
,SFWettedFraction_SEISMO2_7
,SFWettedFraction_SEISMO2_9
,SFWettedFraction_SEISMO3_1
,SFWettedFraction_SEISMO3_3
,SFWettedFraction_SEISMO3_5
,SFWettedFraction_SEISMO3_7
,SFWettedFraction_SEISMO3_9
,SFWettedFraction_SEISMO4_1
,SFWettedFraction_SEISMO4_3
,SFWettedFraction_SEISMO4_5
,SFWettedFraction_SEISMO4_7
,SFWettedFraction_SEISMO4_9
,SFWettedFraction_Corrosion_1
,SFWettedFraction_Corrosion_3
,SFWettedFraction_Corrosion_5
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. The scanner program was modified to report the following.

x, belowleft, aboveleft, belowright, aboveright, belowleft+aboveright, aboveleft+belowright.

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April 11, 2001 through May 17, 2001 – Scanner Modification

During this period of time, I have been working on determining the important parameters using supermodsign. This work is experimental in nature at this point and is not currently used in any formal reports. The work performed during this period is located in the following directories.

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/net/vulcan/home/alozano/scannermean  
/net/vulcan/home/alozano/scannermedian  
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I have not modified any entries previous to this statement

Albert A. Lozano
Albert Lozano Oct. 15, 2001

Printed: October 24, 2002

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INITIAL ENTRIES

Scientific Notebook: #451E

Issued to: S. Mohanty / Albert Lozano

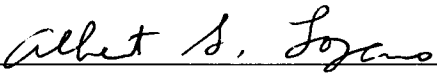
Issue Date: March 20, 2001

Account Number: 20-1402-761

Title: Metric Measure & Other Exploratory Work

Participants: Albert Lozano

I have not modified any entries previous to this statement


Albert Lozano Oct. 15, 2001

This document is being continued from a Microsoft Word document whose last entry was Oct. 15, 2001. All work after Oct. 15, 2001 is documented in this document. The following pages are taken out of a report written by Sitakanta Mohanty on different sensitivity analysis methods.

October 15, 2001 through February 15, 2002

During this time period I was not very active in this project.

February 15, 2001 through March 15, 2002

A significant amount of work was done during this time period. The work performed within this time period is reported in Chapter 6 of a document written by Sitakanta Mohanty. This chapter is titled Distributional Sensitivity Analysis.

DISTRIBUTIONAL SENSITIVITY ANALYSIS

Summary

This study focused on determining the effects on the distribution of the peak expected dose as a function of a change to the distribution of an input parameter. Two sets of input parameters were considered. The first set of parameters were the top ten parameters as determined by other sensitivity analysis methods. The second set of parameters were the five least influential parameters among the top 20. Two types of changes to the distributions were performed. One involved shifting the mean of the distribution while keeping the end points fixed and the other involved changing the distribution type while keeping the end points fixed.

The area between a nominal case CDF and a sensitivity case CDF can be represented as a number called the metric distance. This number is an unsigned number corresponding to the separation of the CDFs. The number was computed and tabulated along with the peak expected dose for the 10,000 year and also for the 100,000 year time periods.

The study involving the shift of the mean of the distribution was performed on both data sets. In most cases the metric distance was proportional to the magnitude of the peak expected dose. WPFlowMF was affected the most by the mean shift in the input distribution followed by PSFDM1. Anomalous results were observed only for ARDSAVNp.

a. Background

Performance assessment model allows for explicit consideration of uncertainties and their propagation through the process models to the assessment results. The data uncertainties are quantitatively represented using probabilistic distributions. These distributions in most cases are represented through probability density functions and associated data ranges. A probability density function for each input parameter relates the possible values of the parameter to its probability of occurrence. In other words, it corresponds to the relative frequency with which randomly sampled values would lie in different intervals of the allowed range of values, in the limit as the number of samples goes to infinity (Stephens, et al., 1993).

The nature of the probability density functions associated with the input variables can substantially influence the peak expected dose. Even if the performance model is constructed to be as realistic as possible within the limits of the computer capability, any bias in input data uncertainty can potentially under- or over-predict the estimates of consequences. Thus, the quality of performance assessment results depends on the quality of the process used for determining the probability distribution function for each sampled input parameter. Numerous sources of uncertainties in the characterization of the distribution function beyond the data uncertainty contribute to the uncertainty in the probability density function.

The following factors or a combination thereof can contribute to the choice of the distribution function for a parameter.

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- Details and accuracy of information that can be obtained for the system or its component may be limited. This could simply be a matter of reaching a practical limit to data collection.
- The level of detailed description and modeling that can practically be included in the performance assessment model may demand data that are not easily obtainable.
- The collected data may have been affected by human error and unknown instrument malfunction.
- There may be ambiguities in relating the value of the parameter actually measured to the parameter of interest (such as the inappropriate constraining in the extrapolation of data).
- Unpredictability of human behavior (e.g., biosphere) into future. This could be a factor, had it not been designated in regulation that the dose must be calculated with respect to a defined receptor.
- Uncertainty arising from numerical approximation and simplification in the calculations used for deriving the distribution function may result in a narrow instead of a wide distribution, or vice versa.
- Some of the measurements may not have been made or may not have been feasible under the conditions near the anticipated extremes. This may lead to narrower than actual range and result in a more pronounced peak value (Dalrymple, 1989; Eslinger and Sagar, 1989)
- If data is sparse, probability encoding could become a function of the experience of the analyst developing the distribution function (Merkhofer and Runchal, 1989). One analyst's interpretation of the information from which the probability density function is derived is not necessarily the same as another's. Different subject matter experts may arrive at different probability values even though they have analyzed, in principle, identical information in which the probability density functions is to be used. The level of differences is proportional to the quantity of data and quality of information regarding the data available to construct the probability density functions. Even if formal elicitation of expert opinion can be used for obtaining a consensus on the specification of the probability density functions, sometimes the difference in opinion is so disparate that one may rely on performing calculations corresponding to each expert's opinion.
- The model developer may have used individual guesses in developing the distribution function.

The purpose of the chapter is to determine to what extent the uncertainties can influence performance assessment results. The effect of distributional uncertainty is studied by conducting sensitivity or relative impact analysis of the uncertainty in the distribution functions representing input parameter uncertainties (supplied by the process model specialist) on the peak expected dose as well as the shape of the peak expected dose CDF. Because of the large number of sampled parameters in the TPA code, only a small set of parameters has been used to estimate the influence of distributional assumptions on the performance prediction. In the following sections, the analysis method is presented, the results from the implementation of the method are presented, and some recommendations are made for future studies.

b. Analysis Method

The general approach for distribution sensitivity involves determination of the relative change to the performance measure with respect to a pre-specified perturbation to the distribution function. The relative change to the performance measure is expressed as (i) the difference between the old (i.e. the nominal case) and the new (i.e. sensitivity case) peak expected dose and (ii) an effective distance between the old and new output distributions. Several notable methods have been proposed in the past by Beckman and McKay (1987) for fast computation. These methods focus on improvement to the computational efficiency by eliminating the need to perform any Monte Carlo runs additional to a standard nominal case run. One of these methods is based on the weighing method (Kahn and Marshall, 1953) and another method is the rejection method (Kennedy and Gentle, 1980). However, these methods appear to have some limitations that could lead to approximations in the analysis if used outside the recommended limits. The efficiency of each method has been shown to decrease rapidly as large differences occur between the old and the new probability density functions. Therefore, for the purposes of the report, the rigorous, but direct or brut-force method has been used.

The direct method involves performing additional Monte Carlo runs corresponding to each change to the distribution function. Only one parameter is changed at a time. Each Monte Carlo run set corresponds to and is identical to the nominal case run except the one input parameter has a distribution function that is different from the nominal case. From the Monte Carlo realization set, expected dose as a function of time is computed. The peak expected dose is then determined from the expected dose-versus time curve. The difference between the nominal case and the sensitivity case is a measure of sensitivity of the dose response to the change in input distribution function. In addition to the peak expected dose, changes to the spread of the dose response should also be measured because in some cases, in response to the changes to the input distribution, the variance of the dose contributing to the peak expected dose may be affected while the peak expected dose may remain the same as the nominal case dose. Therefore, for a more precise quantification, one may investigate the distribution of the dose values corresponding to the peak expected dose. An alternative is to investigate the changes to the distribution of realization peak doses.

For precise quantification of the relative impact of distributional changes of inputs on the change of an output distribution, various measures have been proposed in the literature (Iman and Hora (1990), Khatib-Rahbar et al, (1989), Park and Ahn (1999), and Chun et al., (2000)). In this report, the distributional uncertainty importance measure previously used by Chun et al. (2000) has been used as the second measure. The following is a brief description of this measure.

The change in output distribution can be measured simply by measuring the area between two CDFs (shaded region in Figure 6-1), one for the dose values from the nominal case and other for the dose values from the sensitivity case. Chun et al. (2000) used a distance metric to represent this shaded region based on a Minkowski class of distance, typically used as a measure of fuzziness. The metric distance D is defined as

$$D = \left[\sum_{x \in X} |f_1(x) - f_2(x)|^w \right]^{\frac{1}{w}}, w > 1 \quad (1)$$

where $f_1(x)$ = the nominal case output cumulative distribution function
 $f_2(x)$ = the sensitivity case output cumulative distribution function
 w = an exponent

When $w=2$, D represents the Euclidian metric distance between the two cumulative distribution functions. The two cumulative distribution functions are normalized with the mean of the original cumulative distribution function. The variable x represents the quantile. Then

$$D = \left[\int_0^1 |f_1(x) - f_2(x)|^2 dx \right]^{\frac{1}{2}} \quad (2)$$

As noted earlier, the sensitivity case output cumulative distribution function refers to the case where the input distribution of only one of the variables is changed by pre-specified value. Normalization with the mean value of the nominal case makes the metric distance dimension less.

Metric distance reflects the degree of impact an input variable makes on the output distribution when the input distance is changed. The metric distance is a value ≥ 0 . A large value of the metric distance represents a large impact of the change in shape of the input distribution on the output distribution.

For Monte Carlo or Latin Hypercube Sampling results, the metric distance can be expressed as

$$D = \left[\frac{1}{N} \sum_{n=1}^N [f_1^i(x) - f_2^i(x)]^2 \right]^{\frac{1}{2}} / \frac{1}{N} \sum_{n=1}^N f_2(x)_n \quad (3)$$

where i is the parameter of interest, N is the total number of realizations, n is the current realization, $f_1^i(x)_{n/N}$ is the (n/N) th quantile of the nominal case ($0 < n < N$) and $f_2^i(x)_{n/N}$ is the (n/N) th quantile for its sensitive case. Equation (3) was the method used to compute the metric distance in this report.

The sensitivity case can be created in several ways:

- (i) Change the variance of the distribution function. This changes the range of the data.
- (ii) Shift the mean of the distribution without changing the data range (i.e., fixed variance)
- (iii) Change the mean of the distribution while keeping the end points fixed (the variance changes)

In this report, case iii has been used. The changes have been accomplished by

- (i) Changing the mean by 10 percent of the range while keeping the minimum and maximum values fixed.

(Note: The shifted distribution function will not be symmetrical because the maximum and minimum values are forced to remain fixed.)

- (ii) Changing the distribution function from one type to another while keeping the minimum and maximum values fixed.

c. Implementation Procedure

Distributional sensitivity analysis are performed for two sets of parameters, the first consisting of top 10 influential parameters identified by other parametric sensitivity analysis methods, and the second set consisting of the last 5 of the top 20 influential input parameters identified by one of the parametric sensitivity analysis methods. The rationale for selecting these five parameters is to study the sensitivity with the ones that do not dominate the response values but yet have some influence compared to the parameters that are at the bottom of the list of 330 sampled parameters. For the first set (i.e., top 10 influential parameters), the distribution functions are changed (i) by shifting the mean of the distribution by 10 percent of the data range toward higher values (Figure 6-2) and (ii) by completely changing the type of distribution function (Figure 6-3). For the second set (i.e., last 5 of the top 20), the distribution function is changed by shifting the mean by 10 percent of the data range.

To implement the method, the distribution function for only one parameter is changed at a time. To calculate the metric distance, two TPA Monte Carlo run sets are needed, one for the nominal case and the other for the sensitive case. Each TPA run set involves 330 Monte Carlo realizations. The CDFs are constructed from the peak dose from 330 realizations. The change to the peak expected dose is also computed using the nominal case and the sensitive case. Calculations are performed for both 10,000 and 100,000 yr simulation periods.

A 10% shift to the mean changes the entire distribution function. That means, the new distribution function after a 10% shift to the mean is no longer a normal distribution. Therefore, another distribution function must be used to represent the new distribution function with a new mean value but fixed endpoints. Beta distributions has been chosen to represent the new distribution function because the four-parameters that define a beta distribution provide sufficient flexibility to represent with close approximation a large suite of distribution functions. Log-beta distribution function is used if the original distribution is a log-distribution (e.g., log-uniform or log-normal). Another reason for using beta distribution is that this distribution function is the only one in the LHS code used for Monte Carlo sampling in the TPA code that is flexible enough to represent different distribution functions. Beta distribution is used primarily to represent shifts to normal, uniform, and exponential distribution functions. Several distribution functions in the TPA code representing the nominal case data set do not need beta or logbeta representation of the new distribution function. For example, in a triangular distribution, a 10% shift to the mean can easily be accomplished by appropriately shifting the most likely point.

Because LHS sampling is used, the sampling sequence changes for other parameters when the distribution function is changed for the parameter of interest. This may be merely an artifact of the implementation of the LHS algorithm in the TPA code. Therefore, the original distribution is represented by a beta-equivalent approximation first to obtain a modified nominal case so that when the mean of the original distribution is shifted by 10%, there is no difference in the sampled values for the parameters other than the one that is changed. In

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effect, two Monte Carlo run sets are needed to perform consistent comparison between the nominal case and the sensitive case.

For the top 10 parameters, ideally, 3,660 realizations (i.e., $330 \times 10 + 330$ for the nominal case) would be needed for constructing CDFs and obtaining peak expected dose. However, because of the need for obtaining modified nominal case corresponding to each parameter, 6660 realizations are needed to estimate the metric distance and the differences in the peak expected dose values.

d. Results

In this section, results are presented for the 10 percent shift to the mean of the input parameter distribution functions for the top 10 and the last five of the top 20 influential parameters. Then the results for the cases in which the distribution functions are changed from one type to another are presented. In most cases, results are presented for 10,000 yr and 100,000 yr simulation periods.

The changes to the distribution function for the first parameter set (i.e., 10% change to the mean of the top 10 parameters previously identified by the parametric sensitivity analysis methods) are shown in table 6-1. The top ten parameters used in the distributional sensitivity studies are the top 10 influential parameters based on the 10,000 year simulation. In this table, the 2nd column shows the original distribution, the 3rd column shows the beta distribution equivalent of the original distribution, and the 4th column shows 10% shift to the means in the associated new beta distribution. As mentioned before, this shift is 10% of the range of the distribution function.

Results for the analysis of the first parameter set are shown in table 6-2. These parameters are ordered according to their rank from the parametric studies determined in Chapter 4. In table 6-2, results are shown for 10,000 and 100,000 year simulation period to gain insight into the behavior of these parameters.

The table shows that a 10 percent shift to the mean of the input distribution function results in a definite shift of the sensitivity case CDF in the increasing direction for each input parameter. The sensitivity case CDFs shifted in such a way that in all cases the metric distance and peak expected dose changed. The minus sign for the peak expected dose implies that there is an inverse relationship between the input and output parameters. This shift in the CDF to higher values appears to be intuitively correct because a shift of the mean in the input distribution in the increasing direction corresponds to sampling smaller values with lower and sampling larger values with higher frequency. If the output value is directly proportional to the input value, the sensitivity case peak expected dose CDF also shifts toward higher values and vice versa. The more pronounced the separation between the nominal case and the sensitivity case CDFs, the larger is the magnitude of the metric distance. Because the whole CDF is shifted in the increasing direction without significant overlapping, the metric distance is expected to correlate well with the magnitude of the change in the peak expected dose. Table 6-2 shows good correlation between metric distance and the peak expected dose values indicating that for the top 10 influential parameters, a shift in mean of the input distribution directly results in a correspondingly large shift in the dose values.

Table 6-2 shows that in 10,000 years, WPFlowMF parameter is most sensitive to the change in the distribution

function. For this parameter, the peak expected dose changed nearly 150% with a metric distance of 4.78. Recall that a metric distance of zero means no effect of the distributional change to the input on the output. Another parameter that showed a large change to the peak expected dose (i.e., 57.2%) was PSFDM1. Parameters with a moderate metric distance and change in peak expected dose were DsFailTi, WP-Def%, DTFFAVIF, and SbArWt%. Anomalous results were observed only for one parameter. Although that parameter ARDSAVNp shows a metric distance comparable to WPRRG@20, the metric distance is much smaller compared to the latter. Such a difference in metric distance while the change in peak expected dose are almost identical reveal that while WPRRG@20 equally affects the realization peak as well as the peak expected dose, ARDSAVNp affects the realization peak doses much less than the peak expected dose.

Note that for several parameters in table 6-2, the 10,000 yr peak expected dose is more sensitive than the 100,000-yr peak expected dose (e.g. DsFailTi, WP-Def%, and FOCTR). This finding is consistent with the results from the parametric sensitivity analysis. (However, the distributional sensitivity analysis provides additional support that even a 10% shift in the range to the mean value can result in a negligibly small change in the output distribution.) In contrast, a 10% shift to the mean for parameters such as ARDSAVNp affect the 100,000-yr dose more than the 10,000-yr dose.

Three out of 10 parameters show larger metric distance and change in peak expected dose for both 10,000 and 100,000-yr dose. These parameters are WPFlowMF, PSFDM1, and SbArWt%.

The changes to distribution functions for the second parameter set (i.e, five least influential parameters among top 20) are shown in table 6-3. In this table, the 2nd column shows the original distribution, the 3rd column shows the beta distribution equivalent of the original distribution, and the 4th column shows 10% shift to the means in the associated new beta distribution. Table 6-4 shows the distributional sensitivity analysis results for these five parameters for the 10,000 yr simulation period. Surprising trends were found in the results. For 2 out of 5 parameters, the peak expected dose were found to be higher than several parameters from the list of the top ten in table 6-3. The metric distance for the each of the other three parameters was low. Further analyses are underway to determine why the metric distance for all five parameters are higher than for one of the 10 parameters that showed a moderately large impact (i.e., 75%) are gen_ifi and SFWt%I2. Only one parameter (i.e., InvMPerm) showed a small response to a 10% shift of the range to the mean value. However, this parameter showed significant sensitivity in the 100,000 year calculation compared to most other parameters.

The next set of analyses involve changing the distribution type. Table 6-5 shows the nominal case and the sensitive case distributions with the associated parameters defining these distribution functions. The sensitive cases are obtained by changing the original uniform distributions to normal, loguniform to log normal, and vice versa. All changes in linear scale preserve the mean value. The change from uniform to normal decreases the frequency of values near the high and low limits, and from normal to uniform increases the frequency of the values near the high and low limits while keeping the mean value unchanged. However, the change to the distributions from loguniform to lognormal and vice versa preserves the mean value only in the log scale but not in the linear scale. A change from lognormal to loguniform forces the mean of the parameter to increase. A change from loguniform to lognormal forces the mean to decrease. As figure 6-3 shows, the minimum and maximum for the sensitive case (i.e., the uniform distribution) are identical to the nominal case (i.e., the

triangular distribution).

Table 6-6 shows metric distance and changes to the peak expected dose for 10,000 and 100,000 yr corresponding to the sensitive cases presented in table 6-5. The percentage change in peak expected dose does not appear to correlate well with the metric distance. Three (DTFFAVIF, SbArWt%, WP-Def%) out of six parameters that have linear distribution functions show reasonable high metric distance (~0.7). Only one (DTFFAVIF) out of three showed a greater than a 10% change to the peak expected dose. However, FOCTR showed a surprisingly higher (i.e., ~10%) change in peak expected dose while the corresponding metric distance is lowest among all parameters. Further investigation of this behavior is currently underway.

In the case of the uniform-to-normal change the metric distance will change, but it is possible that the peak expected dose does not change because the mean of the distribution is preserved. The frequency values on both sides of the mean near the limits are decreased symmetrically. The same is true for the normal to uniform case except that the frequency of values on both sides of the mean near the limits are increased symmetrically. If the relationship between the input parameter and the peak expected dose is linear, the metric distance can be large even if the peak expected dose does not change such as is the case for AAMAI@S. If a change in the peak expected dose does occur, that indicates that the relationship between the dose and the parameter under study is nonlinear.

Table 6-6 also shows that changing the distribution from lognormal to loguniform and vice versa resulted in larger changes in the peak expected dose and overall larger metric distances. The percentage change in peak expected dose for the logarithmic distributions (4 out of 10 parameters) ranged between 41.96% and 10.43%, where as for the parameters with linear distributions (6 out of 10) ranged from 0.86% to 16.89%. Note that 3 out of 4 parameters with logarithmic distributions showed the three largest metric distances and change in peak expected dose when the mean of the distributions were shifted by 10 percent. Therefore, it is possible that the larger metric distance and change to the peak expected dose are the symptoms of a shift in the mean (in the linear scale) rather than the change in the distribution type. This analysis, however, reveals that the appropriate selection of distribution functions, especially for the parameters with logarithmic distributions are important. A wrong selection of lognormal distribution instead of a loguniform distribution may have a greater impact than the wrong selection of a uniform distribution instead of a normal distribution. Alternative ways should be used instead (????).

Examination of the 100,000 year columns reveals that there is little or no correlation between the metric distance and the peak expected dose.

e. Risk Significance

Distributional sensitivity analyses show that improper choice of distribution function can significantly affect the dose responses, such as the peak-realization doses and the peak expected dose. These two dose measures showed very high distributional sensitivity, especially when the mean values are changed for the two most-influential parameters identified by the parametric sensitivity analysis methods. The set two parameters are (i) the flow multiplication factor that determines the quantity of water entering the waste package (a 10 percent change to the parameter mean resulted in a 150% change in the dose) and (ii) the pre-exponential term for the

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spent fuel model used in the nominal case (a 10 percent change to the parameter mean resulted in a 57% change in the dose). Peak expected dose showed most sensitivity when the drip shield failure time distribution was changed, followed by the Alluvium matrix retardation factor for neptunium and the distance to the tuff-alluvium interface.

f. Recommendations

1. Although the distributional sensitivity analysis, in this report focuses on top 10 parameters identified by the parametric sensitivity analysis method, the analyses should be extended to all 330 input parameters.
2. Extra attention should be given to the distribution of parameters that show as influential in the parametric sensitivity analyses. However, care should be taken in selecting distribution function for all sample parameters because a small error from each parameter with wrong selection of distribution may accumulate to significantly affect the performance measure.
3. The significance of the metric measure will be analyzed further to identify what additional information can be derived, especially when there is no difference in the peak expected dose between the nominal case and the sensitive case.
4. The study should be extended to (i) changing the variance of the input parameter distribution function and (ii) changing the mean of the distribution while keeping the variance fixed.

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A. L.

Table 6-1. Modified Distribution Functions for the Top 10 Influential Parameters for Creating Sensitivity Cases				
Parameter		Original Distribution	Nominal	Sensitivity
Abbreviation	Description			
WPFlowMF	Waste Package Flow Multiplication Factor	lognormal 3.15e-2, 1.05e3	logbeta 1.6e3,1.7e4, 5.0,5.0	logbeta 1.6e3,1.7e4, 7.5,5.0
PSFDM1	Pre-exponential term for the spent fuel dissolution model 2	loguniform 1.2e3, 1.2e6	logbeta 1.2e3,1.2e6, 1.0,1.0	logbeta 1.2e3,1.2e6, 1.97,1.0
SbArWt%	Subarea wet fraction	uniform 0.0, 1.0	beta 0.0,1.0, 1.0,1.0	beta 0.0,1.0, 1.5,1.0
AAMAI@S	Areal average mean annual-infiltration at start [mm/yr]	uniform 4.0,13.0	beta 4.0,13.0, 1.0,1.0	beta 4.0,13.0, 1.5,1.0D
DSFailTi	Drip shield failure time [yr]	lognormal 2700.0, 20400.0	logbeta 2700.0, 20400.0, 5.0, 5.0	logbeta 2700.0, 20400.0, 7.8, 5.0
WPRRG@20	Well pumping rate at the 20-km receptor Group location [gal/day]	uniform 4.5e6, 1.3e7	beta 4.5e6, 1.3e7, 1.0, 1.0	beta 4.5e6, 1.3e7, 1.5, 1.0
WP-Def%	Fraction of total waste packages in a subarea that fail at time t=0	uniform 1.0e-4, 1.0e-2	beta 1.0e-4, 1.0e-2, 1.0, 1.0	beta 1.0e-4, 1.0e-2, 1.5, 1.0
DTFFAVIF	Distance traveled in Tuff [km]	uniform 10.0, 19.9	beta 10.0, 19.9, 1.0, 1.0	beta 10.0, 19.9, 1.5, 1.0
FOCTR	Fraction of water condensate moving towards repository	uniform 0.05, 1.0	beta 0.05, 1.0, 1.0, 1.0	beta 0.05, 1.0, 1.5, 1.0

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ARDSAVNp	Matrix retardation for neptunium in the saturated zone of the Amargosa Valley alluvium	lognormal 1.0, 3.9e3	logbeta 1.0, 3.9e3, 5.0, 5.0	lognormal 1.0, 3.9e3, 8.2, 3.5
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A. L.

Table 6-2. Metric Distances for 10,000 and 100,000 yr Simulations for the Top 10 Influential Parameters with 10 Subareas and 330 Realizations Where the Mean of the Distribution Is Shifted by 10 Percent of the Range

Top Ten Parameters		Distribution Type	10,000 yr		100,000 yr	
			Metric Distance	Changes in Peak Expected Dose (%)	Metric Distance	Changes in Peak Expected Dose (%)
Abbreviation	Description					
WPFlowMF	Waste package flow multiplication factor	Lognormal	$4.78 \times 10^{+00}$	149.88	$1.93 \times 10^{+00}$	59.00
PSFDM1	Pre-exponential term for the spent fuel dissolution model 2	Loguniform	$1.40 \times 10^{+00}$	57.20	$1.51 \times 10^{+00}$	75.18
SbArWt%	Subarea wet fraction	Uniform	4.98×10^{-01}	24.93	5.32×10^{-01}	21.14
AAMAI@S	Areal average mean annual-infiltration at start [mm/yr]	Uniform	2.09×10^{-01}	5.28	1.51×10^{-01}	4.94
DSFailTi	Drip shield failure time[yr]	Lognormal	9.98×10^{-01}	-24.83	3.63×10^{-03}	-0.01
WPRRG@20	Well pumping rate at the 20-km receptor group location [gal/day]	Uniform	3.24×10^{-01}	-8.62	2.74×10^{-01}	-9.68
WP-Def%	Fraction of total waste packages in a subarea that fail at t=0	Uniform	5.30×10^{-01}	22.06	6.16×10^{-03}	0.22
DTFFAVIF	Distance traveled in TUFF [km]	Uniform	5.16×10^{-01}	19.89	6.05×10^{-01}	19.31
FOCTR	Fraction of water condensate moving towards the repository	Uniform	2.15×10^{-01}	4.41	1.05×10^{-03}	0.03
ARDSAVNp	Matrix retardation for neptunium in the saturated zone of the Amargosa Valley alluvium	Lognormal	8.88×10^{-02}	-8.35	$1.84 \times 10^{+00}$	-68.10

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Table 6-3. Modified Distribution Functions for the Five Least Influential Parameters within the Top 20 for Creating Sensitivity Cases				
Parameters		Original Distribution	Base	Sensitivity
Abbreviation	Description			
SFWt%I2	Spent fuel wetted fraction for initially defective waste packages in subarea 2	uniform 0.0,1.0	beta 0.0,1.0, 1.0,1.0	beta 0.0,1.0, 1.5,1.0
InvMPerm	Matrix permeability of the invert [m ²]	lognormal 2.0e-18,2.0e-16	logbeta 2.0e-18,2.0e-16, 5.0,5.0	logbeta 2.0e-18,2.0e-16, 9.0,5.0
SFWt%I9	Spent fuel wetted fraction for initially defective waste packages in subarea 9	uniform 0.0,1.0	beta 0.0,1.0, 1.0,1.0	beta 0.0,1.0, 1.5,1.0
SFWt%I1	Spent fuel wetted fraction for initially defective waste packages in subarea 1	uniform 0.0,1.0	beta 0.0,1.0, 1.0,1.0	beta 0.0,1.0, 1.5,1.0
gen_ifi	Irrigation interception fraction	triangular 0.06,0.4,1.0	triangular 0.06,0.4,1.0	triangular 0.06,0.7,1.0

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Table 6-4. Metric Distances for 10,000-yr Simulations for the 5 least Influential Parameters within the Top 20 with 10 Subareas and 330 Realizations Where the Mean of the Distribution Is Shifted by 10 Percent of the Range

Parameters			10,000 yr	
Abbreviation	Description	Distribution Type	Metric Distance	Changes in Peak Expected Dose (%)
SFWt%l2	Spent fuel wet fraction for initial failures in subarea 2	Uniform	2.21×10^{-01}	5.49
InvMPerm	Matrix permeability of the invert [m ²]	Lognormal	1.03×10^{-02}	0.02
SFWt%l9	Spent fuel wet fraction for initial failures in subarea 9	Uniform	1.12×10^{-01}	1.68
SFWt%l1	Spent fuel wet fraction for initial failures in subarea 1	Uniform	1.74×10^{-01}	2.89
gen_ifi	Irrigation interception fraction	Triangular	3.34×10^{-01}	9.80

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Influential Parameter		Nominal Case (Input)	Sensitivity Case (Input)
Abbreviation	Description		
WPFlowMF	Waste package flow multiplication factor	lognormal 3.15e-2, 1.05e3	loguniform 3.15e-2, 1.05e3
PSFDM1	Pre-exponential term for the spent fuel dissolution model 2	loguniform 1.2e3, 1.2e6	lognormal 1.2e3, 1.2e6
SbArWt%	Subarea wet fraction	uniform 0.0, 1.0	normal 0.0, 1.0
AAMAI@S	Areal average mean annual-infiltration at start [mm/yr]	uniform 4.0,13.0	normal 4.0,13.0
DSFailTi	Drip shield failure time[yr]	lognormal 2700.0, 20400.0	loguniform 2700.0, 20400.0
WPRRG@20	Well pumping rate at the 20-km receptor Group location [gal/day]	uniform 4.5e6, 1.3e7	normal 4.5e6, 1.3e7
WP-Def%	Fraction of total waste packages in a subarea that fail at time t=0	uniform 1.0e-4, 1.0e-2	normal 1.0e-4, 1.0e-2
DTFFAVIF	Distance traveled in Tuff [km]	uniform 10.0, 19.9	normal 10.0, 19.9
FOCTR	Fraction of water condensate moving towards repository	uniform 0.05, 1.0	normal 0.05, 1.0
ARDSAVNp	Matrix retardation for neptunium in the saturated zone of the Amargosa Valley alluvium	lognormal 1.0, 3.9e3	normal 1.0, 3.9e3

Table 6-6. Metric Distances for 10,000 and 100,000 yr Simulations for the Top 10 Influential Parameters with 10 Subareas and 330 Realizations Where Distribution Type Is Change						
Top Ten Parameters		Distribution Type	10,000 yr		100,000yr	
			Metric Distance	Changes in Peak Expected Dose (%)	Metric Distance	Changes in Peak Expected Dose (%)
WPFlowMF	Waste package flow multiplication factor	Loguniform to lognormal	9.54×10^{-01}	14.49	2.23×10^{-01}	-4.76
PSFDM1	Pre-exponential term for the spent fuel dissolution model 2	Loguniform to lognormal	6.94×10^{-01}	-10.43	1.87×10^{-01}	-42.86
SbArWt%	Subarea wet fraction	Uniform to normal	7.01×10^{-01}	-6.13	5.25×10^{-01}	0.38
AAMAI@S	Areal average mean annual-infiltration at start [mm/yr]	Uniform to normal	2.50×10^{-01}	-0.86	1.08×10^{-01}	1.45
DSFailTi	Drip shield failure time [yr]	Lognormal to loguniform	9.77×10^{-01}	-41.96	1.88×10^{-03}	0.00
WPRRG@20	Well pumping rate at the 20-km receptor Group location [gal/day]	Uniform to normal	3.77×10^{-01}	-3.56	2.00×10^{-01}	1.59
WP-Def%	Fraction of total waste packages in a subarea that fail at time t=0	Uniform to normal	6.08×10^{-01}	-3.31	6.07×10^{-03}	0.04
DTFFAVIF	Distance traveled in Tuff [km]	Uniform to normal	7.81×10^{-01}	-16.89	7.65×10^{-01}	-10.96

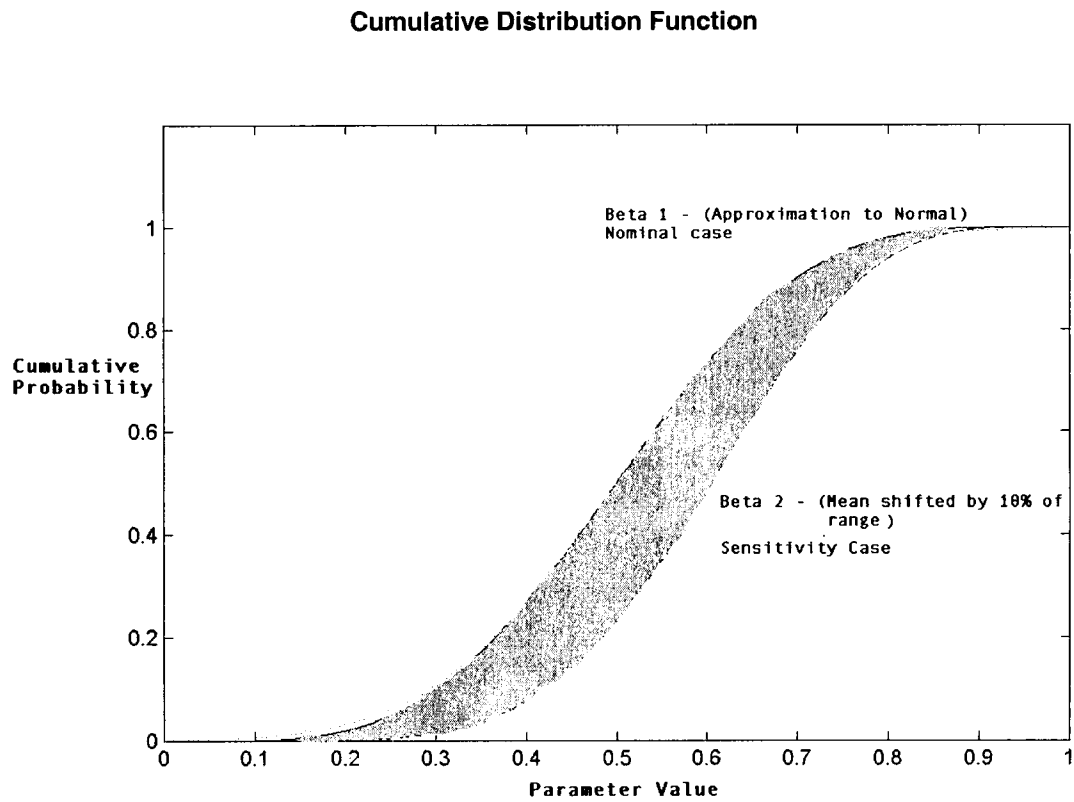


Figure 6-1 - Example of a shifted output CDF from a shift in the input distribution for a shift in the mean of 10% of the range

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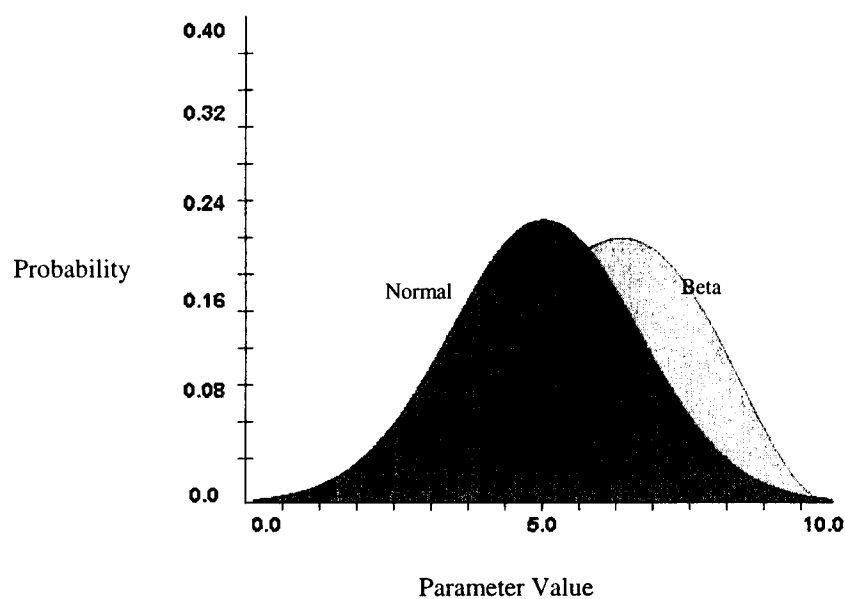


Figure 6-2 - Example of changing the probability density function for an input parameter by shifting the mean value of a Normal distribution without changing the end points. This is done by approximating the Normal distribution with a Beta distribution and then modifying the shape parameters.

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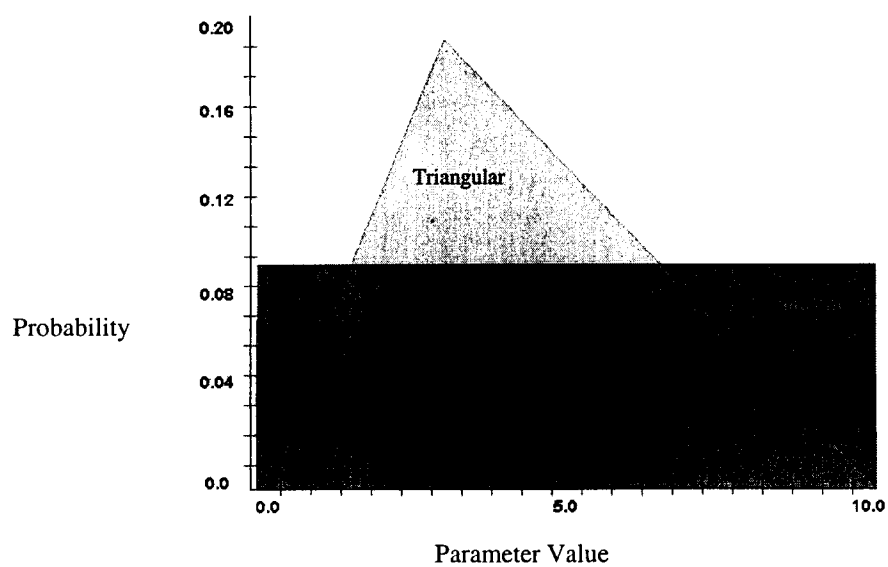


Figure 6-3 - Example of changing the probability density function by changing the distribution Type from Uniform to Triangular

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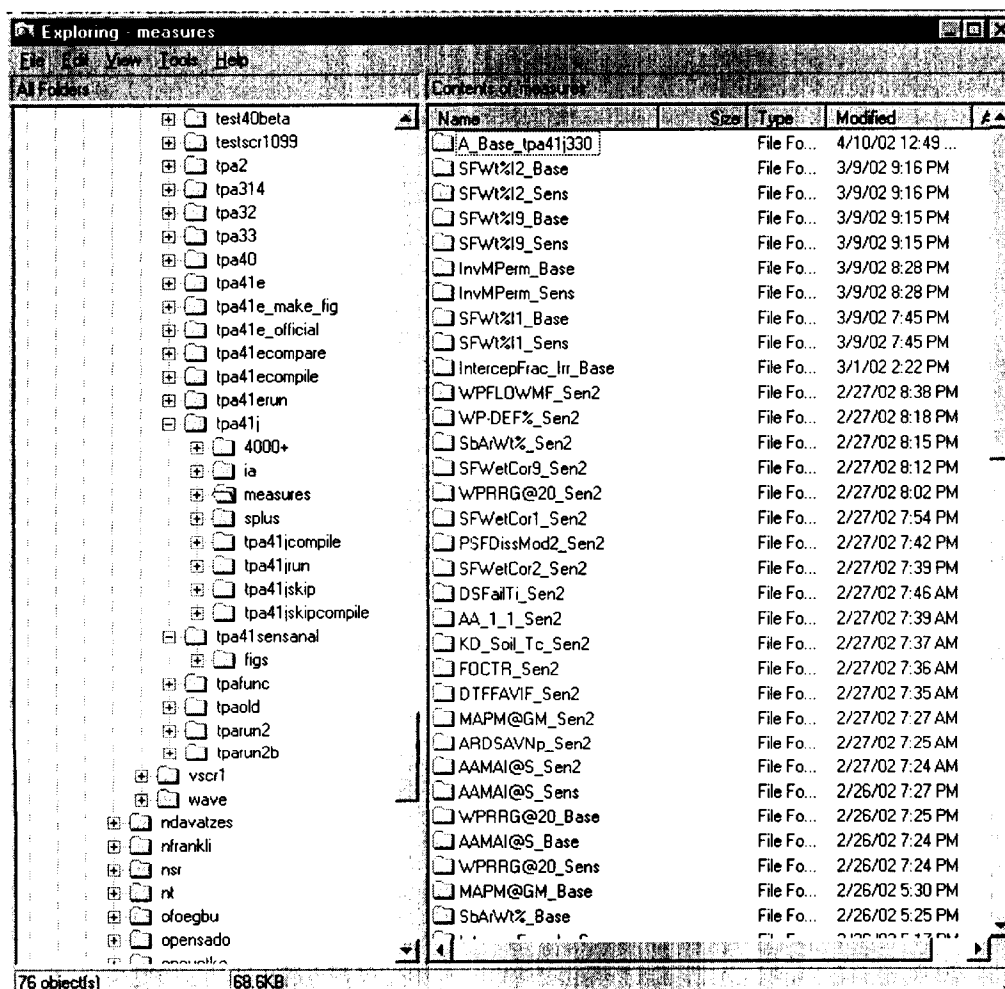
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The results for these runs are stored in the following directory path.

(SPOCK) /home/muller/tpa/tpa41j/measures/...

The folders with the data are shown in the following figure.

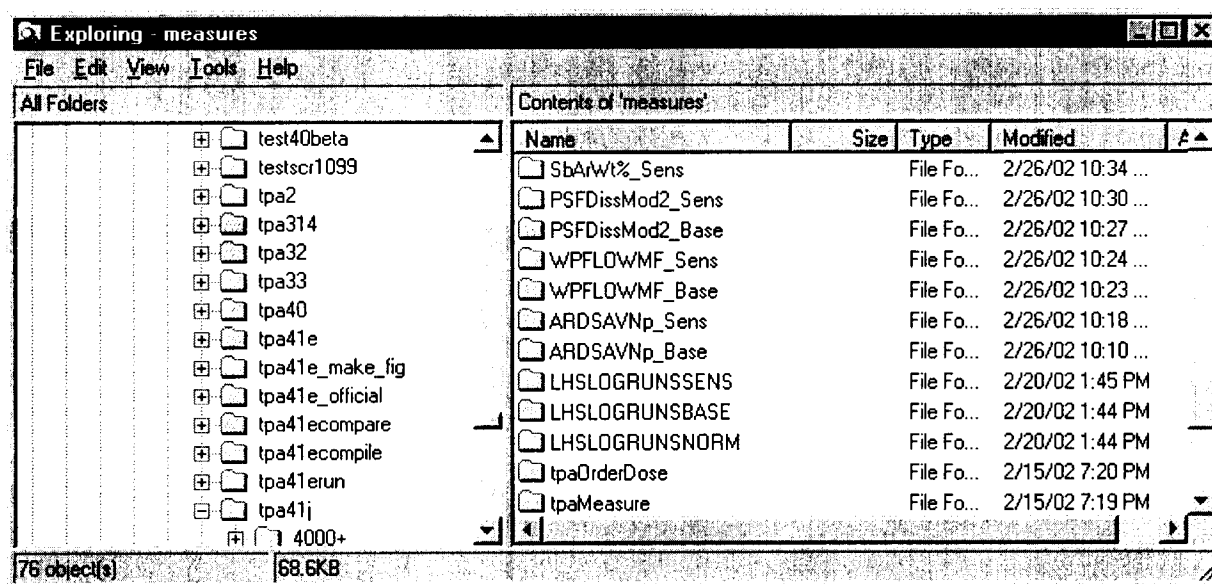


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February 15, 2001 through March 15, 2002

Supermodsign work. (Parameter Tree method)

The work performed within this time period is reported in Chapter 4 of a document written by Sitakanta Mohanty. The section of chapter 4 is titled Results from the parameter tree method.

The method used for examining system sensitivity to combinations of parameters found to be most important is to treat each realization of a parameter value as either a + or a - depending on whether the realized value is greater or less than a specified value. This is similar to the procedure followed in a Sign Test (Bowen and Bennet, 1988). Next the realizations are sorted based on the commonality of their parameters being either + or a -. For example, realizations with all five important parameters sampled above the median would be placed in the same bin. Similarly, all realizations where the first four parameters are a + and the last parameter is a - would be placed in another bin and so on. The following page shows the result of a supermodsign run with the chosen parameters.

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* Modified Signs Test Based on Median Values *

median of gwpkdoses= 0.363E-06
median of PSFDM1 = 0.380E+05
median of WPFlowMF= 0.575E+01
median of SbArWt% = 0.500E+00
median of DSFailTi= 0.742E+04
median of FOCTR = 0.525E+00

	+ output/ # in bin	mean dose in bin (rem/y)	fractional contribution	amplification factor
11111	70 / 122	0.180E-03	0.1037	3.4015
11110	55 / 131	0.716E-04	0.0443	1.3513
11101	123 / 127	0.557E-03	0.3340	10.5208
11100	98 / 129	0.250E-03	0.1524	4.7244
11011	59 / 124	0.324E-04	0.0190	0.6114
11010	37 / 114	0.290E-04	0.0156	0.5480
11001	120 / 130	0.118E-03	0.0727	2.2359
11000	75 / 125	0.451E-04	0.0266	0.8504
10111	45 / 114	0.141E-04	0.0076	0.2668
10110	34 / 135	0.114E-04	0.0073	0.2156
10101	110 / 124	0.106E-03	0.0618	1.9931
10100	76 / 121	0.399E-04	0.0228	0.7524
10011	31 / 126	0.446E-05	0.0026	0.0841
10010	26 / 132	0.196E-05	0.0012	0.0369
10001	88 / 128	0.225E-04	0.0136	0.4250
10000	48 / 118	0.563E-05	0.0031	0.1063
01111	62 / 122	0.138E-04	0.0079	0.2602
01110	41 / 133	0.841E-05	0.0053	0.1587
01101	117 / 123	0.498E-04	0.0289	0.9408
01100	105 / 133	0.501E-04	0.0314	0.9450
01011	49 / 119	0.421E-05	0.0024	0.0795
01010	34 / 113	0.993E-05	0.0053	0.1874
01001	118 / 132	0.202E-04	0.0126	0.3815
01000	66 / 123	0.103E-04	0.0060	0.1943
00111	29 / 134	0.196E-05	0.0012	0.0370
00110	14 / 110	0.361E-06	0.0002	0.0068
00101	94 / 122	0.967E-05	0.0056	0.1825
00100	58 / 120	0.471E-05	0.0027	0.0888
00011	19 / 138	0.209E-06	0.0001	0.0039
00010	13 / 133	0.499E-06	0.0003	0.0094
00001	46 / 115	0.150E-05	0.0008	0.0284
00000	40 / 130	0.170E-05	0.0010	0.0322

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A 1 represents a + and a 0 represents a -. Supermodsign chose these five parameters because they produced the largest amplification factor. This case occurred at 11101 median of PSFDM1(+), WPFlowMF(+), SbArWt%(+), DSFailTi(-), and FOCTR(+).

Results using super modsign using different combinations of mean, median, and percentile values are shown below for the latest 4000 vector tpa run.

10 K Year
Based on New Code

All 4000 Vectors

	10KYearMean	10KYearMedian	50KYearPerc_50_90
1	WPFlowMF	PSFDM1	PSFDM1
2	PSFDM1	WPFlowMF	WPFlowMF
3	SbArWt%	SbArWt%	SbArWt%
4	genKDsPb	DSFailTi	DSFailTi
5	SSMOV503	FOCTR	FOCTR
6	MAPM@GM	*Chlorid	*Chlorid
7	AAMAI@S	Solbl-Np	Solbl-Np
8	MATI@GM	gen_hirP	gen_hirP
9	gen_dwcl	SSMOV404	SSMOV404
10	SSMO-JS1	AAMAI@S	AAMAI@S

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3999 Vectors (Vector 265 removed)

	10KYearMean	10KYearMedian	50KYearPerc_50_90
1	WPFlowMF	PSFDM1	PSFDM1
2	PSFDM1	WPFlowMF	WPFlowMF
3	SbArWt%	SbArWt%	SbArWt%
4	genKDsPb	DSFailTi	DSFailTi
5	SSMOV503	WP-Def%	WP-Def%
6	MAPM@GM	TempGrBI	TempGrBI
7	AAMAI@S	FPrm_TSw	FPrm_TSw
8	MATI@GM	WPFD-ThD	WPFD-ThD
9	gen_dwcl	SSMO-RE	SSMO-RE
10	SSMO-JS1	AAMAI@S	AAMAI@S

3999 Vectors (Vector 2267 removed)

	10KYearMean	10KYearMedian	50KYearPerc_50_90
1	WPFlowMF	PSFDM1	
2	PSFDM1	WPFlowMF	
3	SbArWt%	SbArWt%	
4	genKDsPb	DSFailTi	
5	SSMOV503	WP-Def%	
6	MAPM@GM	TempGrBI	
7	AAMAI@S	FPrm_TSw	
8	MATI@GM	WPFD-ThD	
9	gen_dwcl	SSMO-RE	
10	SSMO-JS1	AAMAI@S	

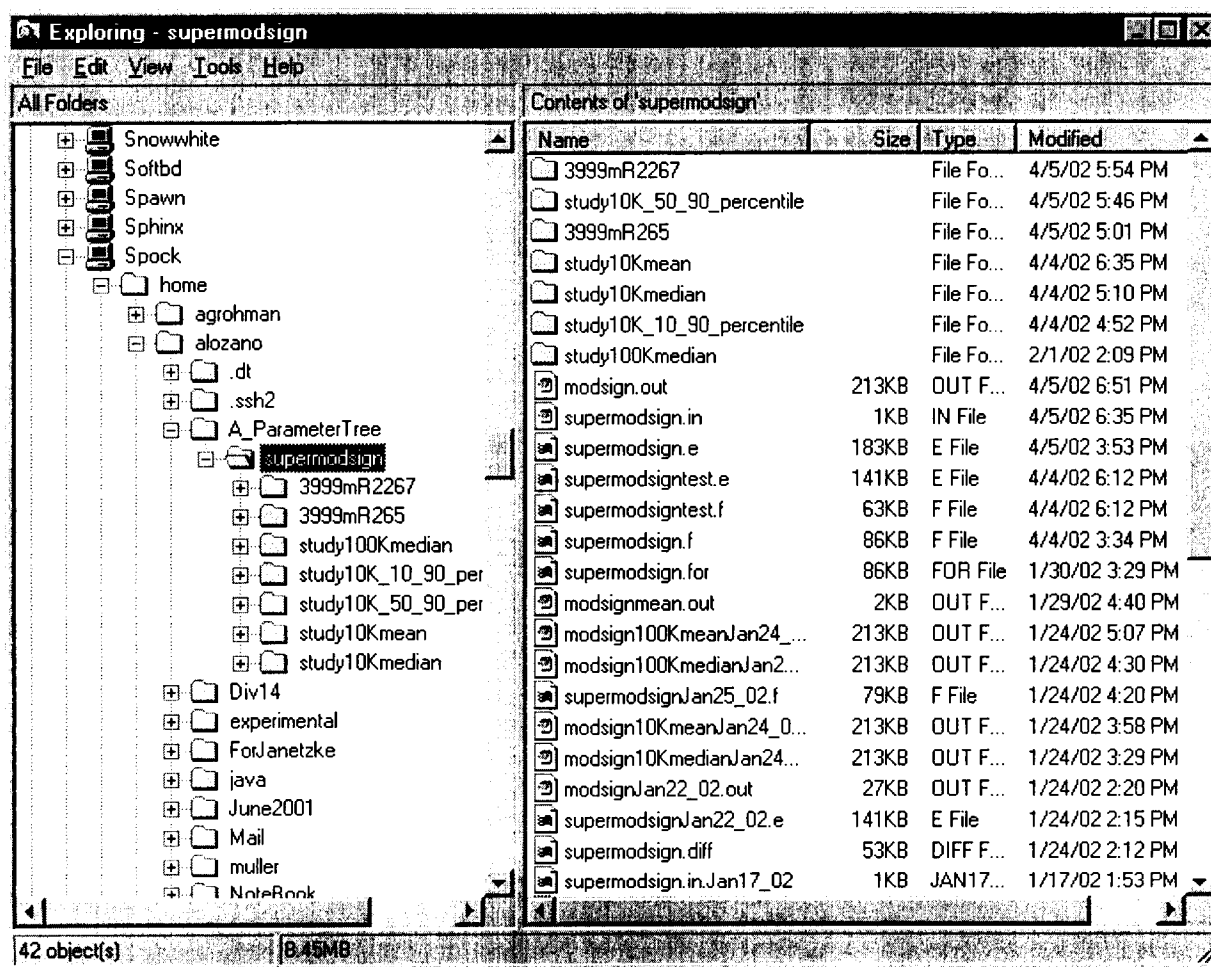
The data for these runs is stored as shown in the following figure.

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have not modified any entries previous to this statement

Albert S. Lozano
Albert Lozano Apr. 16, 2002

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INITIAL ENTRIES

Scientific Notebook: #451E

Issued to: S. Mohanty / Albert Lozano

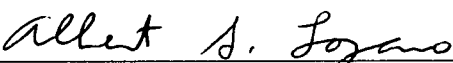
Issue Date: March 20, 2001

Account Number: 20-1402-761

Title: Metric Measure & Other Exploratory Work

Participants: Albert Lozano

I have not modified any entries previous to this statement


Albert Lozano Apr. 16, 2002

This document is being continued from a Word Perfect document whose last entry was April 16, 2002. All work after April. 16, 2002 is documented in this document.

April 16, 2002 through May 13, 2002

During this time period I was not very active in this project.

May 14, 2001 through June 30, 2002

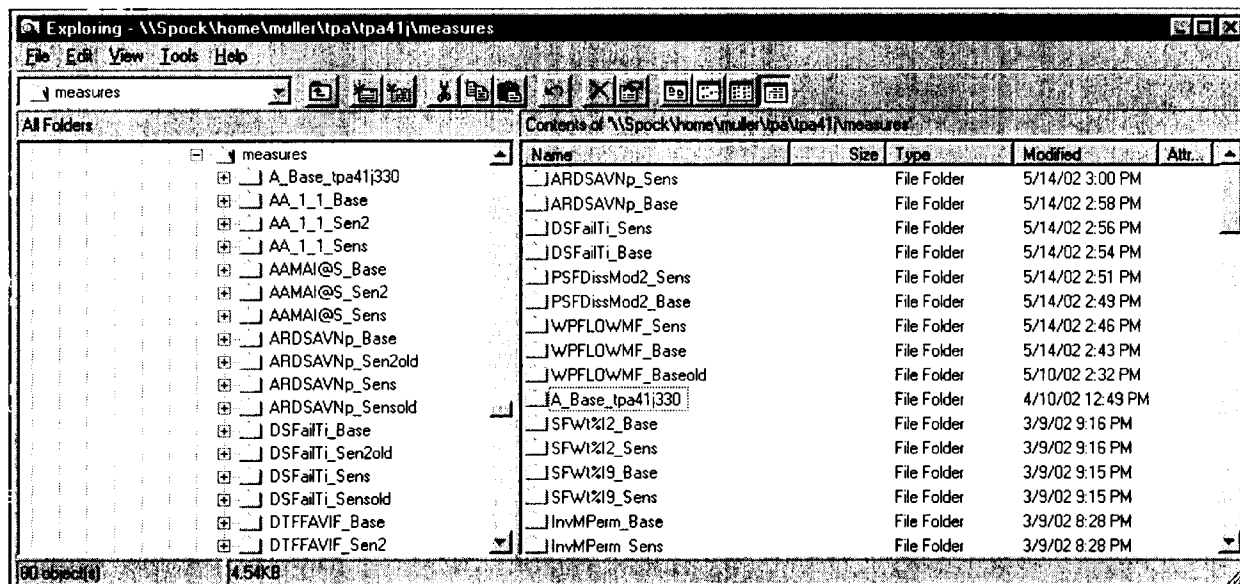
Work done during this period was in support of Sitakanta Mohanty on his Sensitivity Analysis report. New tpa runs had to be made for the following reason. The chapter on distributional sensitivity describes results that were obtained when the distribution of an input was changed from one type, such as normal, to another such as uniform for the same range of values. For linear distributions, the mean value of the input remains the same. When changing from a non linear distribution type, such as lognormal, to another, such as loguniform, the mean values do not remain the same. The new set of runs were made in an attempt to change the distribution types of the nonlinear distributions while keeping the mean values the same.

Printed: October 24, 2002

A. Lozano

SCIENTIFIC NOTEBOOK No.

451E INITIALS: A. L.



The parameters that were rerun are WPFLOWMF, PSFDM1, DSFailTi, and ARDSAVNp. The data is stored in the subdirectories shown in the Exploring window above. The metric measure results are found at the end of the measure.res file in each ..._Base directory.

July 1, 2002 - Oct.4, 2002

During this period, I was not active on this project.

Albert S. Lozano

Albert Lozano Oct 8, 2002

Printed: October 24, 2002

A. Lozano

SCIENTIFIC NOTEBOOK No.

451E

INITIALS: A. L.

INITIAL ENTRIES

Scientific Notebook: #451E

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Issue Date: March 20, 2001

Account Number: 20-1402-761

Title: Metric Measure & Other Exploratory Work

Participants: Albert Lozano

I have not modified any entries previous to this statement

Albert S. Lozano
Albert Lozano October 8, 2002

This document is being continued from a Word Perfect document whose last entry was October 8, 2002. All work after October 8, 2002 is documented in this document.

October 8, 2002 through --- 2002

During this time period I was not very active in this project.

~~May 14, 2001 through June 30, 2002~~

~~Work done during this period was in support of Sitakanta Mohanty on his Sensitivity Analysis report. New tpa runs had to be made for the following reason. The chapter on distributional sensitivity describes results that were obtained when the distribution of an input was changed from one type, such as normal, to another such as uniform for the same range of values. For linear distributions, the mean value of the input remains the same. When changing from a non linear distribution type, such as lognormal, to another, such as loguniform, the mean values do not remain the same. The new set of runs were made in an attempt to change the distribution types of the non-linear distributions while keeping the mean values the same.~~

A. L.
12/20/2002

Printed: October 24, 2002

A. Lozano

SCIENTIFIC NOTEBOOK No.

451E INITIALS: A. L.

A. L. 12/20/2002

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July 1, 2002 - Oct. 4, 2002

During this period, I was not active on this project.

Albert S. Lozano

Albert Lozano Oct 8, 2002

I have very briefly reviewed this SD and on that basis conclude that a scientist with the correct background in probability, statistics, mathematics, and risk assessment along with strong skills in the use of MATLAB would be able to reproduce the work described herein.

Josh Wilkey 12/30/2002

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK No.: 451E

Document Date:	03/20/2001
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
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Application Used: (including version number)	WordPerfect; Microsoft Word
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD
File Types: (.exe, .bat, .zip, etc.)	wpd, doc
Remarks: (computer runs, etc.)	Media contains: Metric measure and other exploratory work