SCIENTIFIC NOTEBOOK

612-22E

by

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INITIAL ENTRIES

Scientific Notebook: #612E

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Title: TPA 5.0 Code Development

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Objective:

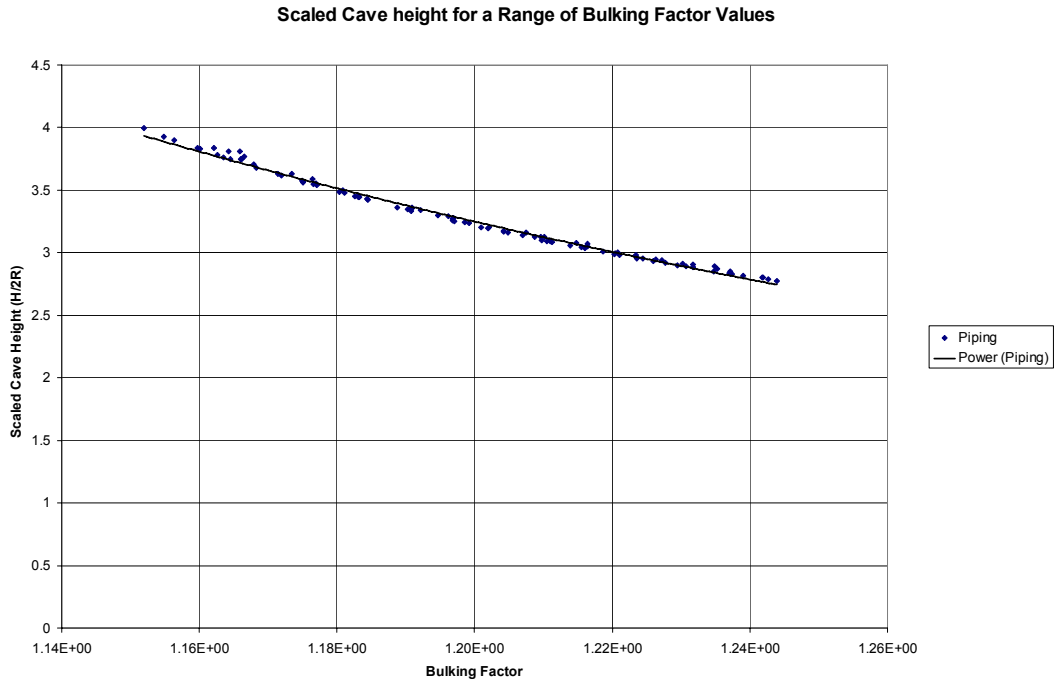
This scientific notebook will document the work performed in the development and validation of the TPA code.

7.5.06

Tests were run for driftfail from TPA5.1BetaC. Several 100-realization long runs of the TPA code are to be performed. The output will then be graphed and compared to page 7 of Fernando Ferrante's scientific notebook (#782 E) which contains graphs he made in Matlab. Seismicity was turned off and the maximum drift height was extracted from driftfail.rlt. In the graphs height is scaled by H/2R where R is 2.75m. The DS width is 2.505m and the DS height is 2.521m. To get the correct bulking factor, since lhs.out gives bulking factors for each rock type, the two were combined with 85% of rock type 1 and 15% of rock type 2.

7.6.06

Graphed the output from the Driftfail test. The graphs do not compare to Fernando's (pg 7). All the cave height values are generally higher than in the reference which has a range of 2.7m- 2.2m in cave height compared to values of 3.6m to 2.8m across the same span of bulking factors. This graph only shows the piping geometry which is when the drift degrades like a chimney. The line shown is a trendline made by using the "power" option.



Figure

7.11.06

Mechfail tests performed are as follows:
All have 450 realizations and are run for 100,000 years.

Base Case:
Both seismicity and drift degradation are turned on. Can take the tpa.inp file "as is" and only change the years and number of realizations.
No Seismic:
Turned off the value of SeismicDisruptiveScenarioFlag in tpa.inp
No Drift Degradation:
Turned off the value DriftDegradationScenarioFlag in tpa.inp
Special Case:
tpa.inp provided by George Adams with correlated parameters

Note: TPA output shows the label "MAPE" for seismic event size. This is the mean annual probability of exceedance. References refer to the "MAFE" or mean annual frequency of exceedance. For these purposes, the two are interchangeable.

Edited the WPSfail spreadsheet to include seismic information for the base case run of the TPA code. This includes finding the distribution density for the MAFE values, which should match with the copy of page 5-20 of Drip Shield-Waste Package Mechanical Interaction shown below:

$P(\text{MAFE} < 10^{-4}) = 100.0$ percent
$P(10^{-5} < \text{MAFE} < 10^{-4}) = 90.1$ percent
$P(10^{-6} < \text{MAFE} < 10^{-5}) = 9.2$ percent
$P(10^{-7} < \text{MAFE} < 10^{-6}) = 0.7$ percent
$P(\text{MAFE} < 10^{-7}) = 0.08$ percent

TPA run results (realizations with some type of failure in them)

	Number of Columns with the MAFE value	% of MAFE distribution
MAFE 1E-4:	0	0.0%
MAFE 1E-5:	1264	85.9%
MAFE 1E-6:	176	12.0%

MAFE 1E-7:	32	2.2%

The code does not allow for events in the range of 1E-4, however, like the reference, it is true that 100% of the MAFEs are greater than 1E-4. The summary of the table data in terms of the reference can be represented as:

P(MAFE < 1E-4) = 100%
P(1E-5 < MAFE < 1E-4) = 85.9%
P(1E-6 < MAFE <1E-5)= 12.0%
P(1E-7 < MAFE <1E-6) = 2.2%
P(MAFE < 1E-7) = 0%

7.19.06

MAFE vs. percent waste packages failed was graphed as shown below. These results were lower than expected, however. One realization for example experienced a MAFE value of 9.19E-08, and all of the waste packages did NOT fail. The Capacity for one subarea in this realization, in which no packets failed due to the seismic event was 1.49529E+04 kPA while the dynamic pressure was 3.06944E+03 kPA. The reason for these differences may be the drift geometry. Some events were a trapezoid geometry and therefore experienced less waste package failures.

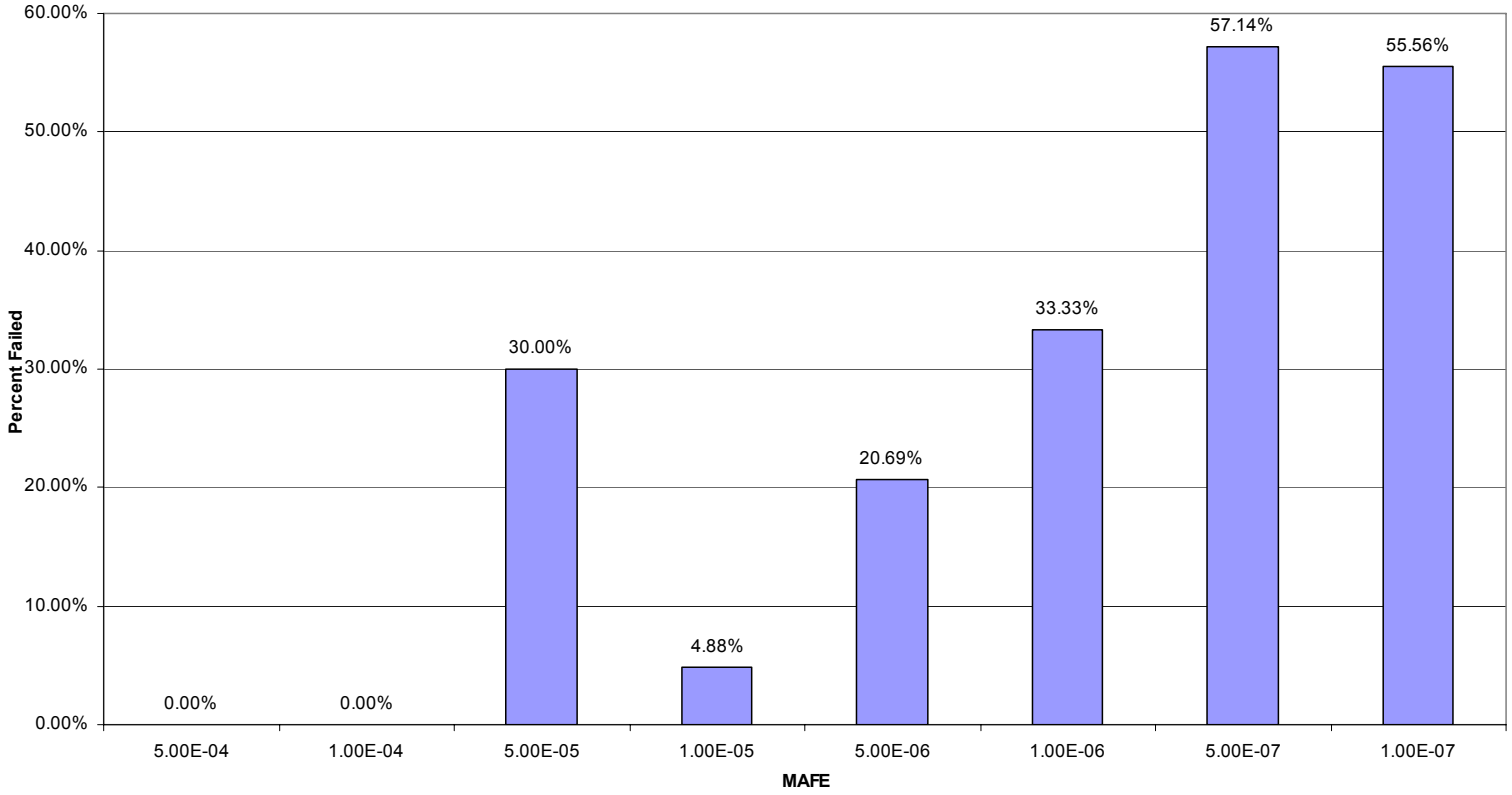


Figure 2

Note that each bar represents a range from the listed value to the preceding bar's value.

100% failures were expected in cases with a MAFE to the degree of 1.0E-7 and below. This expectation is inaccurate because of the combination of a low MAFE with a high bulking factors and low contact angles will prevent total WP failure. Failure in this case of this data is defined as a seismic event that produced <u>any</u> number of waste package failures. It is not necessary that all waste packages fail. This graph measures the probability of failure falling in one of the

specified bins *once* it has been determined that failure occured. For the bin representing the MAFE range 5.0 x10^{-5} -1.0 x 10^{-4} there is an unexpected leap in the percentage. This is currently under investigation.

Code to obtain the values used in Figure 2 (found in file Macros.xls hosted on machine Storm):

```
'Macro to get the average percent failure for each bin
Sub mean_percentage_histogram()
   Dim count As Integer

   Dim mape4 As Integer
   Dim mape5 As Integer
   Dim mape6 As Integer
   Dim mape7 As Integer
   Dim mape4_5 As Integer
   Dim mape5_5 As Integer
   Dim mape6_5 As Integer
   Dim mape7_5 As Integer

   Dim tot4 As Integer
   Dim tot5 As Integer
   Dim tot6 As Integer
   Dim tot7 As Integer
   Dim tot4_5 As Integer
   Dim tot5_5 As Integer
   Dim tot6_5 As Integer
   Dim tot7_5 As Integer

   mape4 = 0                    'for mape(mafe) totals
   mape5 = 0
   mape6 = 0
   mape7 = 0
   mape4_5 = 0
   mape5_5 = 0
   mape6_5 = 0
   mape7_5 = 0

   tot4 = 0
   tot5 = 0
   tot6 = 0
   tot7 = 0
   tot4_5 = 0
   tot5_5 = 0
   tot6_5 = 0
   tot7_5 = 0

   Range("AB6").Select

   Do Until count = 50
```

```
count = 0

    If Selection.Value >= 0.0005 And Selection.Value < 0.001 Then
        mape4 = mape4 + 1
        tot4 = tot4 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.0001 And Selection.Value < 0.0005 Then
        mape4_5 = mape4_5 + 1
        tot4_5 = tot4_5 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.00005 And Selection.Value < 0.0001 Then
        mape5 = mape5 + 1
        tot5 = tot5 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.00001 And Selection.Value < 0.00005 Then
        mape5_5 = mape5_5 + 1
        tot5_5 = tot5_5 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.000005 And Selection.Value < 0.00001 Then
        mape6 = mape6 + 1
        tot6 = tot6 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.000001 And Selection.Value < 0.000005 Then
        mape6_5 = mape6_5 + 1
        tot6_5 = tot6_5 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.0000005 And Selection.Value < 0.000001 Then
        mape7 = mape7 + 1
        tot7 = tot7 + Selection.Offset(0, 2).Value
    End If

    If Selection.Value >= 0.0000001 And Selection.Value < 0.0000005 Then
        mape7_5 = mape7_5 + 1
        tot7_5 = tot7_5 + Selection.Offset(0, 2).Value
    End If

    Selection.Offset(1, 0).Select
    Do Until count = 50 Or Selection.Value <> ""
        Selection.Offset(1, 0).Select
        count = count + 1
    Loop

Loop
```

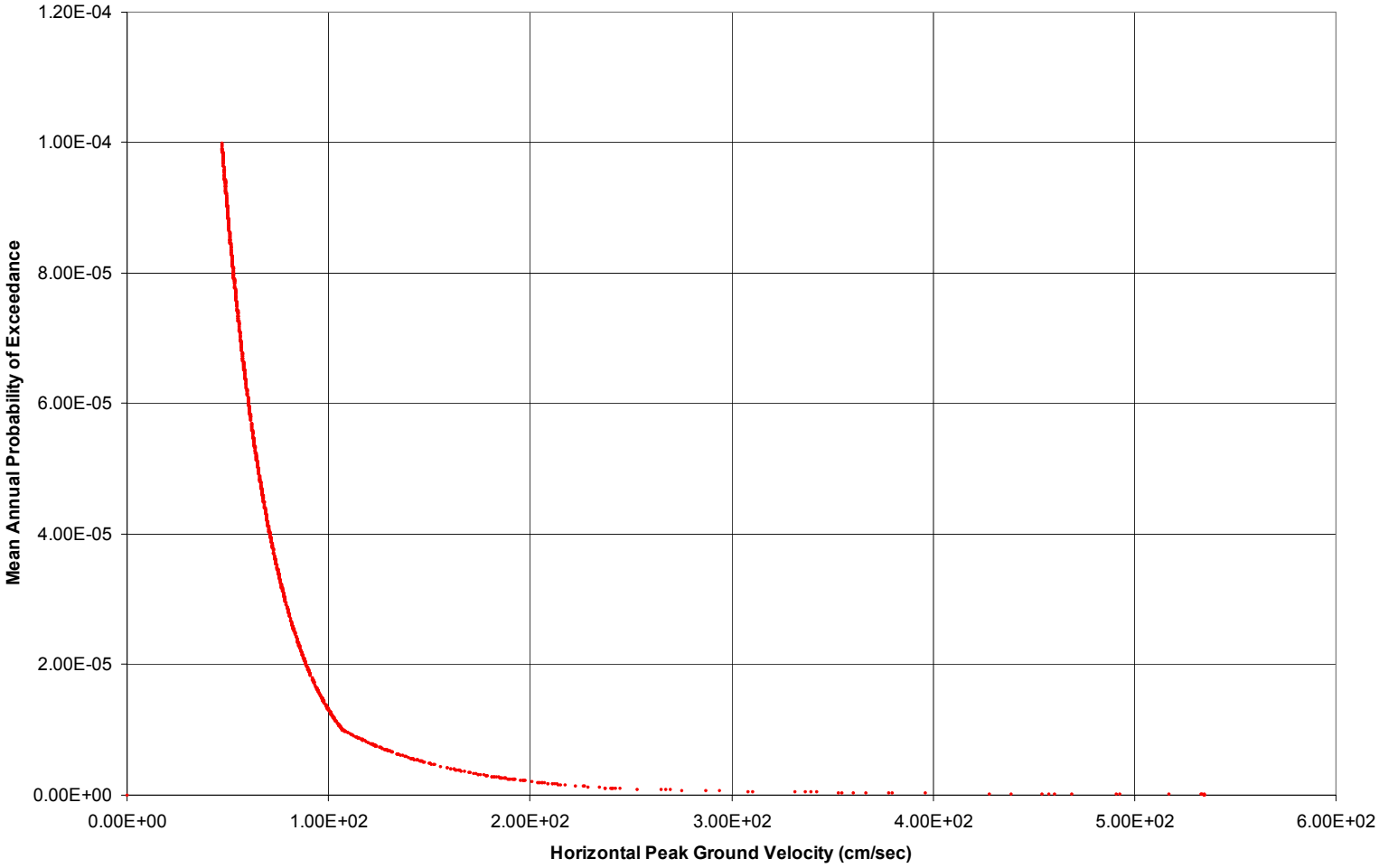
```
    Selection.Offset(-48, 0).Select  'go back up to where the data stops to begin output

    'print out the average pgv values
    Selection.Offset(4, 0).Select
    Selection.Value = "PGA E-4:"
    Selection.Offset(0, 1).Value = 0 'tot4 / mape4
    Selection.Offset(0, 2).Value = mape4


    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-4.5:"
    Selection.Offset(0, 1).Value = 0 'tot4 / mape4
    Selection.Offset(0, 2).Value = mape4_5

    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-5:"
    Selection.Offset(0, 1).Value = tot5 / mape5
    Selection.Offset(0, 2).Value = mape5

    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-5.5:"
    Selection.Offset(0, 1).Value = tot5_5 / mape5_5
    Selection.Offset(0, 2).Value = mape5_5

    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-6:"
    Selection.Offset(0, 1).Value = tot6 / mape6
    Selection.Offset(0, 2).Value = mape6

    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-6.5:"
    Selection.Offset(0, 1).Value = tot6_5 / mape6_5
    Selection.Offset(0, 2).Value = mape6_5

    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-7:"
    Selection.Offset(0, 1).Value = tot7 / mape7
    Selection.Offset(0, 2).Value = mape7

    Selection.Offset(1, 0).Select
    Selection.Value = "PGA E-7.5:"
    Selection.Offset(0, 1).Value = tot7_5 / mape7_5
    Selection.Offset(0, 2).Value = mape7_5
End Sub
```

Note: Statements like Selection.Offset(0, 2) are referencing a cell in an excel sheet from the point of view of the currently selected cell. The arguments are (y,x), unlike most coordinates.

Selection.Offset(0, 2) would reference the cell 2 to the right of the selected cell. Negative values go to the left.

This graph of unbounded hazard curves at the emplacement level when compared to a similar one on page 5-17 of the Mechfail report, shows many differences. The curve of the data is concave in this case, whereas it is convex in the reference.

Figure 3



The problem with the graph is merely the scale, rather than the information. When set to logarithmic, the data matches the reference material for the unbounded hazard curves at the emplacement level. The corrected graph below is convex as expected.

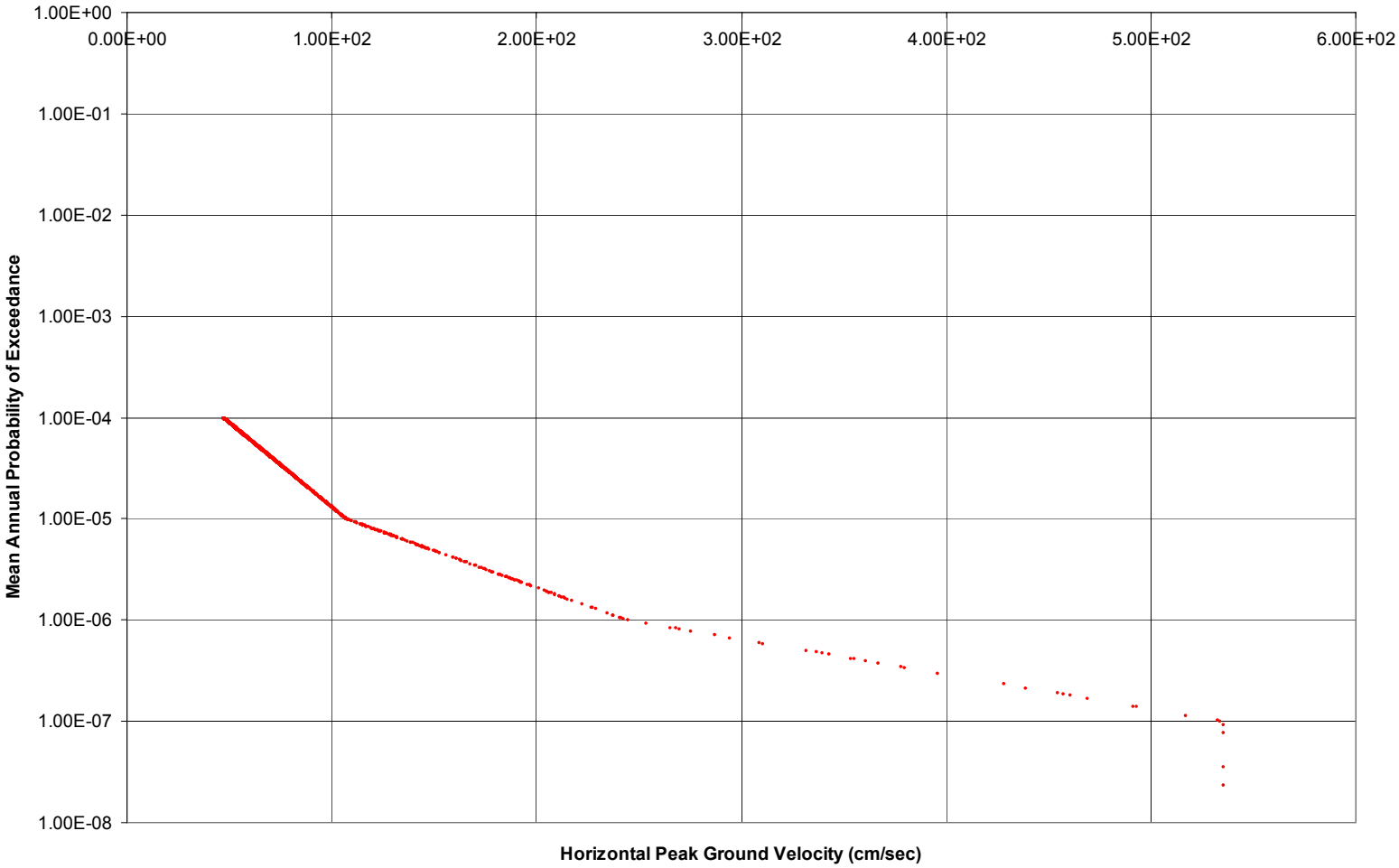


Figure 4

7.24.06

Page 5-3 of Ibarra, L. et. al. identifies the bulking factor distribution as follows:

P(BF<1.1) = 0.08 percent
P(BF<1.15) = 8.0 percent
P(BF<1.25) = 90.6 percent
P(1.15<BF<1.25) = 82.5 percent
P(BF<1.35) = 100.0 percent

The TPA run results show the actual distribution as:

P(BF<1.1)=	0	0%
P(BF<1.15)=	0	0%
P(BF<1.25)=	9000	100%
P(1.15<BF<1.25)=	9000	100%
P(BF<1.35)=	9000	100%
Total:	9000	

Note that included in the total amount of bulking factors is a factor for each of two rock types and each of 10 subareas totaling 9000 bulking factors.
(450 realizations*10 subareas*2 rock types)

The reason for these discrepancies is because the minimum bulking factor is set to 1.15 and the maximum is set to 1.25 in the tpa.inp. The reference assumes that 82% of the bulking factor values will fall between 1.15 and 1.25, whereas the code assumes all of them will. Page 2 of the mechfail primer document specifies that bulking factor should only be in the range of 1.15 and 1.25. Ibarra, L. et. al. also states that the bulking factor should have a mean of 1.2 and a standard deviation of 0.037. In this aspect, the data matches. The bulking factor data, located in moreMECH.xls, has a mean of 1.2 and a standard deviation of 0.029. The difference in deviation can be attributed to not using as large a range of values. I believe the TPA code matches the intentions of developers and the listing in Ibarra, L. Et. Al. Is an unbounded representation of bulking factors.

Page 5-3 Also identifies the probability density areas for different drift degradation times as:

$P(t < 400$ years) – 0.3 percent
$P(t < 500$ years) – 3.9 percent
$P(t < 1{,}000$ years) – 89.5 percent
$P(t < 1{,}280$ years) – 99.0 percent

The TPA run results show the distribution of drift degradation times as:

400 Years:	280	3.1%	P(t<400 years) 3.1%
500 Years:	95	1.1%	P(t<500 years) 4.2%
1000 Years:	6883	76.5%	P(t<1000 years) 80.6%
1280 Years:	1555	17.3%	P(t<1280 years) 97.9%
More than 1280:	187	2.1%	
Total:	9000		

All the intervals agree within 9%. The largest discrepancy being with times less than 1000 years which differs by 8.9%. The occurrence of seismic events which are not part of the tpa.inp degradation time distribution may be part of the reason why these values do not match as closely as some of the other variables.

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7.26.06

For the following data, I extracted my data from the readsp2.exe created by George Adams. The program takes a variable to search for in its readsp.inp file. In order to run, the files samplpar.res and samplpar.hdr need to be placed in the same directory as the .exe and .inp files.

Lateral-to-vertical load pressure is found in the TPA code as the variable DripShieldHorizToVertLoadRatioRock1Subarea_1 (with the subarea number changing). This was put into readsp.inp to extract the ratios for each subarea of each realization. Page 5-5 of reference material indicates the probability density areas for lateral-to-vertical load pressure ratios at certain intervals as:

$P(Ph/Pv < 0.20)$ – 0.17 percent

$P(Ph/Pv < 0.50)$ – 50.0 percent

$P(Ph/Pv < 0.80)$ – 99.8 percent

$P(Ph/Pv < 1.00)$ – 100.0 percent

The data retrieved from the TPA run shows the probability density for this horizontal (lateral) to vertical load ratio to be:

P(Ph/Pv < 0.20) =	7	0.2%
P(Ph/Pv < 0.50) =	2253	50.1%
P(Ph/Pv < 0.80) =	4495	99.9%
P(Ph/Pv < 1.00) =	4500	100.0%
Total:	4500	

These results closely correspond with the reference values.

TEMPERATURE MULTIPLIER

Temperature multiplier is not a sampled value like many of the other mechfail inputs. Instead it is produced in the code. Page 5-7 of the reference catalogs the discrete values for temperature multipliers as follows:

F_{temp} ' 1.0 for $T \leq$ 150 ˚C [302 ˚F]

F_{temp} ' 0.78 for T = 260 ˚C [500 ˚F]

F_{temp} ' 0.64 for $T \geq$ 316 ˚C [601 ˚F]

The value of the temperature multiplier was not recorded anywhere, and therefore, could not be analyzed, however, the following code from the function dtempFactor in mechfail.f shows how the variable is determined. This function returns the temperature multiplier that modifies ds capacity.

```
      DOUBLE PRECISION dtempDS

c     Adjust the capacity for the temperature of the drip shield
      IF(dtempDS .LE. 150.0D0)THEN
        dtempFactor = 1.0D0
      ELSEIF(dtempDS .LE. 260.0D0)THEN

c       Interpolate between 0.78 and 1.0 for temperatures of
c       260 C and 150 C respectively
c       0.78 - 1.0   factor - 1.0
c       ---------- = -------------
c       260 - 150    dtempDS - 150

        dtempFactor =(-2.0D-3 * (dtempDS - 150.0D0) + 1.0D0)

      ELSEIF(dtempDS .LT. 316.0D0)THEN
c       Interploate between 0.64 and 0.78 for temperatures of
c       316 C and 260 C respectively
c       0.64 - 0.78   factor - 0.78
c       ----------- = -------------
c       316 - 260     dtempDS - 260

        dtempFactor = (-2.5D-3 * (dtempDS - 260.0D0) + 0.78)

      ELSE
        dtempFactor = 0.64D0
      ENDIF
```

CONTACT ANGLE

Page 5-11 indicates probabilities of occurrence for some contact angle (α) at intervals of interest

$P(-30 \leq \alpha \leq 30)$ – 99.7 percent

$P(-20 \leq \alpha \leq 20)$ – 95.5 percent

$P(-10 \leq \alpha \leq 10)$ – 68.3 percent

$P(-5 \leq \alpha \leq 5)$ – 38.3 percent

The variable name: ContactAngleSubarea_1[degrees] was input into readsp.inp to retrieve the values needed to perform this examination. The TPA run results indicated the following probabilities for the occurrence of a contact angle:

$P(-30< \alpha <30)$	4491	99.8%
$P(-20< \alpha <20)$	4297	95.5%
$P(-10< \alpha <10)$	3079	68.4%
$P(-5< \alpha <5)$	1727	38.4%
Total:	4500	

Note that the number of contact angles used for this probability extraction comes from the 10 subareas for each of 450 realizations (450 realizations * 10 subareas). These results closely match those of the reference material and therefore the sampled values for contact angle are successfully accurate.

8.7.06

Discussion of the mechfail results revealed that abnormal percent failures may not be abnormal depending on the contact angle. There is a high probability of contact angles between -10 and 10 degrees which creates higher resilience for the capacity. In some cases, the PGA (peak ground acceleration) and PGV (peak ground velocity) do not correspond as they should, however the two values are reached independently so the possibility of this occurring is present.

Many of the large events (those with lower MAFE values) and small percent failures can be explained due to their proximity to the next MAFE interval.

MAFE Bin	# of Seismic events	Percentage of Seismic events	Number with partial WP failures	Percentage of partial WP failures
[$1x10^{-4}$ $1x10^{-5}$]	4036	90%	51	1.3%
[$1x10^{-5}$ $1x10^{-6}$]	405	9%	74	18%
[$1x10^{-6}$ $1x10^{-7}$]	43	.9%	25	58%
[$1x10^{-7}$ $1x10^{-8}$]	4	.09%	4	100%

8.10.06

Tests on Ebsfail/Weldfail began, however they are still in process. The object of this test is to prove that 30% of realizations experience weld failures and 5% experience surface failures. TPA5.1BetaD must be run instead of BetaC because new additions allow the types of corrosion failure to be distinguished. The variables WeldCritChlorideConc and CritChlorideConcForFirstLayer can be disabled by setting them to a high number such as 100. In the case of WeldCritChlorideConc which contains a range, the variable was set as follows:

loguniform

WeldCritChlorideConc[mol/L]

100.0, 101.0

The preceding variables can be changed in tpa.inp.

Three test cases were run:

1.A base case with both types of localized corrosion on

2. A case with weld corrosion turned off leaving only surface corrosion (by changing WeldCritChlorideConc to 100)

3. A case with surface corrosion turned off leaving only weld corrosion (by changing CritChlorideConcForFirstLayer to 100)

The first time we ran the series of tests, the results were inconclusive. An excerpt of the results are shown below. Complete results can be found in ebs_weldfail.xls on the machine Storm. Notice that surface failures are overshadowed by Weld Failures when both are present in the base case. Performance Assessment staff have verified that this can be expected.

Realization		Base Case		Only Weld		Only Surface
1		3532		3532		1062
2		1793		1793		0
3		2909		2909		0
4		723		723		0
5		3430		3430		0
6		6444		6444		3540
7		1405		1405		0

8		5775		5775		1452
9		6010		6010		2904
10		4482		4482		2855

It was then determined that only one subarea should be examined over the 500 realizations. The test will be run again under these circumstances.

Entries into Scientific Notebook #612-22E for pages 3-20 have been made by Nicole Epps.

It should be noted that periodic printing of sections of this notebook may result in non-sequential page numbers even though there is no missing content. This may be caused by different printers having different fonts from the ones used for the original document.

No original text entered into this Scientific Notebook has been removed.

Nicole Epps August 11, 2006.

NO Further Entries

JR Wu 1/28/10
manager, PA Group

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 612E-22

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