SCIENTIFIC NOTEBOOK
NUMBER 185, VOLUME 6

by

Roberto T. Pabalan

Southwest Research Institute
Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

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10/03/97 (CANE)

A new tpa.inp file was generated by copying the file tpa.inp.meanvalues1 and commenting out (with **) the three "correlateinputs" parameters at the end of the input file. This will set every parameter, including the 6 that were sampled using the tpa.inp.meanvalues1 file, to their mean. Subsequently, all four parameters that were sampled for Cases 1m, 2m, 3m, and 4m were set to their respective range and PDFs. Thus, all four of these parameters will be sampled. The number of realizations was set to 400. The TPA 3.1.1 code was then initiated. This run will be referred to as CASE-6mm.

10/06/97 (CANE)

A new tpa.inp file was generated by copying the tpacase1m.inp file and commenting out the "correlateinputs" parameters at the end of the file. The TPA 3.1.1 code was then initiated. This run will be referred to as CASE-1mm. In this case, only one parameter is sampled: **Matrix Permeability**.

Below is a copy of the guidelines for conducting the sensitivity analysis provided by V. Colten-Bradley:

Sensitivity Analysis for October 22, 1997

The objective of the module sensitivity analysis is to provide insights concerning modelling approaches input data needs in the total-system performance assessment and ultimately feed into the importance analysis.

Each KTI needs to establish sensitivity at the overall system level AND the subsystem level. The sensitivity analysis is for parameters to dose AND the output from the module that each KTI helped to construct the data set for.

The first step in the analysis is to establish a baseline result. This will be done by executing the TPA code using the meanvalue data file tpa.input.meanvalues1. One hundred realizations will be obtained to establish the baseline results . Since this baseline will be common to all KTIs, TPA KTI will make this run and provide outputs (*.res files) to KTIs. These outputs will be the baseline outputs.

Note: Even though the input file name implies meanvalues, the data set has four flow parameters that are sampled (this is done to prevent the flow under mean parameter conditions to be either all in the matrix or in the fractures).

<u>First approach for sensitivity analysis at the KTI level:</u>

A KTI can vary all [i.e., assign probability distributions to all stochastic (uncertain or sampled)] parameters of its module(s) simultaneously (rather than varying them one by one). For example, SDS KTI can vary all stochastic parameters of FAULTO module in one execution of the TPA. This can be done easily by replacing the FAULTO segment from tpa.inp.meanvalues1 by that in the tpa.inp.master file. The number of realizations one should obtain depend upon the number of sampled parameters; larger the number of such parameters, more the number of realizations required. But for consistency, use 100 vector runs which would be sufficient to do the first cut sensitivity work. Most KTIs do not have enough parameters that they need to worry about convergence of the random errors in the sampler.

One could plot CCDFs for dose and releases. But the CCDFs may be very subtle and difficult to discern. However, the ccdf files are easily and readily available using tccdf after a tpa run. Data in these files can be plotted easily.

Parameter sensitivities then can be studied using S-plus following the procedure provided by Virginia Colten-Bradley (VCB). In this approach, step-wise regression is used (VCB has provided the S-plus object) to rank parameters of importance. Ranking of the parameters will be obvious by the correlation coefficients. Note that we shall obtain all of the graphs that VCB had in her handout during the training.

Scatter plots should be used as the first tool for evaluating sensitivity. Two object files (lotsa.plots.obj and scatter.obj) have been provided by VCB for the purpose of getting a lot of scatter plots done quickly.

Unless a KTI has "billions and billions" (à la C.Sagan) of parameters, the stepwise routine will not tell any more than the scatter plots will. In general, the stepwise routine will select the parameters in the order of their correlation coefficient to the performance measure. If the stepwise routine must be used, use the stepwise command in the S-plus command screen, entering all of the appropriate arguments. [VCB]

Second approach to sensitivity analysis by the KTIs:

Vary one parameter at a time in the meanvalues input file and obtain appropriate number of realizations. If you adopt this approach, you may have to make at least two runs per parameter, using the minimum and maximum value of the parameter. The result will be two CCDFs for each run which can be compared to the baseline CCDF to determine the sensitivity. This is more time consuming for the person doing the sensitivity analysis, as one would have to change the parameter values manually for the various runs. Therefore, generally, the first approach is preferred.

Caveat: This approach to sensitivity analysis is too time-consuming and will require very careful interpretation of the results. If it's a matter of changing a constant, then this approach should be used. But, not for sampled parameters. [VCB]

What is Expected:

1. Determine overall sensitivity of input parameters to peak dose. Some KTIs may need to use other performance measures such as release rate, number of WP failures, ground water travel time (GWTT). One can start with the result from the meanvalues data set and compare other results against it. This will give qualitative idea that can be presented in the graphical form.

2. Rank in order of sensitivity the parameters that the user has varied.

3. Based on the findings, determine if the data provided for the base case is reasonable or the best that should be used in the overall sensitivity analyses. Propose changes of sampled paramters to constants, changes in ranges and distibtutions, etc.

4. Provide recommendations about the necessary improvements to the modules or data used in TPA. If sensitivity needed to be obtained with respect to a parameter distribution different from the distribution in the master input file, the rationale for picking the alternate distribution should be documented.

Note: We are interested in the "big stuff", not "nits". [VCB]

Materials to Use:

S-Plus 3.4
S-plus training materials from VCB and MRB (all KTI co-leads should have a copy)

nawk files from VCB (please come by to make a photocopy of the fax) object files from VCB (check the directory /solapps/cnwra/goodies/vcb) Files from M. Rose Byrne (check the directory /solapps/cnwra/goodies/mrb)

10/7/97

0830 hrs - The TPA run for CASE-1mm is completed. However, based on the list of sampled parameters listed in file samplpar.res, it appears that seven parameters were sampled, the same as for Case-1m:

```
Input file tpa.inp as supplied with TPA Version 3.1 Code.
 Generated from Base case data set Rev 3.1.1  9/22/97
 TPA 3.1, Job started: Mon Oct  6 16:04:44 1997
 Names for Sampled Parameters (Nonconstant)
 Specified in "tpa.inp" - Values for Each Vector
   1 AAMAI@S   ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
   2 MAPM@GM   MeanAveragePrecipitationMultiplierAtGlacialMaximum
   3 MATI@GM   MeanAverageTemperatureIncreaseAtGlacialMaximum[degC]
   4 Fow*      FowFactor
   5 Fmult*    FmultFactor
   6 SbArWt%   SubAreaWetFraction
   7 MPrm_TSw  MatrixPermeability_TSw_[m2]
```

A check of S. Mohanty's e-mail dated 09/23/97 indicated that, indeed, three UZFLOW and three EBSREL parameters were sampled for the tpa.inp.meanvalues1 case. Thus, a new TPA run was initiated for CASE-1mm. The old output files were deleted. In this new run, the input file was changed so that parameters 1 to 6 in the box above was set to their mean value. Thus, only one parameter, #7, should be sampled in the run.

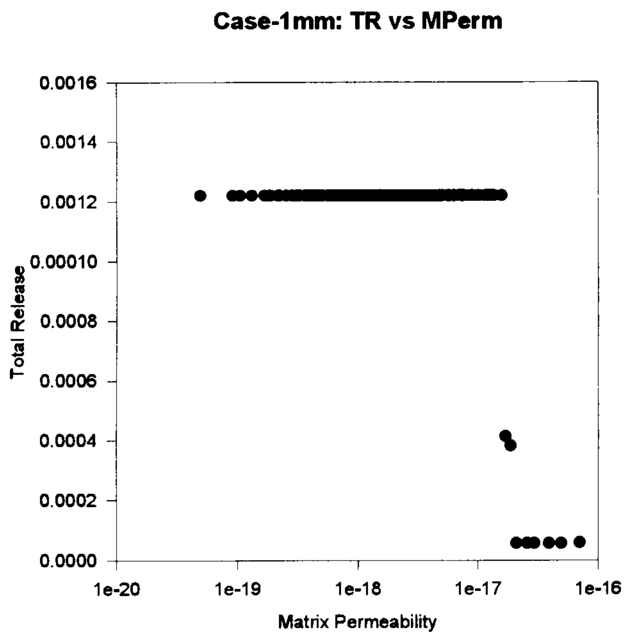
1500 hrs - CASE-1mm run was completed. The CASE-2mm run, with only the Matrix Porosity as the sampled parameter, was initiated.

1700 hrs - The CASE-3mm run, with only the Fracture Permeability as the sampled parameter, was initiated.

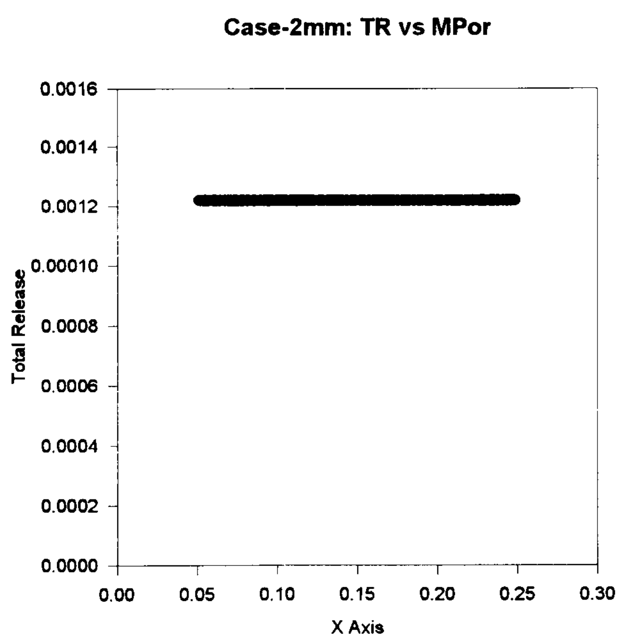
10/08/97 (CANE)

0815 hrs - The runs for CASE-2mm and CASE-3mm are complete. Input files for CASE-4mm and CASE-5mm were generated, and the TPA runs were initiated. For CASE-4mm, only the FRACTURE POROSITY was sampled, whereas in CASE-5mm, MATRIX PERMEABILITY and MATRIX POROSITY were sampled at low values.

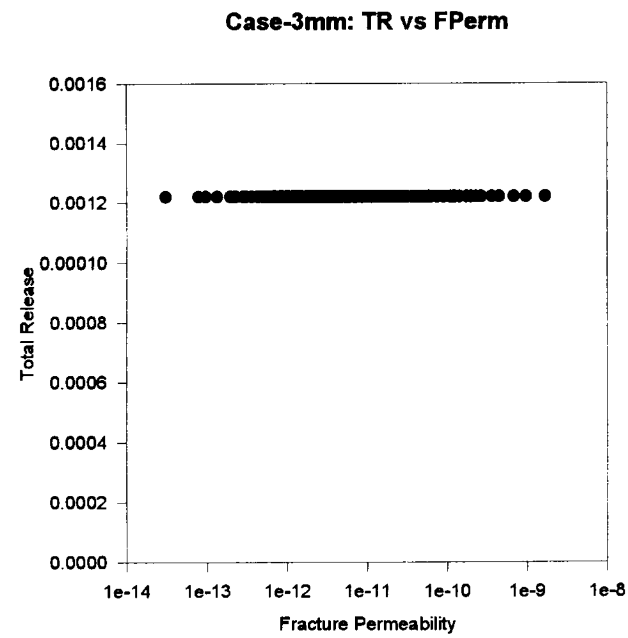
1300 hrs - Below is a plot of total release vs matrix permeability for CASE-1mm:



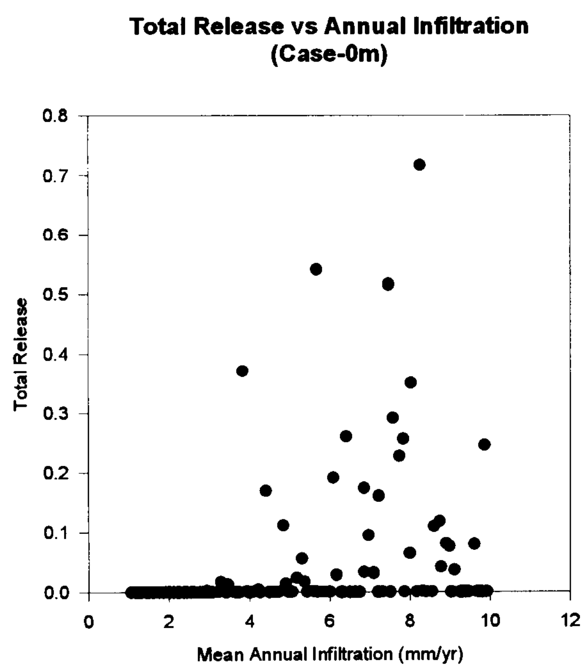
Below is a plot of total release vs matrix porosity for CASE-2mm:



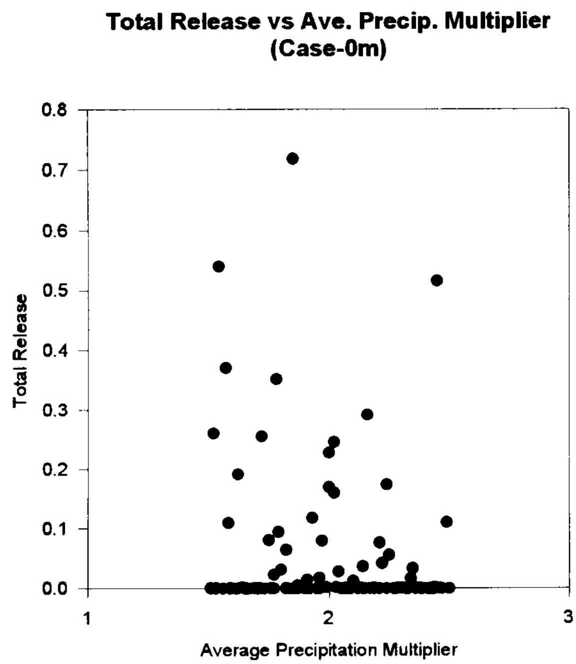
Below is a plot of total release vs FRACTURE PERMEABILITY for CASE-3mm:



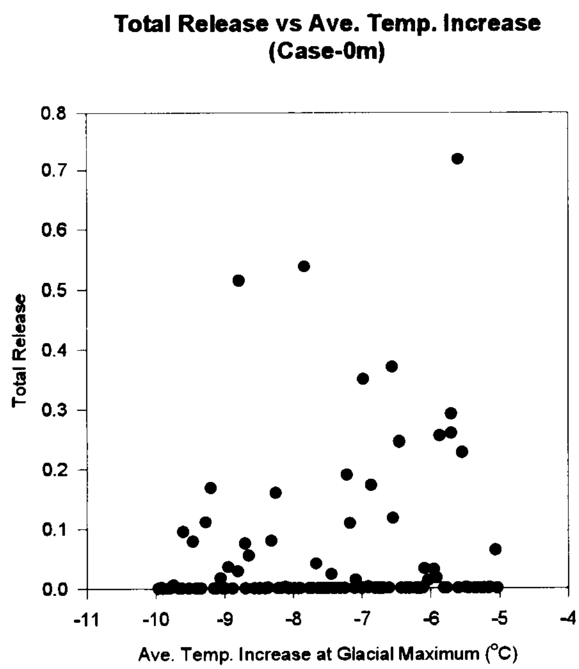
Below is a plot of total release vs ArealAverageMeanAnnualInfiltration for Case-0m:



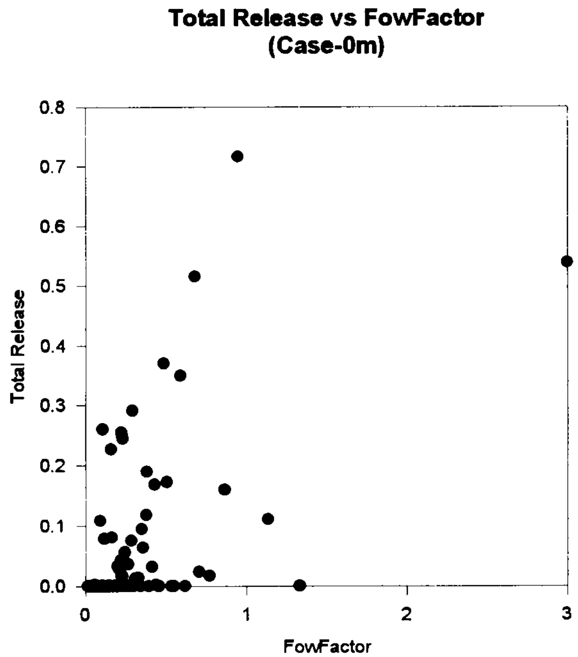
Below is a plot of total release vs MeanAveragePrecipitationMultiplierAtGlacialMaximum for CASE-0m:



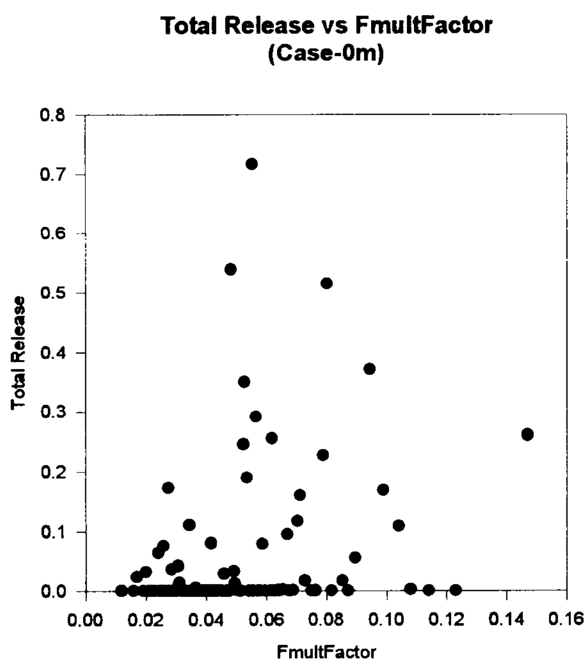
Below is a plot of total release vs MeanAverageTemperatureIncreaseAtGlacialMaximum for CASE-0m:



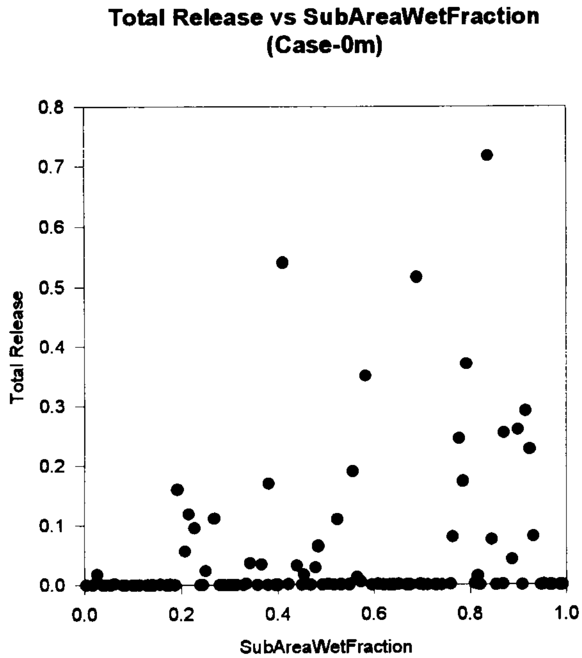
Below is a plot of total release vs the FowFactor for CASE-0m:



Below is a plot of total release vs the FmultFactor for CASE-0m:



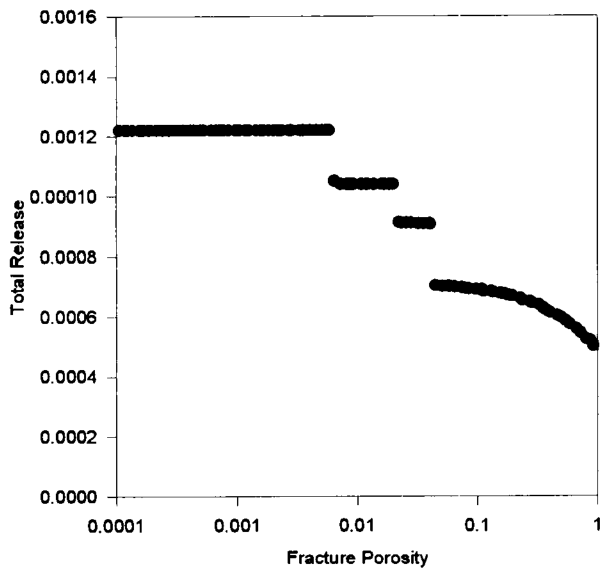
Below is a plot ot total release vs SubAreaWetFraction for CASE-0m:



10/09/97 (CANE)

0815 hrs - The TPA run for CASE-4mm is done. Below is a plot of total release vs fracture porosity for CASE-4mm:

Case-4mm: Total Release vs Fracture Porosity



1300 hrs - A TPA run, to be referred to as COLLOID, was initiated relevant to determining the effect of iron colloids on repository performance. The values of matrix Kds and fracture Rds were allowed to be sampled over certain ranges. The ranges of values used in the simulations were specified by D. Turner, and are listed below:

uniform
MatrixKD_TSw_Am[m3/kg]
1.0 5.0
**
uniform
MatrixKD_TSw_Np[m3/kg]
0.5 1.0
**
constant
MatrixKD_TSw_I[m3/kg]
0.0
**
constant
MatrixKD_TSw_Tc[m3/kg]
1.0000000000000D-05
**
constant
MatrixKD_TSw_Cl[m3/kg]
0.0
**
uniform
MatrixKD_TSw_Cm[m3/kg]
1.0 5.0
**
uniform
MatrixKD_TSw_U[m3/kg]
0.1 1.0
**
uniform
MatrixKD_TSw_Pu[m3/kg]
1.0 5.0
**

uniform
MatrixKD_TSw_Th[m3/kg]
1.0 5.0
**
triangular
MatrixKD_TSw_Ra[m3/kg]
0.0 0.03 0.75
**
uniform
MatrixKD_TSw_Pb[m3/kg]
0.1 1.0
**
constant
MatrixKD_TSw_Cs[m3/kg]
0.36000000000000
**
logtriangular
MatrixKD_TSw_Ni[m3/kg]
0.003 0.9 1.00
**
constant
MatrixKD_TSw_C[m3/kg]
0.0
**
uniform
MatrixKD_TSw_Se[m3/kg]
0.10 1.0
**
uniform
MatrixKD_TSw_Nb[m3/kg]
1.0 5.0
**

uniform
FractureRD_TSw_Am
0.90 1.0
**
uniform
FractureRD_TSw_Np
0.90 1.0
**
constant
FractureRD_TSw_I
1.0
**
constant
FractureRD_TSw_Tc
1.0
**
constant
FractureRD_TSw_Cl
1.0
**
uniform
FractureRD_TSw_Cm
0.90 1.0
**
uniform
FractureRD_TSw_U
0.90 1.0
**
uniform
FractureRD_TSw_Pu
0.90 1.0
**
uniform
FractureRD_TSw_Th
0.90 1.0
**
uniform
FractureRD_TSw_Ra
0.90 1.0
**
uniform
FractureRD_TSw_Pb
0.90 1.0
**
constant
FractureRD_TSw_Cs
1.0
**
uniform
FractureRD_TSw_Ni
0.90 1.0
**
constant
FractureRD_TSw_C
1.0
**
uniform
FractureRD_TSw_Se
0.90 1.0
**
uniform
FractureRD_TSw_Nb
0.90 1.0
**

1600 hrs - A TPA run for CASE-5mm was initiated. This case is similar to CASE-5m, with both matrix porosity and permeability sampled over a range of small values to simulate plugging of the matrix/fracture interface, except that all other parameters were set to their mean values. The results for CASE-5mm, tabulated below, indicate no change in total release if matrix porosity and permeability varies over a range of low values.

MatrixPerm	TotalRel	MatrixPor	TotalRel
2.02E-28	1.22E-03	8.49E-02	1.22E-03
7.31E-26	1.22E-03	9.92E-02	1.22E-03
6.85E-27	1.22E-03	6.21E-02	1.22E-03
1.01E-22	1.22E-03	7.68E-02	1.22E-03
7.46E-23	1.22E-03	7.55E-02	1.22E-03
1.73E-24	1.22E-03	1.12E-01	1.22E-03
8.99E-24	1.22E-03	1.30E-02	1.22E-03
1.50E-22	1.22E-03	3.52E-02	1.22E-03
1.98E-21	1.22E-03	6.75E-02	1.22E-03
3.66E-24	1.22E-03	5.99E-02	1.22E-03
1.32E-24	1.22E-03	1.16E-01	1.22E-03
1.19E-24	1.22E-03	1.10E-01	1.22E-03
1.39E-25	1.22E-03	4.45E-02	1.22E-03
5.48E-25	1.22E-03	7.67E-02	1.22E-03
4.87E-27	1.22E-03	1.07E-01	1.22E-03
1.31E-27	1.22E-03	1.40E-02	1.22E-03
5.99E-27	1.22E-03	2.81E-02	1.22E-03
1.79E-26	1.22E-03	1.09E-01	1.22E-03
3.33E-22	1.22E-03	3.30E-02	1.22E-03
2.22E-25	1.22E-03	3.11E-02	1.22E-03
6.11E-23	1.22E-03	6.97E-02	1.22E-03
2.30E-24	1.22E-03	7.25E-02	1.22E-03
9.54E-27	1.22E-03	1.15E-01	1.22E-03
1.01E-25	1.22E-03	9.80E-02	1.22E-03
3.27E-26	1.22E-03	2.67E-02	1.22E-03
5.46E-24	1.22E-03	7.38E-02	1.22E-03
5.55E-25	1.22E-03	2.00E-02	1.22E-03
4.83E-26	1.22E-03	8.11E-03	1.22E-03
2.74E-27	1.22E-03	7.13E-02	1.22E-03
1.23E-25	1.22E-03	1.20E-01	1.22E-03
7.23E-29	1.22E-03	9.44E-02	1.22E-03
2.49E-26	1.22E-03	1.03E-02	1.22E-03
2.02E-26	1.22E-03	1.00E-01	1.22E-03
3.58E-24	1.22E-03	1.18E-01	1.22E-03
5.03E-24	1.22E-03	3.82E-02	1.22E-03
6.44E-25	1.22E-03	4.33E-02	1.22E-03
1.12E-23	1.22E-03	4.20E-02	1.22E-03
1.47E-24	1.22E-03	7.06E-03	1.22E-03
6.04E-22	1.22E-03	3.39E-02	1.22E-03

3.49E-27	1.22E-03	2.39E-02	1.22E-03
7.47E-24	1.22E-03	5.49E-02	1.22E-03
4.05E-28	1.22E-03	1.66E-02	1.22E-03
2.52E-22	1.22E-03	1.03E-01	1.22E-03
4.46E-23	1.22E-03	1.02E-01	1.22E-03
4.10E-25	1.22E-03	3.18E-02	1.22E-03
1.87E-23	1.22E-03	8.69E-02	1.22E-03
3.18E-23	1.22E-03	8.54E-02	1.22E-03
1.89E-22	1.22E-03	4.61E-02	1.22E-03
6.58E-26	1.22E-03	2.97E-02	1.22E-03
3.08E-25	1.22E-03	2.85E-03	1.22E-03
2.70E-25	1.22E-03	8.28E-02	1.22E-03
2.40E-25	1.22E-03	6.41E-02	1.22E-03
1.98E-24	1.22E-03	1.14E-01	1.22E-03
8.94E-22	1.22E-03	1.14E-02	1.22E-03
2.76E-26	1.22E-03	3.62E-02	1.22E-03
2.06E-25	1.22E-03	1.47E-03	1.22E-03
1.06E-20	1.22E-03	9.34E-02	1.22E-03
5.42E-28	1.22E-03	1.80E-02	1.22E-03
1.79E-25	1.22E-03	7.96E-02	1.22E-03
4.34E-27	1.22E-03	8.91E-02	1.22E-03
3.83E-21	1.22E-03	6.64E-02	1.22E-03
1.59E-26	1.22E-03	5.36E-02	1.22E-03
2.26E-24	1.22E-03	8.06E-02	1.22E-03
1.43E-26	1.22E-03	9.18E-02	1.22E-03
1.35E-25	1.22E-03	4.96E-02	1.22E-03
4.91E-25	1.22E-03	6.05E-02	1.22E-03
1.59E-25	1.22E-03	5.88E-02	1.22E-03
9.57E-26	1.22E-03	7.82E-02	1.22E-03
8.96E-25	1.22E-03	2.41E-02	1.22E-03
2.33E-27	1.22E-03	8.22E-02	1.22E-03
4.15E-24	1.22E-03	9.28E-03	1.22E-03

3.54E-25	1.22E-03	2.09E-02	1.22E-03
1.24E-29	1.22E-03	1.06E-01	1.22E-03
1.18E-23	1.22E-03	5.64E-02	1.22E-03
2.60E-24	1.22E-03	5.57E-02	1.22E-03
1.81E-27	1.22E-03	2.55E-02	1.22E-03
8.21E-23	1.22E-03	4.12E-03	1.22E-03
5.88E-26	1.22E-03	1.13E-01	1.22E-03
1.09E-28	1.22E-03	5.21E-02	1.22E-03
8.99E-28	1.22E-03	9.04E-02	1.22E-03
8.13E-25	1.22E-03	1.47E-02	1.22E-03
1.13E-24	1.22E-03	6.87E-02	1.22E-03
7.57E-25	1.22E-03	4.75E-02	1.22E-03
1.48E-23	1.22E-03	3.89E-02	1.22E-03
2.18E-23	1.22E-03	9.66E-02	1.22E-03
5.15E-26	1.22E-03	1.88E-02	1.22E-03
1.21E-26	1.22E-03	5.09E-02	1.22E-03
3.59E-26	1.22E-03	1.06E-01	1.22E-03
8.66E-24	1.22E-03	4.86E-02	1.22E-03
1.68E-23	1.22E-03	3.99E-02	1.22E-03
3.83E-25	1.22E-03	2.24E-02	1.22E-03
8.31E-28	1.22E-03	1.10E-03	1.22E-03
9.88E-25	1.22E-03	4.15E-02	1.22E-03
3.07E-24	1.22E-03	9.60E-02	1.22E-03
4.31E-26	1.22E-03	8.84E-02	1.22E-03
8.12E-26	1.22E-03	6.24E-02	1.22E-03
4.19E-23	1.22E-03	1.12E-01	1.22E-03
8.45E-27	1.22E-03	6.51E-02	1.22E-03
5.98E-24	1.22E-03	1.04E-01	1.22E-03
2.91E-23	1.22E-03	4.99E-03	1.22E-03

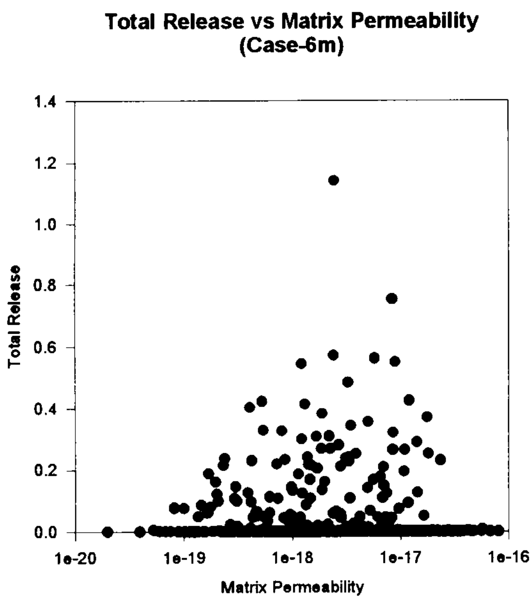
10/10/97 (CANE)

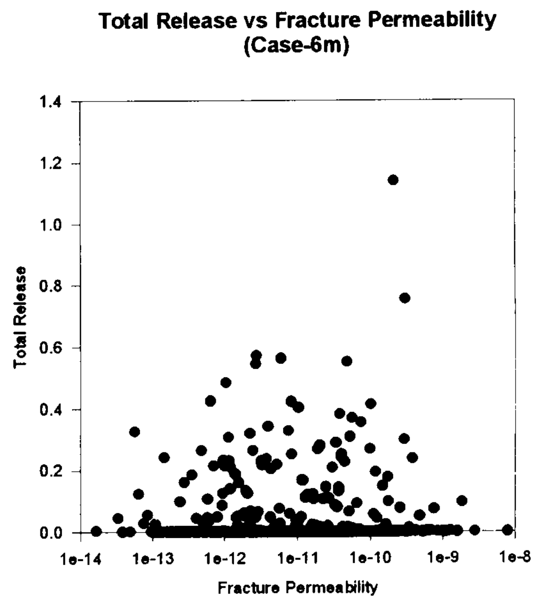
0930 hr - TPA runs for CASE-7mm and CASE-8mm were initiated to determine the effect of fracture plugging on repository performance. CASE-7mm is similar to CASE-3mm, except that the fracture permeability is sampled from 1.0e-30 (approximating zero) to 8.0e-13 (the mean value). CASE-8mm is similar to CASE4mm, except that fracture porosity is sampled from 1.0e-30 to 1.0e-3 (the mean value).

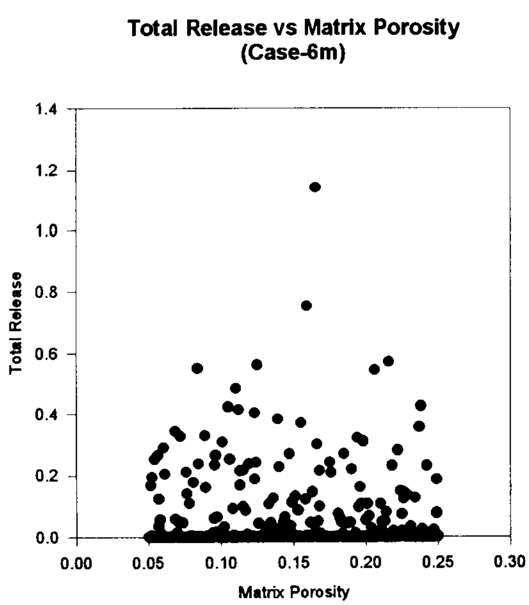
1300 hrs - Based on discussions during a telecon yesterday with NRC PA (Tim McCartin, V. Colten-Bradley), the cumrel.res files were checked to see if the parameters of interest in CANE had an effect on cumulative release from the unsaturated zone. The Fortran program READCUMR.FOR was modified to calculate the total curies released from the unsaturated zone based on the individual radionuclide release for each realization. The results for CASE-1mm, -2mm, -3mm, -4mm, and -5mm show that the unsat. zone cumulative release is insensitive to the four parameters studied. However, the results for CASE-6mm are different from the others - the total release from the unsat. zone in many cases are one or two orders of magnitude higher than for CASE-1mm to -5mm, although many CASE-6mm results are equal to zero. Thus, there appears to

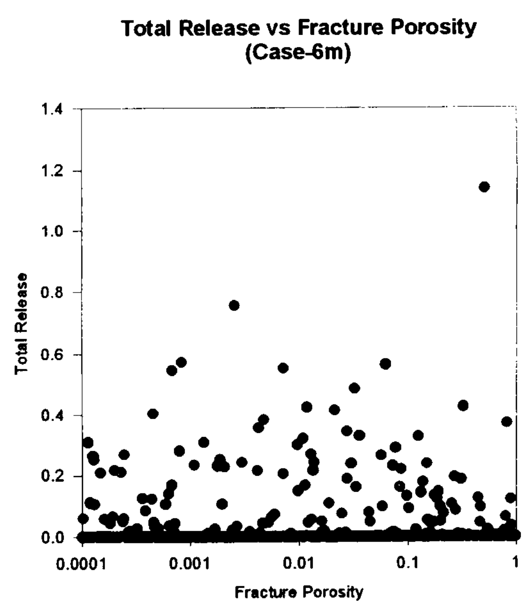
be some synergistic effect among the four parameters varied in CASE-6mm. **HOLD IT!** A check of the samplpar.hdr file for CASE-6mm indicates that **ten** parameters were sampled, instead of four. The mean values were not set for the six parameters originally sampled in the tpa.inp.meanvalues1 case. Thus the results really should be referred to as **CASE-6m**. Another TPA run will have to be done for CASE-6mm.

Below is a plot of total release vs matrix permeability, matrix porosity, fracture permeability, and fracture porosity for CASE-6m:







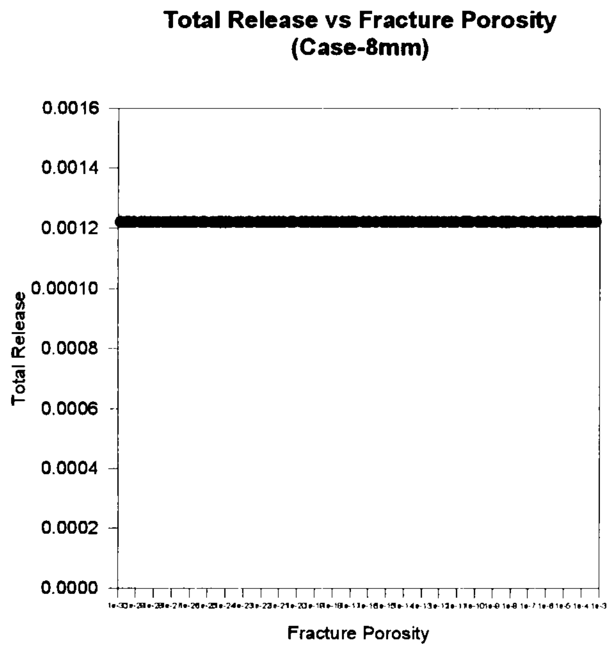


10/13/97 (CANE)

0815 hrs - TPA runs for CASE-7mm and CASE-8mm are complete. However, the samplpar.res output file for CASE7mm indicates that only 66 realizations were completed instead of 100 specified in the input file. No error messages were listed. Thus, another TPA run for CASE7mm will be initiated.

0830 hrs - TPA run for CASE-6mm was initiated.

For CASE-8mm, below is a plot of total release vs fracture porosity:



1500 hrs - A second TPA run for CASE-7mm was initiated.

1530 hrs - The second TPA run for CASE-7mm terminated after the 7th realization due to an arithmetic error. Could be due to the use of 1.0e-30 as the lower bound for FracturePermeability of Tsw. The input file was modified to change the lower bound to 1.0e-25. The third run for CASE-7mm was initiated.

10/14/97 (CANE)

0830 hrs - The TPA runs for CASE-7mm and CASE-6mm terminated due to errors. The system manager (R. Juhl) rebooted the computer system (Bigbend).

0945 hrs - CASE-7mm and CASE-6mm were rerun.

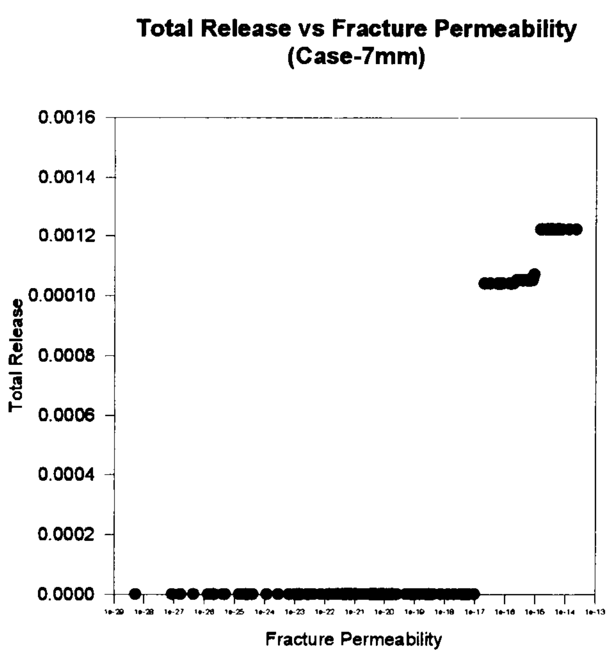
1300 hrs - The TPA run for CASE-7mm terminated due to an arithmetic error in NEFTRAN. S. Mohanty suggested a probable cause of the abrupt termination. He said that it is likely due to the very low value of the fracture permeability (lower bound = 1.0e-25) compared to the value of matrix permeability (constant at 2.0e-19). He suggested using a fracture permeability value equal to that of the matrix permeability. This was done. The tpa.inp file was changed to set fracture permeability, the only parameter to be sampled, equal to 2.0e-19. Case-7mm was rerun.

1600 hrs - The TPA run for CASE-7mm terminated again with the same error message as in previous ones:
>>>Error in runnefmks <<<
NEFTRAN failure. Status = 34304.
Note: the following IEEE floating-point arithmetic exception exceptions occurred and were never cleared; see ieee_flags(3M): Inexact; Underflow

The tpa.inp file was modified. The value of fracture permeability was changed to 1.0e-19 from 2.0e-19. The code was rerun.

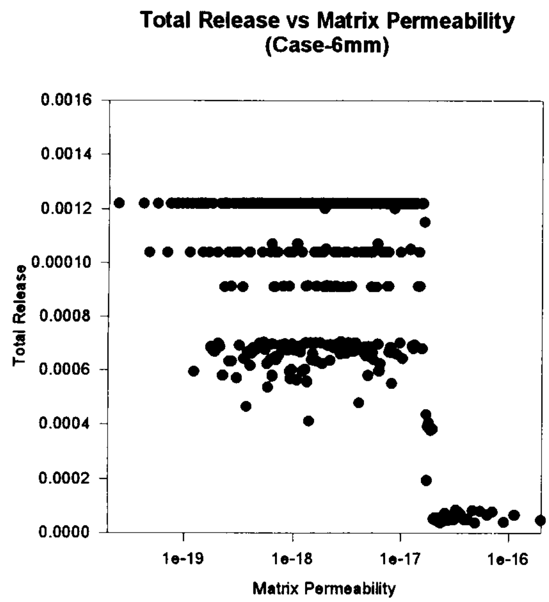
10/15/97 (CANE)

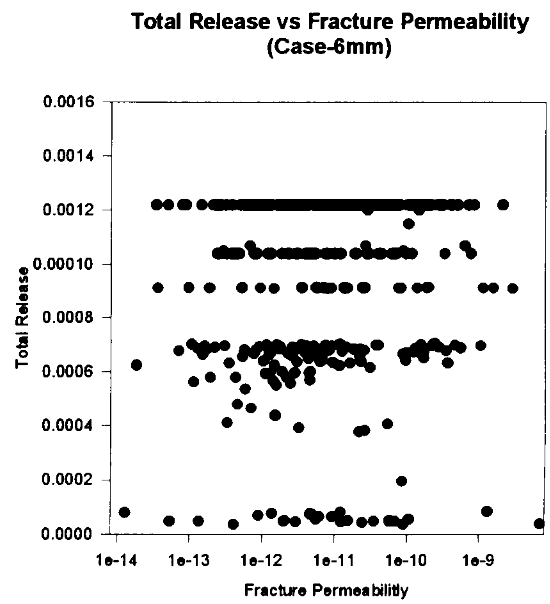
0900 hrs - The TPA run for CASE-6mm is complete. However, the run for CASE-7mm again terminated with an error message as in previous attempts. The job terminated at the 28th realization. At this point it is not clear the real reason for early termination of the CASE-7mm runs. The output from two terminated runs, one with 66 realizations completed and another with 28 realizations completed, were combined to generate the following plot of total release vs fracture permeability:

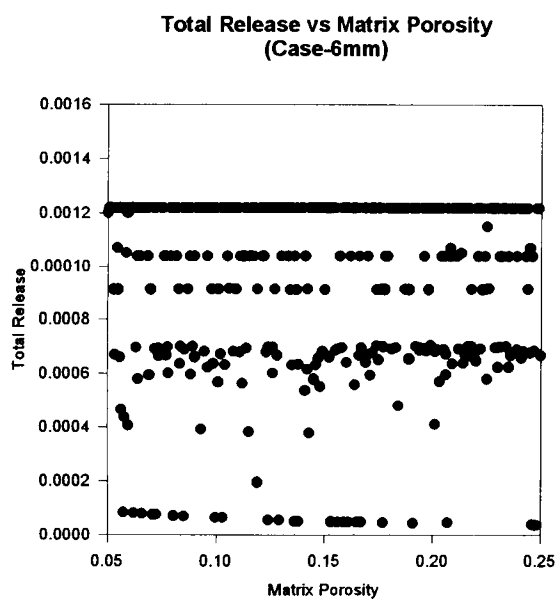


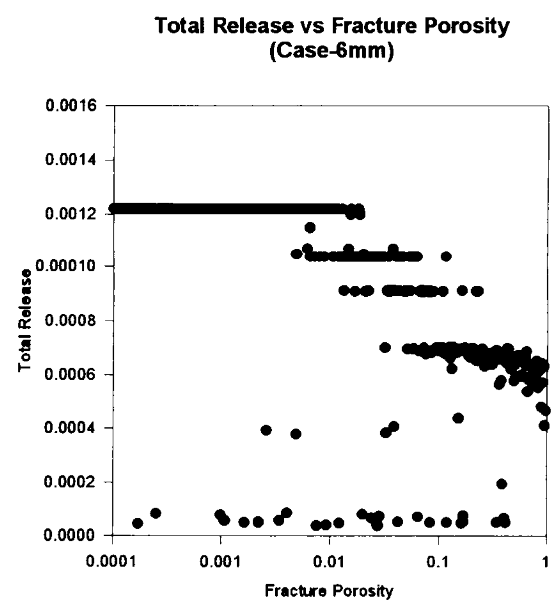
10/16/97 (CANE)

1000 hrs - Below are plots of total release vs each of the four parameters allowed to be sampled in CASE-6mm: matrix permeability, matrix porosity, fracture permeability, and fracture porosity:





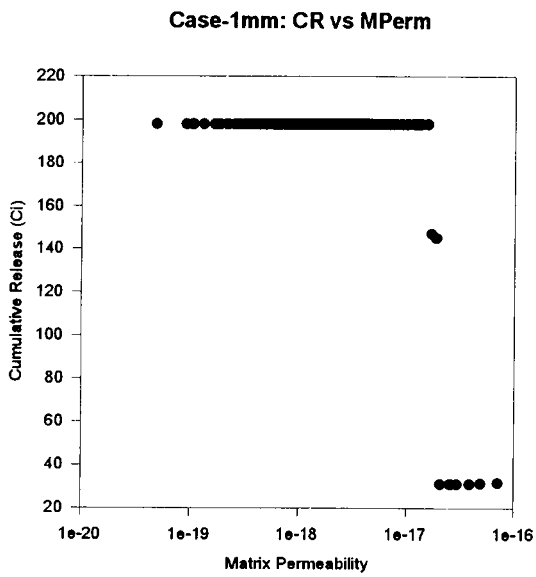


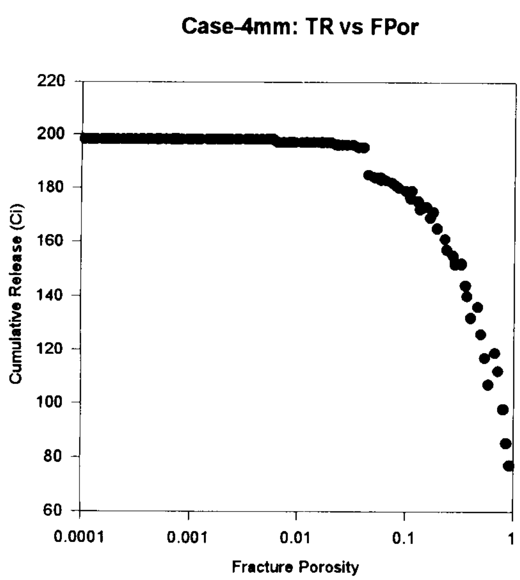


10/22/97 (CANE)

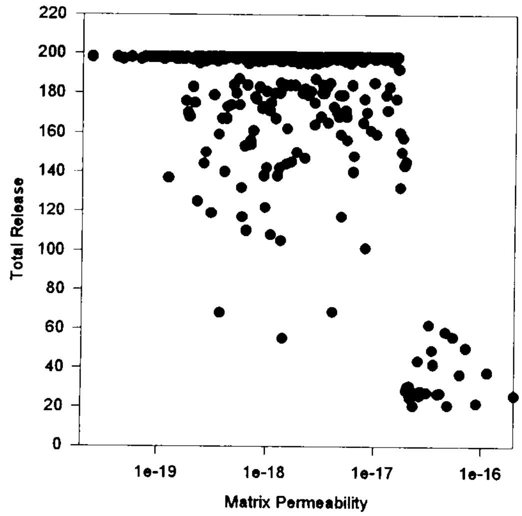
Below are plots of cumulative cumulative release from the unsaturated zone at 10,000 yrs versus matrix permeability (CASE-1mm) and versus fracture porosity (CASE-4mm). Following those are

plots of cumulative release vs matrix permeability/porosity and fracture permeability/porosity for CASE-6mm. The cumulative release from UZ for CASE-2mm, Case-3mm, Case-5mm, and Case-8mm are all the same constant value for all realizations: 198 ci. No values were generated in the CASE-7mm cumrel.res file.

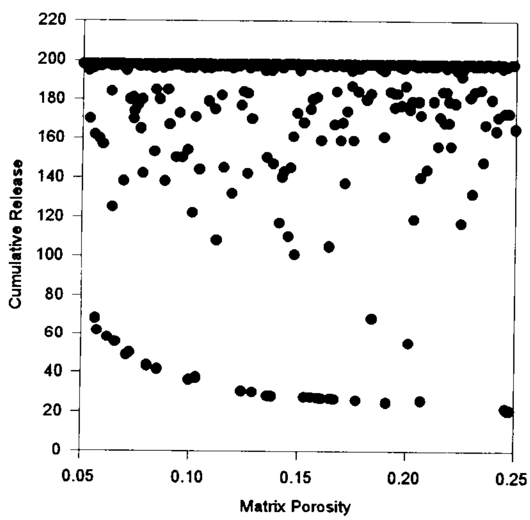


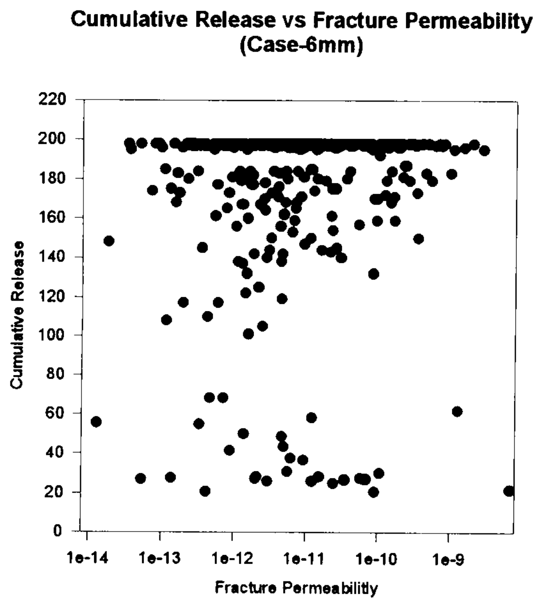


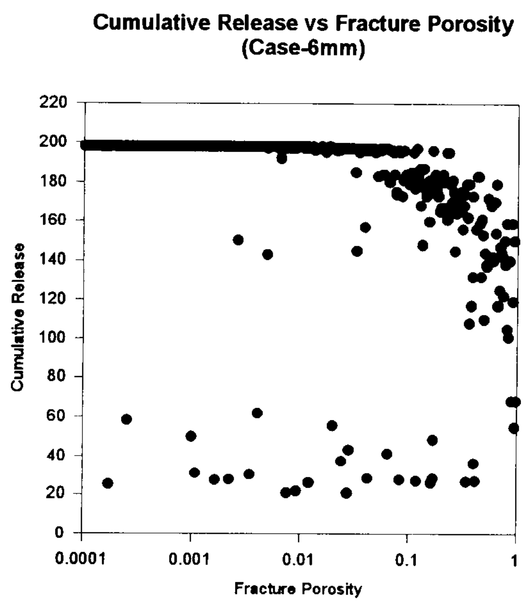
Cumulative Release vs Matrix Permeability (Case-6mm)



Cumulative Release vs Matrix Porosity (Case-6mm)




Cumulative Release vs Fracture Permeability
(Case-6mm)
220
200
180
160
140
120
100
80
60
40
20
0
Cumulative Release
1e-14
1e-13
1e-12
1e-11
1e-10
1e-9
Fracture Permeabilitiy


Cumulative Release vs Fracture Porosity
(Case-6mm)
220
200
180
160
140
120
100
80
60
40
20
0
Cumulative Release
0.0001
0.001
0.01
0.1
1
Fracture Porosity