308 --- Q200304070004
Scientific Notebook # 298: TPA Simulations of WP Performance and Sensitivity Analyses

LABORATORY NOTEBOOK

CNWRA/SwRI

NOTEBOOK NO. ______________

ISSUED TO SEAN BROSSIA

ON ______________ **19** ____

DEPARTMENT DIV 20

RETURNED ______________ **19** ____

20-1402-571

Container Life and Source Term (TPA)

CNWRA CONTROLLED COPY 298

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INSTRUCTIONS

1. **The primary purpose of this notebook is to protect your and the Company's Patent-Rights by keeping records of all original work in a form acceptable as evidence if any legal conflict arises.**

2. • When starting a page, enter the title, project number, and book number.
   • Use ink for permanence -- avoid pencil.
   • Record your work as you progress, including any spur-of-the-moment ideas which may be developed later.
   • Avoid making notes on loose paper to be recopied.
   • Record your work in such a manner that a co-worker can continue from where you stop. You might be ill and to protect your priority it could be urgent that the work continue while you are absent.

3. • Give a complete account of your experiments and the results, both positive and negative, including your observations.
   • Record all diagrams, layouts, plans, procedures, new ideas, or anything pertinent to your work including the details of any discussions with suppliers, or other people outside the Company.
   • Do not try to erase any incorrect entries; draw lines deleting them, note the corrections, sign and date the changes. This extra care is worthwhile because of the necessity of original data to prove priority of new discoveries.

4. • After entering your data, sign and date the entries.
   • Explain your work to at least two witnesses who are not co-inventors, and have them sign and date the pages in the place provided.
   • Record the names of operators and witnesses present during any demonstration and have at least two witnesses sign the page. If no witnesses are present during an experiment of importance, repeat it in the presence of two witnesses.

5. Since computer programs can be patented these instructions apply to the development of computer software. In this case a description of the structure and operation of the program should be recorded in the notebook, together with a basic flow diagram which illustrates the essential features of the program. In the course of developing the code, the number of lines of code written each day should be recorded in the notebook, together with a statement of the portion of the flow diagram to which the section of code is directed.

6. This notebook and its contents are the exclusive property of the Company. It is confidential and the contents are not to be disclosed to anyone unless authorized by the Company. You must return it when completed, upon request, or upon termination of employment. It should be kept in a protected place. **If loss occurs, notify your supervisor immediately, and make a written report describing the circumstances of the loss.**

Table of Contents

TITLE ________ Project No. ____ Book No. ____

From Page No. ____

Initial Scientific notebook entry for TPA 3.2 code testing and sensitivity analyses.

Title: TPA simulations of WP performance and sensitivity analyses

Tests Performed by: Sean Brossia

Objectives: Learn use of TPA 3.2 and perform simulations to examine WP performance sensitivity to various corrosion parameters. Example parameters include, Erp for carbon steel and C-22, ipass for carbon steel and C-22, [Cl^-] and pH of the solution impacting the WP and couple potential for galvanic coupling.

Equipment: Access to Sun computer to run computations.

Materials: None.

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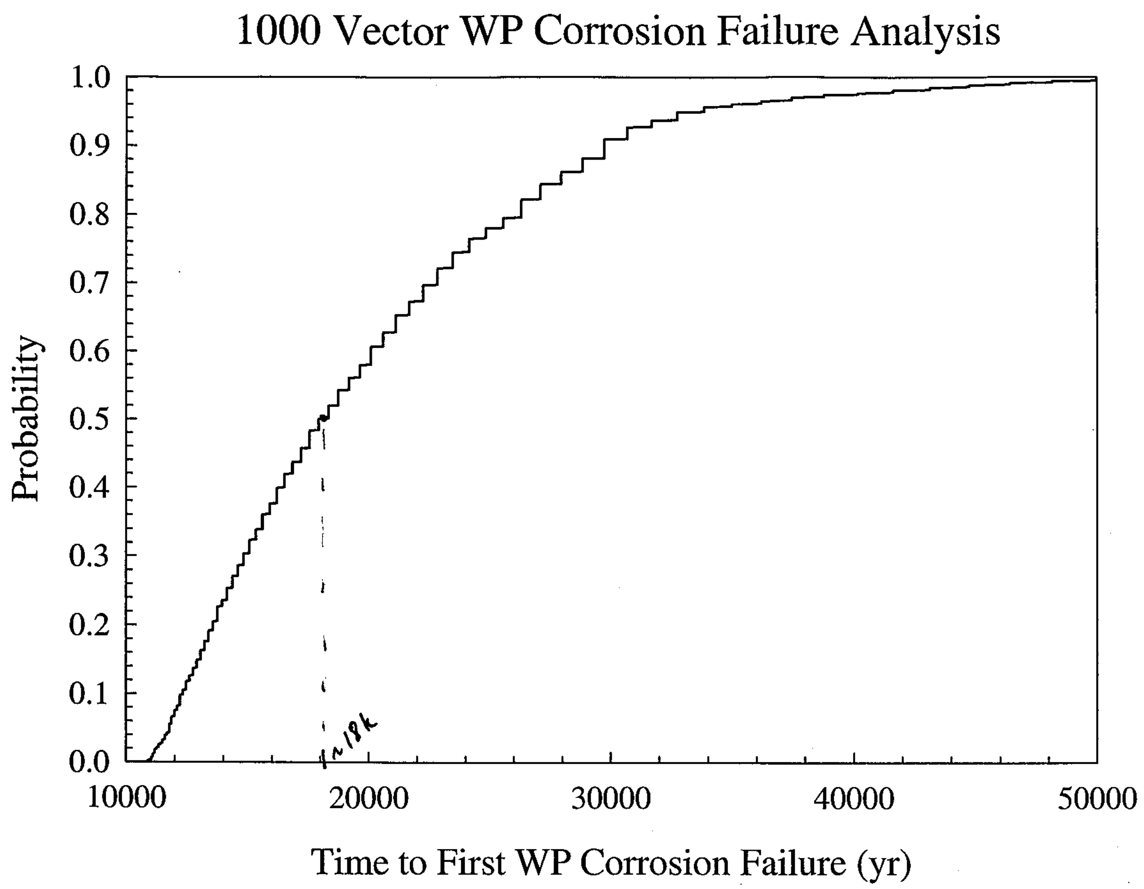
TITLE Analysis of 1000 Vector TPA runs

From Page No.



First Corrosion failure only considered. Failure by seismic and volcanic events ignored.

files:
\1000 vector
totdose.res
wpcfail.res
wpcfail.JNB (Sigma Plot)

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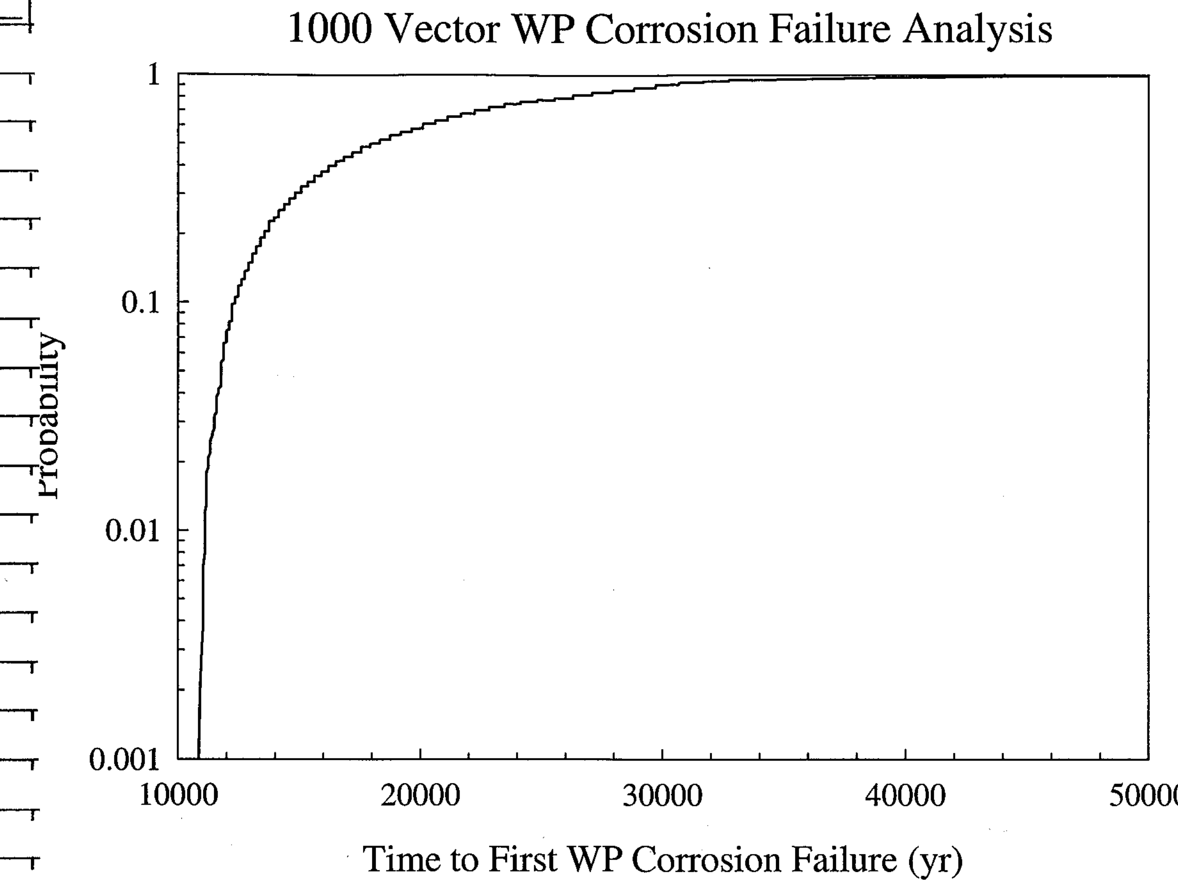

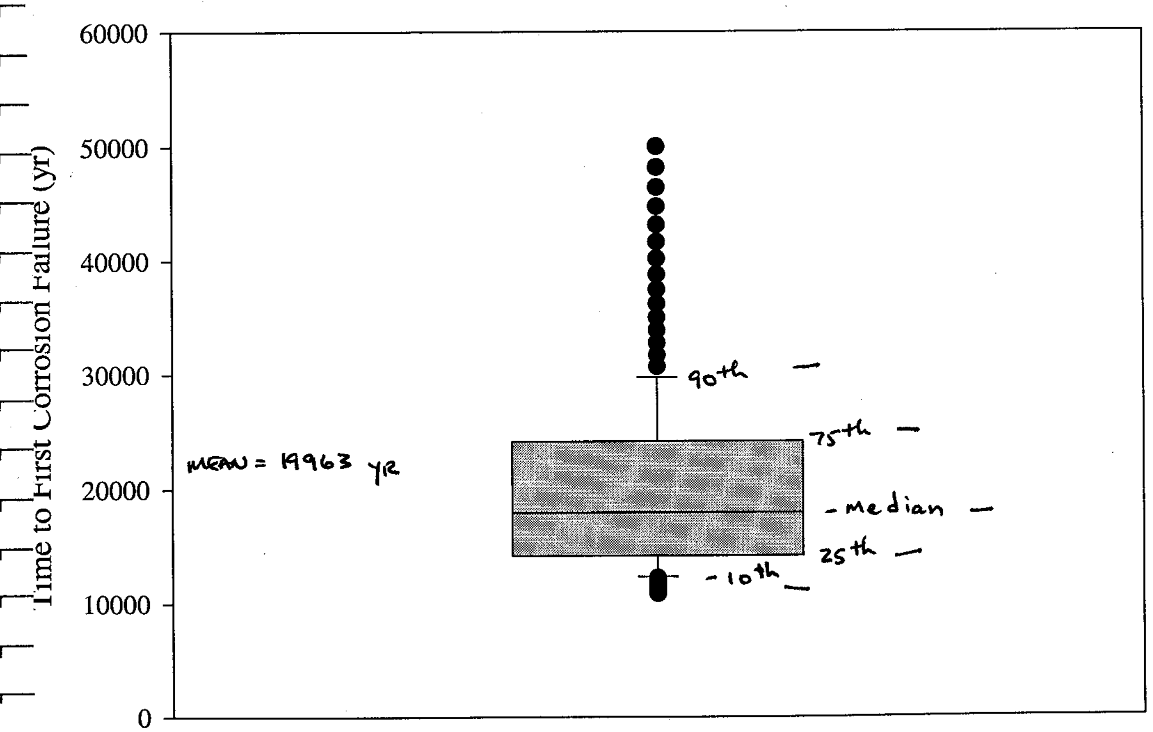

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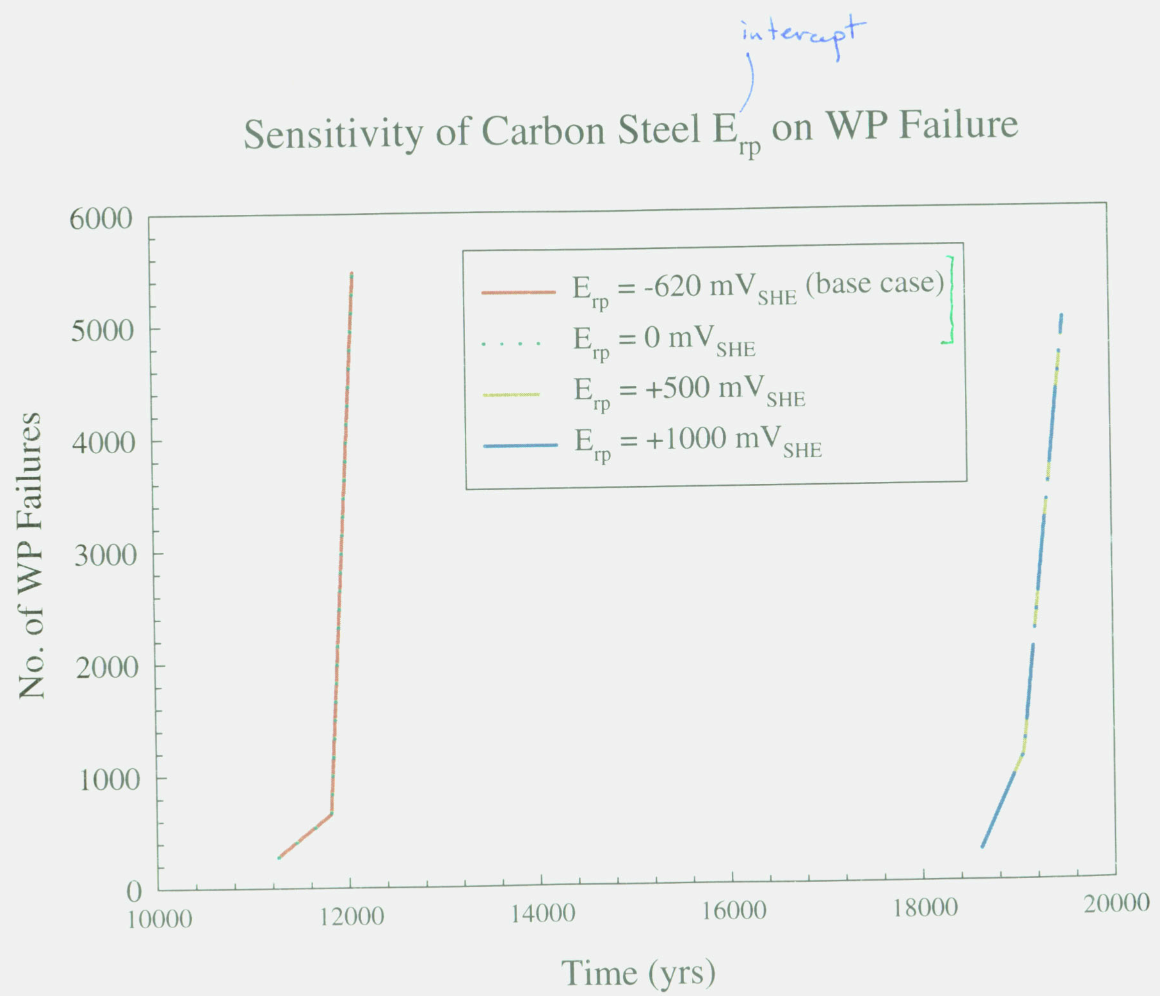
Book No.____
TITLE Sensitivity Analyses

From Page No. ____

Sensitivity of Carbon Steel Erp intercept on WP failure by corrosion.

1 Realization TPA ver 3.2
"OuterOverpackErpIntercept" parameter varied



files: \carbon steel Erp
\basecase carbon steel Erp sensitivity WP. JNB
totdose.res carbon steel Erp sensitivity.JNB
wpsfail.res

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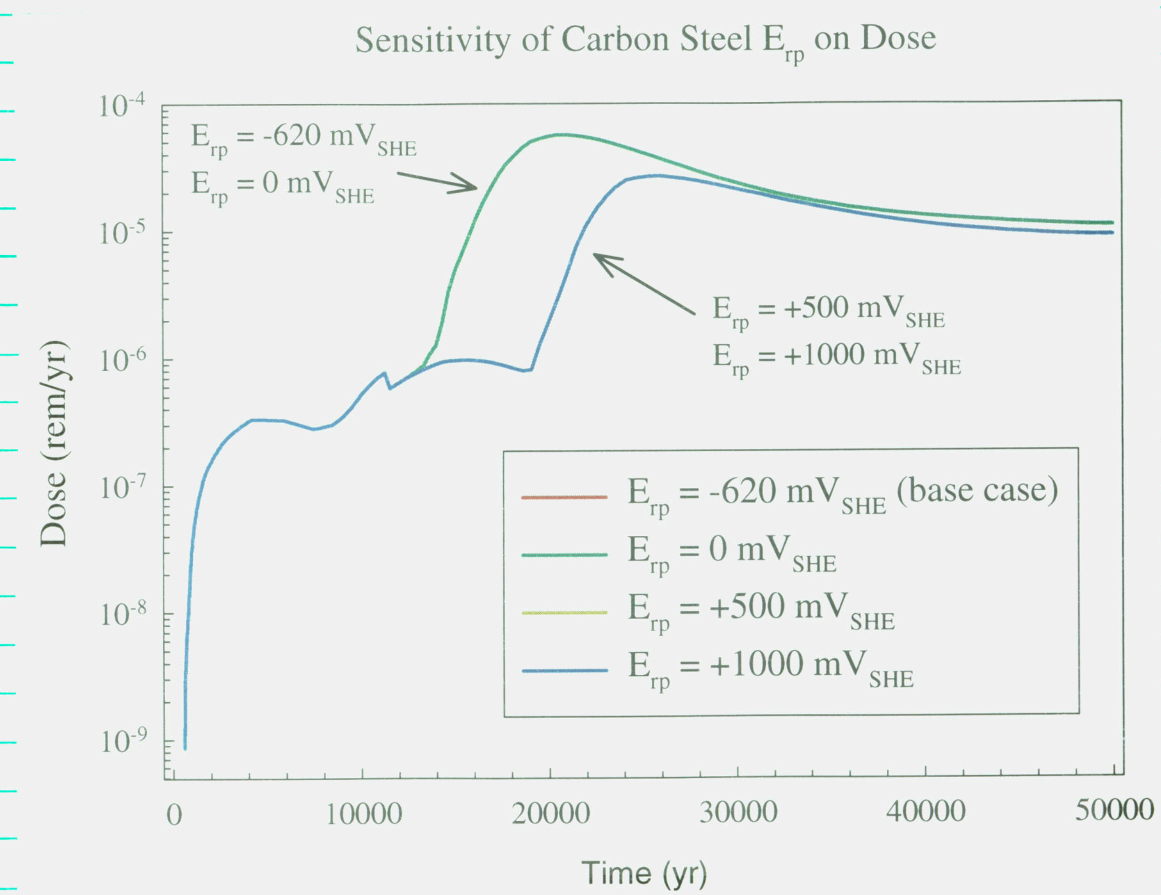
Same as p 4, but considering dose instead of WP failure
→ same performance @ t < ~ 12,000 yr due to initial WP failures included in base case



\carbon steel Erp
totdose.res (Erp int = 0 mVshe)
wpsfail.res —— " ——
totdose2, wpsfail2.res (Erp int = +500)
totdose3, wpsfail3.res (Erp int = +1000)

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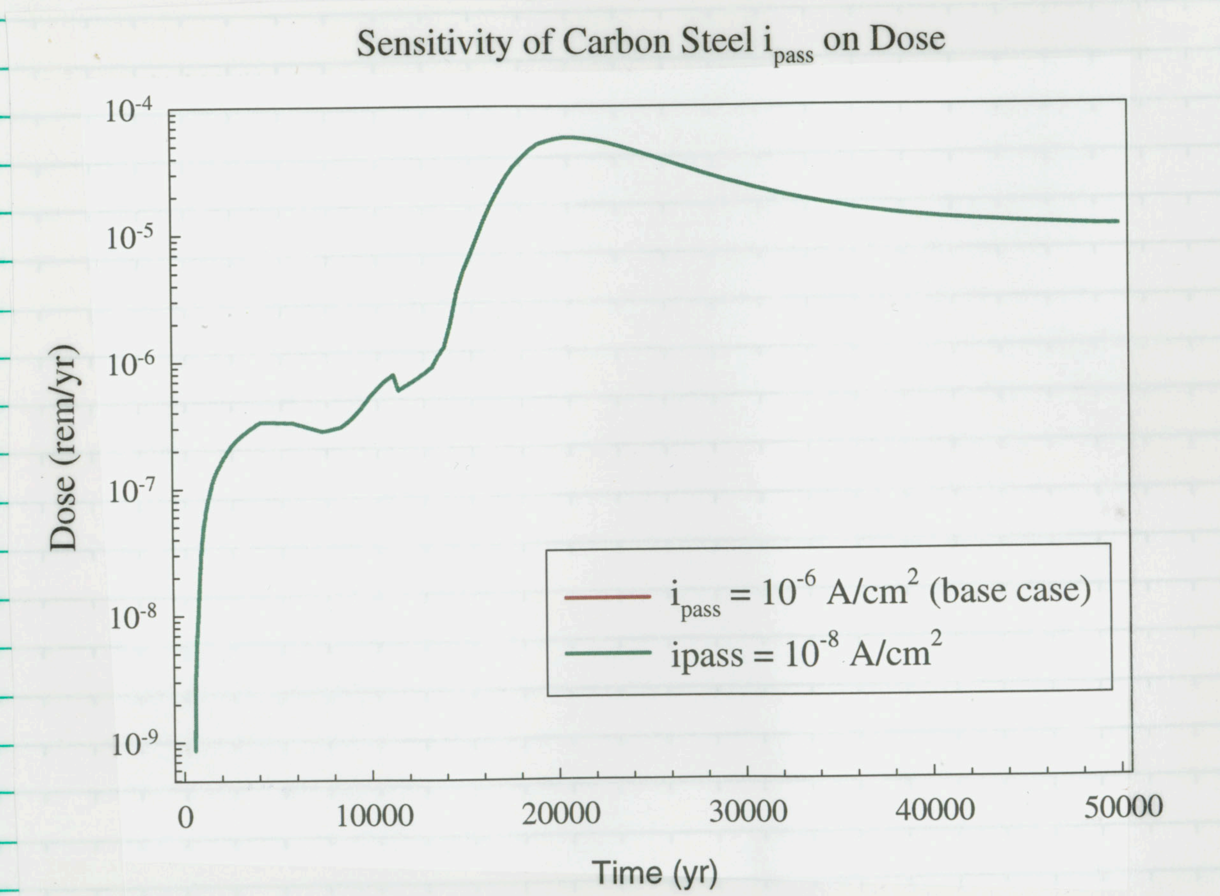
Sensitivity of dose on carbon steel ipass
→ As Lc (localized corrosion) rather than passive dissolution dominates in base case, thus parameter has no influence.

1 Realization, TPA 3.2
"AA-1-1"



files:
\basecase - see p 5
\carbonsteel ipass
carbonsteel ipass sensitivity.JNB
totdose, wpsfail.res

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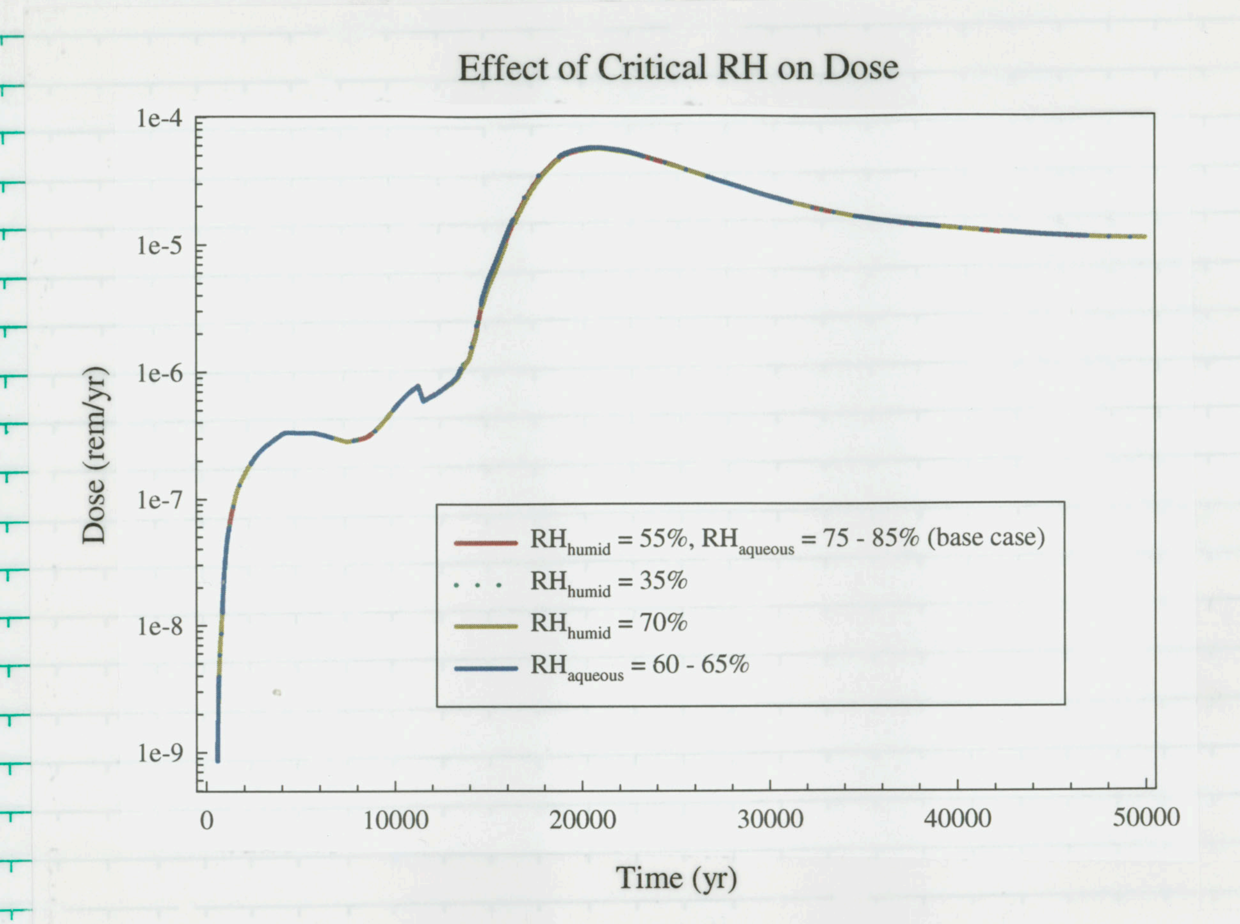
Sensitivity of dose on critical RH for Humid Air Corrosion

page tear → wrong page initially placed in notebook CSB 11/23/98



→ No effect of RH as localized corrosion likely dominates process (at least at RH values studied)

files: \RH
RH on dose.JNB
totdose35, wpsfail35.res (Humid Air Crit = 35%)
totdose70, wpsfail70.res (Humid Air Crit = 70%)
totdose60-65, wpsfail60_65.res (Aq. Crit = 60-65%)

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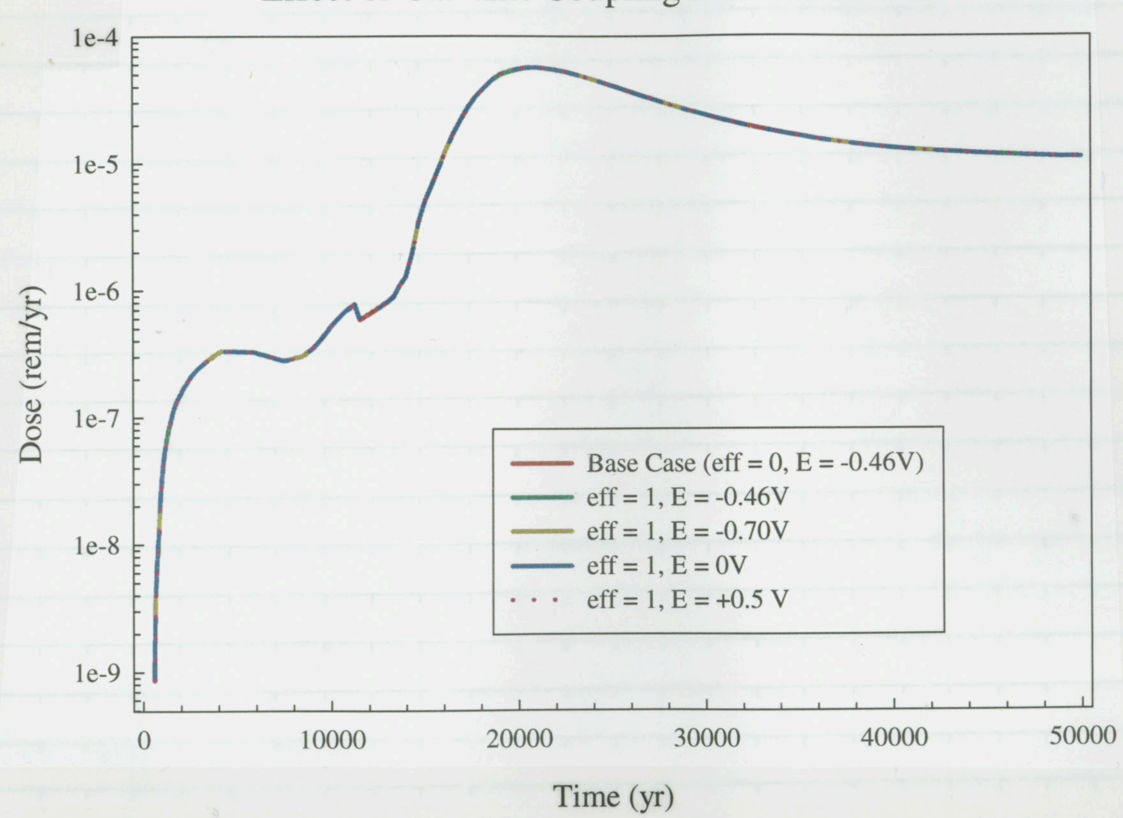
SB 8/16/2000 ~~Effect of the critical RH for onset of humid air and aqueous corrosion on dose~~

Effect of Galvanic coupling on dose

— no effect

Effect of Galvanic Coupling Potential on Dose



files: \Galvanic Couple

galvanic couple on dose. JNB – sigma Plot

eff_1_-460 — efficiency = 1, Ecouple

totdose_eff_1_-460, _1_-700, _1_0, ~~#1~~_1_+500.res

tpa ————— " ————— .inp

wpsfail ————— " ————— .res

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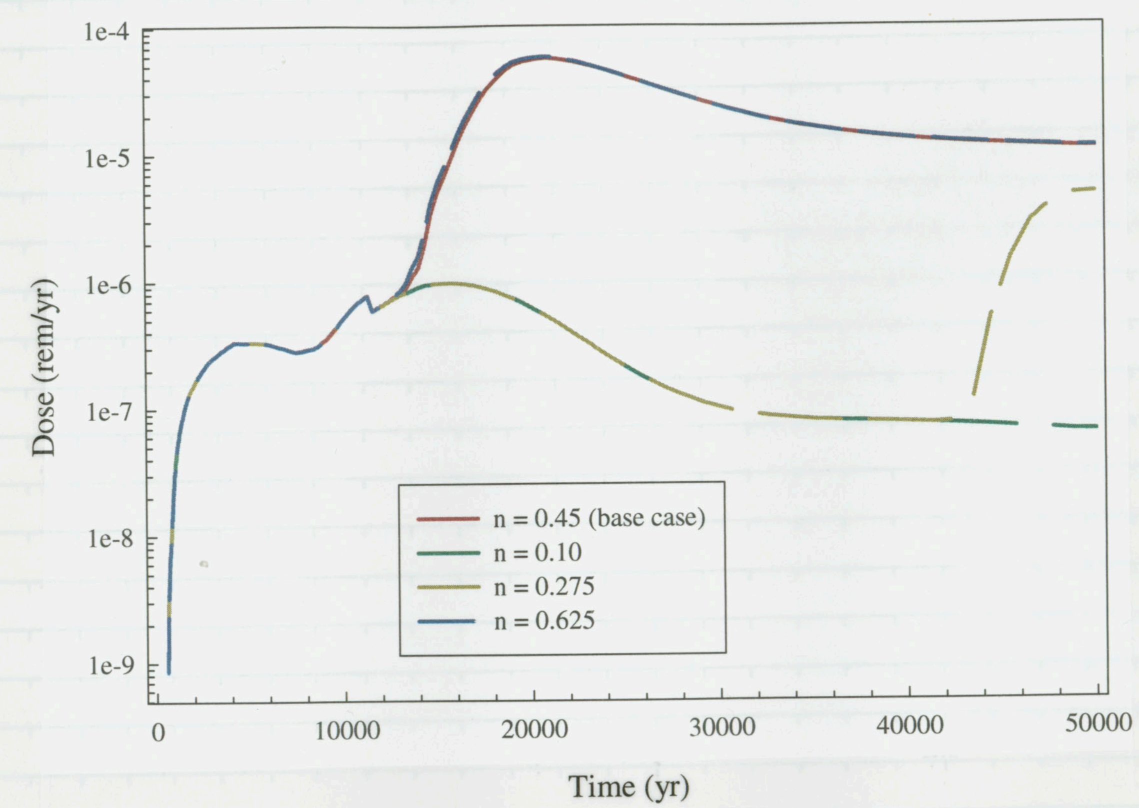
$P \propto At^n$

Effect of carbon steel pit growth exponent on dose

→ decreasing n symbolizes lower propagation rates and making repassivation and arrest of pits in carbon steel easier ⇒ n = 0.1 delayed corr^n to beyond 50 kyr

Effect of Carbon Steel Pit Growth Exponent on Dose



files: \CS_Exp

carbon steel pit exponent. JNB – sigma plot

01 ⇒ n = 0.10 totdose 01, 0275, 0625.res

0275 ⇒ n = 0.275 wpsfail ——— " ———, res

0625 ⇒ n = 0.625 tpa ——— " ——— .inp

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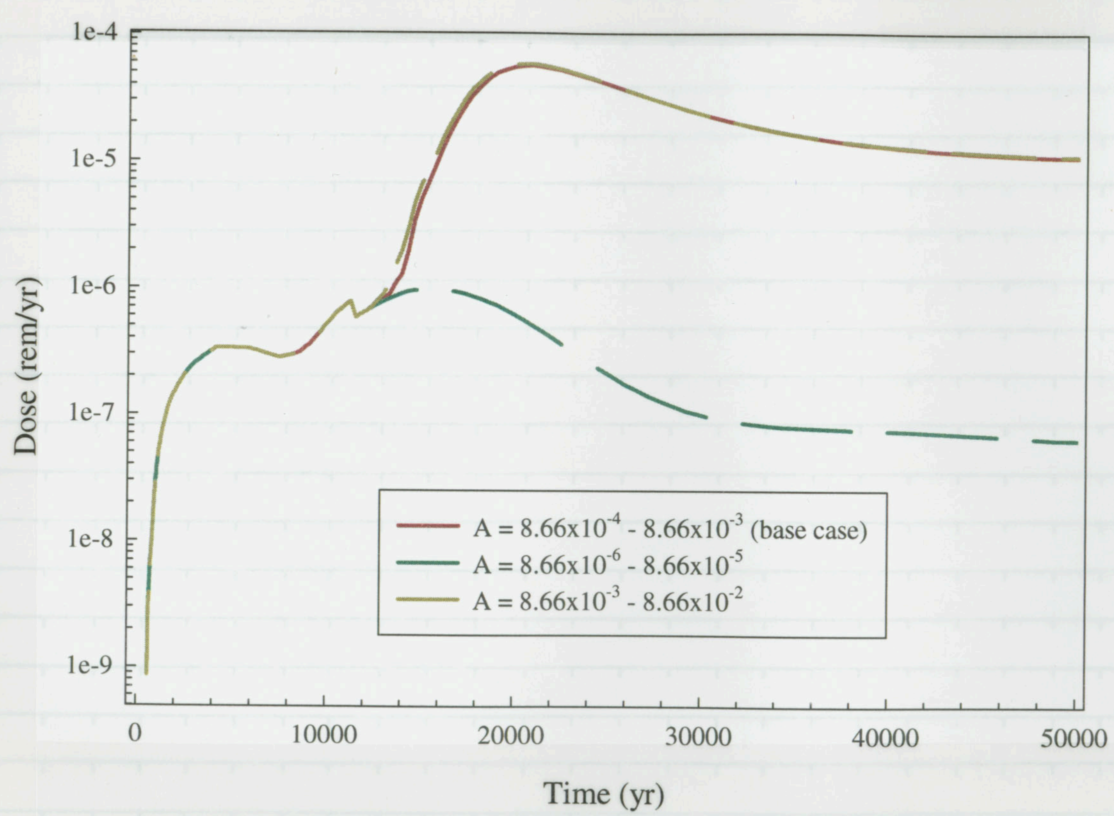
Effect of pre-exponent of carbon steel pit growth rate on dose.

- by decreasing A by a factor of 100, failure delayed beyond 50 kyr
- Increasing A by a factor of 100, failure slightly earlier

→ Changing A has the same effect as changing n ⇒ making repassivation easier or decreasing propagation rate

Effect of Carbon Steel Pit Growth Pre-Exponent on Dose



files: \ CS_Rate_Coef

carbonsteel rate coef. JNB sigma Plot

A

$-3\_-2 = 8.66\times10^{-3} - 8.66\times10^{-2}$

$-6\_-5 = 8.66\times10^{-6} - 8.66\times10^{-5}$

totdose_-3_-2, _-6_-5 ~~,~~ VJ 4/7/03 .res

wpsfail ——— " ——— .res

tpa ——— " ——— .res

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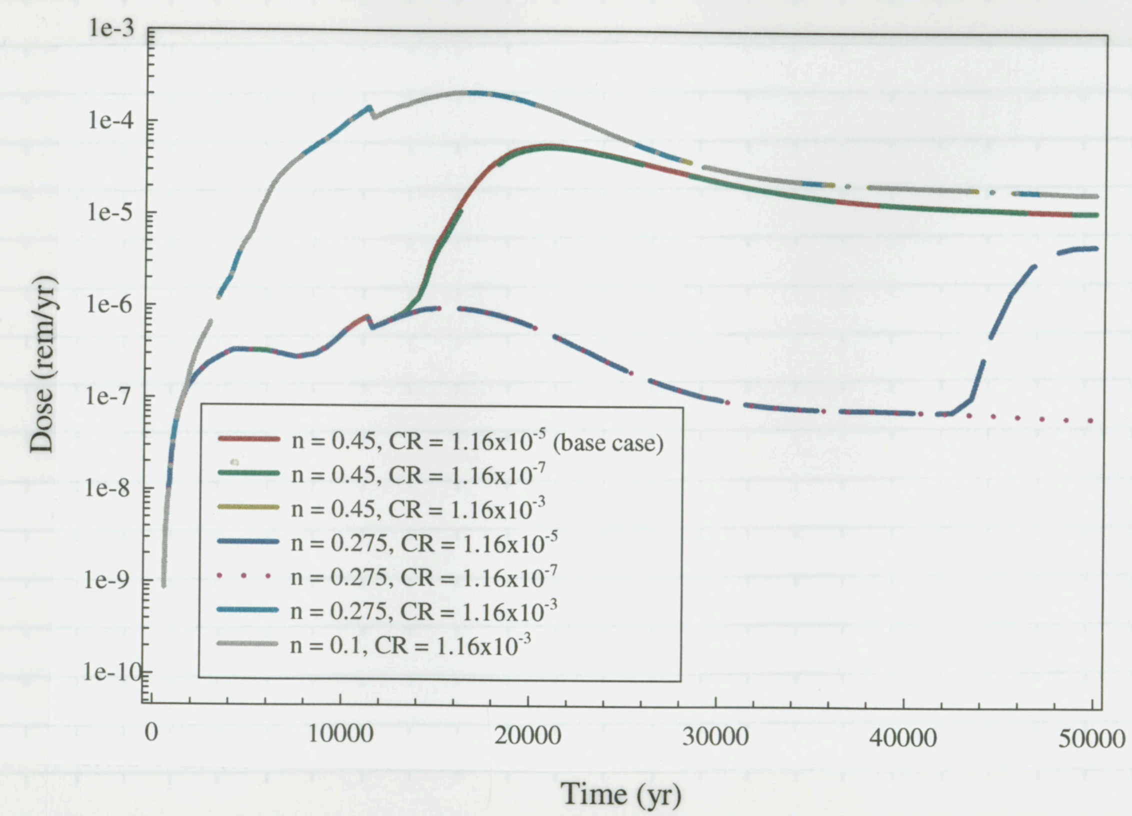
Effect of humid corrosion rate on dose including influence when repassivation is easier ($n = 0.275$, 0.1 vs 0.45).

→ decr. by 100x had only minimal influence @ $n = 0.45$, but VJ 4/8/03 ~~did for~~ did further delay WP failure @ $n = 0.275$

→ incr. by 100x had dramatic infl. on WP failure

⇝ these likely due to small time window in which this mech. dominates prior to onset of localized.

Effect of Carbon Steel Humid Air Corrosion Rate on Dose



files: \ Humid_CR

carbon steel humid air corrosion. JNB

totdose -310, -3275, -3b, -7275, -7b .res

wpsfail ——— " ——— .res

tpa ——— " ——— .inp

-3, X _ n

CR exponent

n

b = base case

10 = 0.10

275 = 0.275

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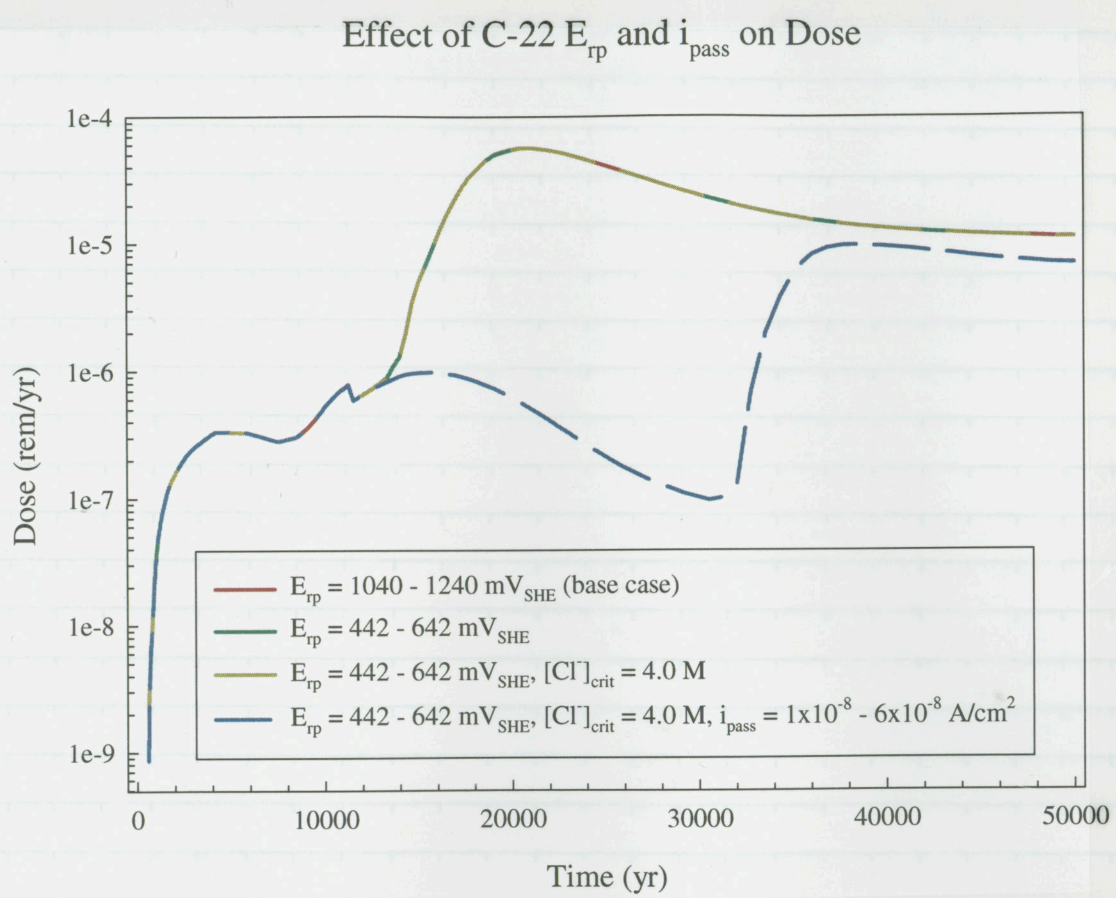
Effects of changing C-22 Erp and ipass on dose



files: \C-22 Erp

SB 8/16/2020 ~~ipass~~ C-22 Erp . JNB Sigma Plot

totdose, wpsfail, tpa 442_642 – Erp = 442-642 mV_{SHE}

totdose, wpsfail, tpa 442_642_Cl4 – Erp = 442-642 + $[Cl^-]_{crit}$ = 4.0M

_ipass – as above + ipass = 1×10^{-8} - 6×10^{-8} A/cm^2

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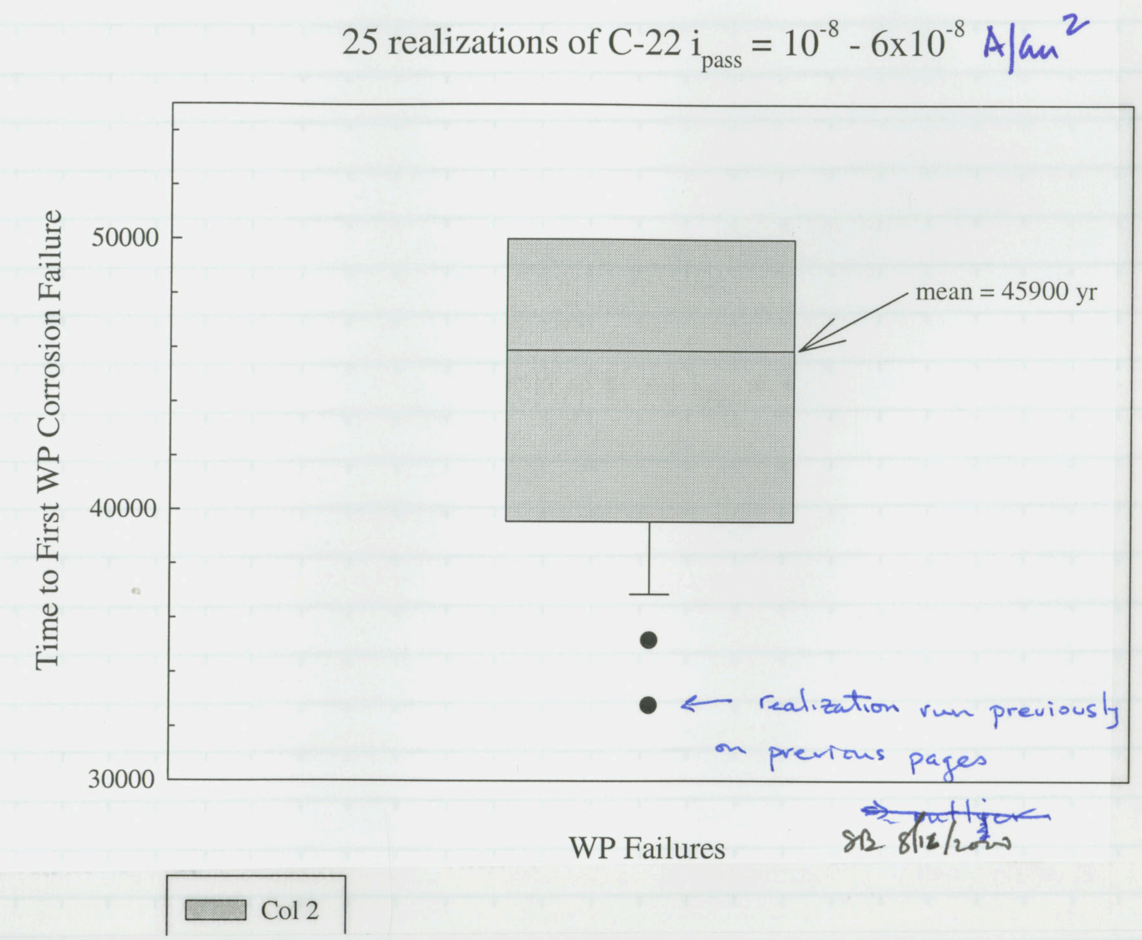
25 realization run to examine distribution of initial WP corrosion failure times → several did not fail @ 50 kyr



files:\ C-22 Erp

wp fail times 25 runs. JNB – Sigma plot

wpsfail, totdose, ~~tpp~~ tpa _ ipass _ 25 runs

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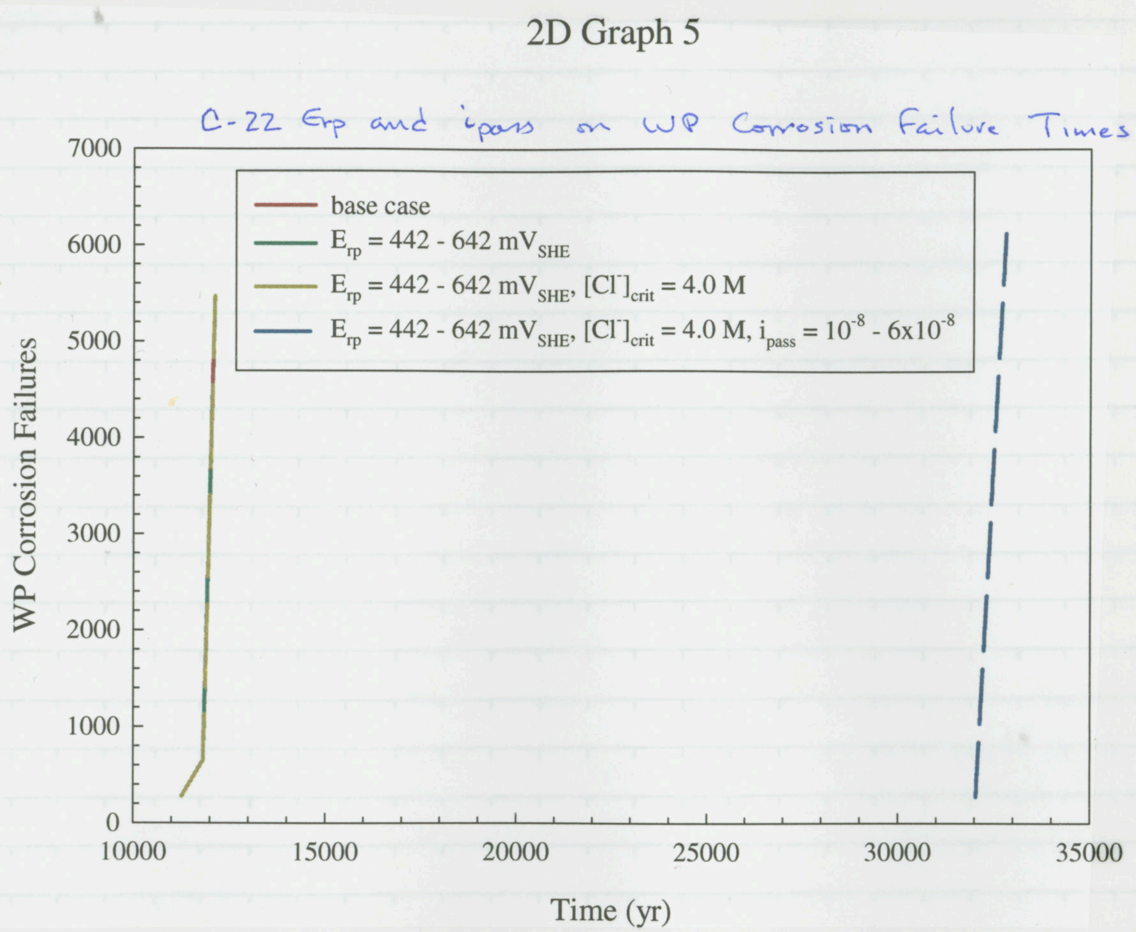
SB 8/16/2000

from p ~~13~~ 12 - WP fail times corresponding to dose calc. shown on p ~~13~~ 12

C-22 Erp and ipass on WP Corrosion Failure Times



files - \ C-22 Erp
c22 Erp WP.JNB - Sigma Plot
other files same as on p 12

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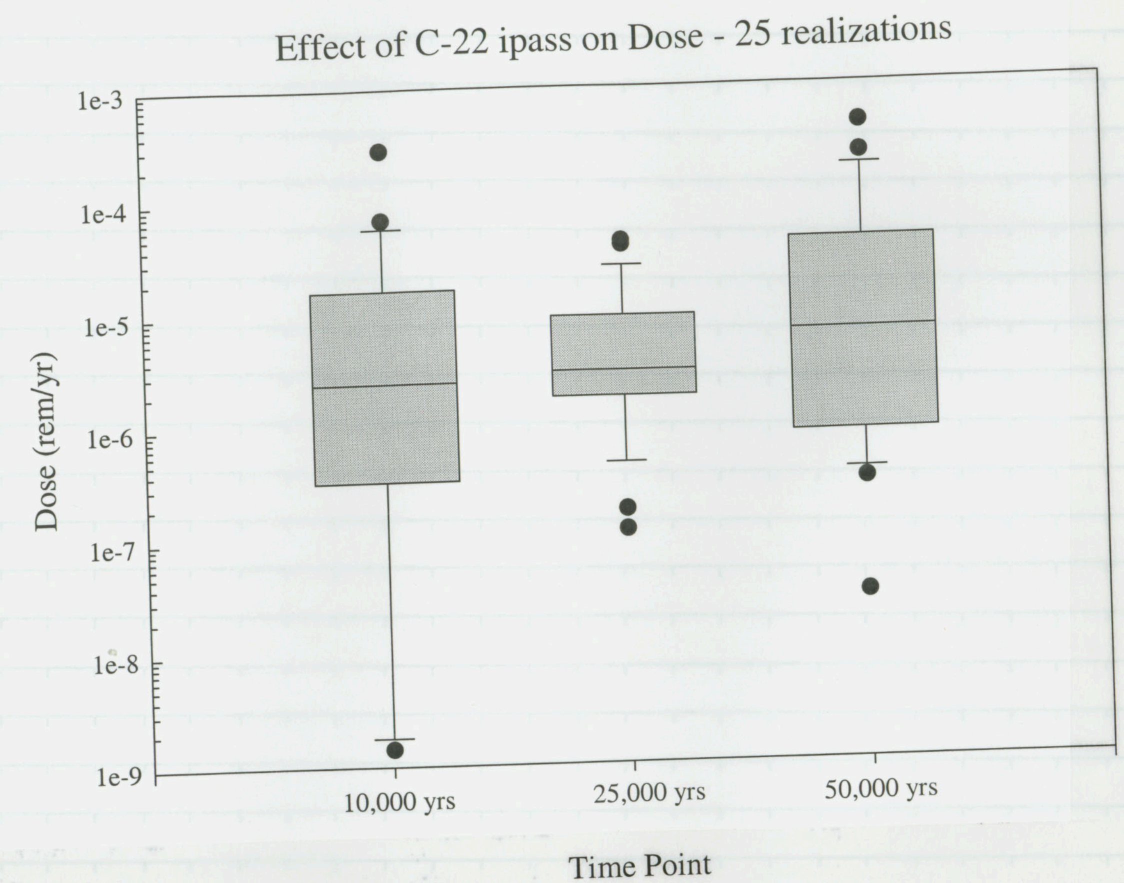
continuation of p 13 → dose distribution @ varied times



files: \ C-22 Erp
ipass dose distribution. JNB - sigma plot
others same as p 13

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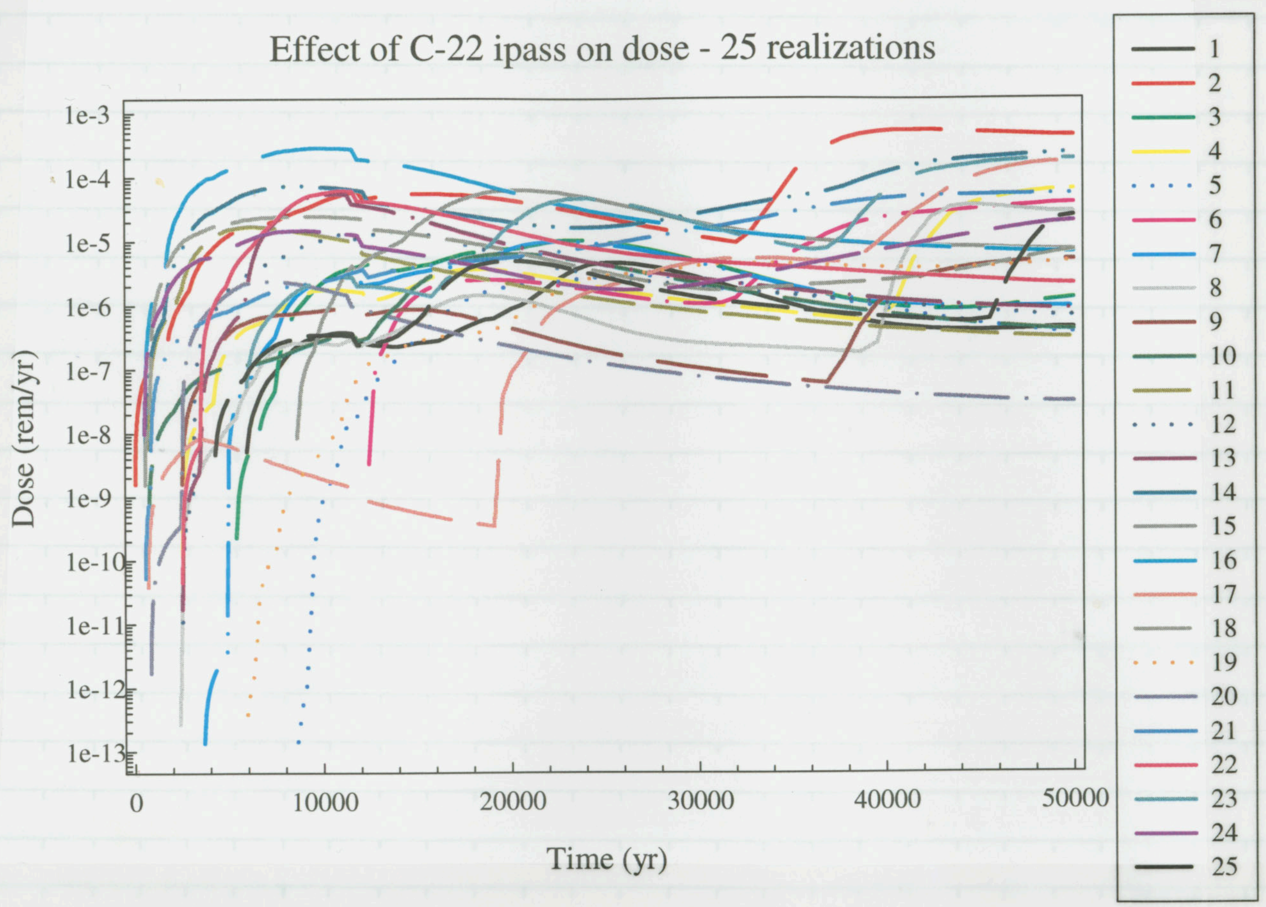
25 realizations – dose predictions



files: \ C-22 Exp
ipass on dose. JNB – Sigma Plot

others same as p13

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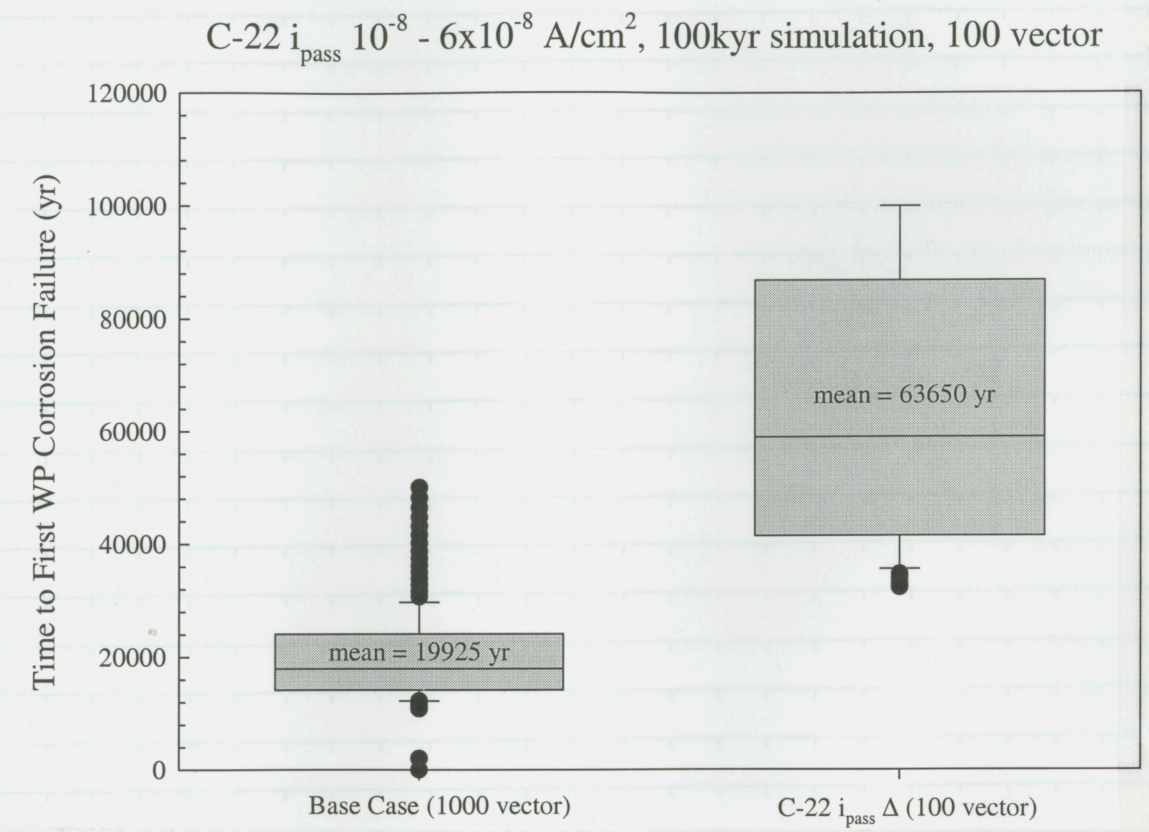
100 realization, 100 kyr simulation – C-22 ipass on WP failure times



files: \ C-22 Exp
100yr 100 vector wp. JNB – Sigma plot
totdose, wpsfail, tpa – 100kyr – 100 run

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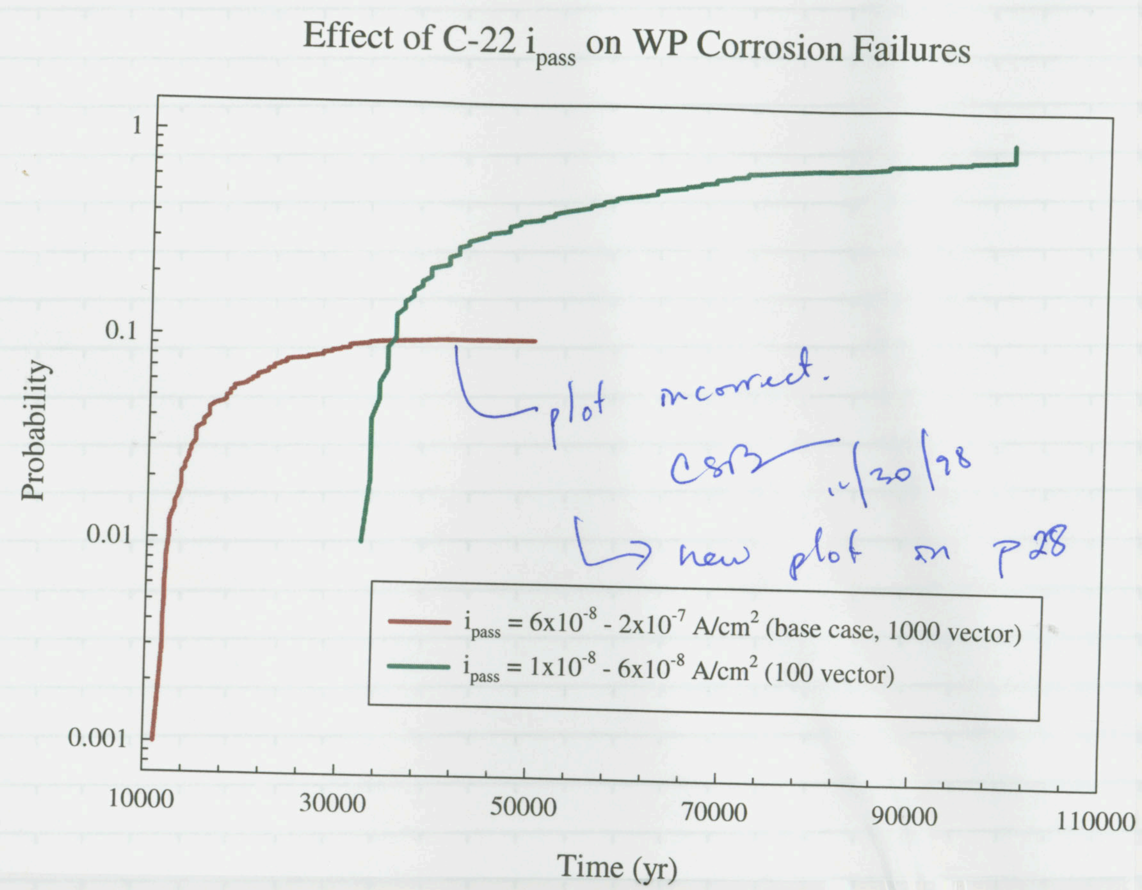
probability of WP failure by corrosion



plot incorrect.
CSB 11/30/98

→ new plot on p28

files:
same as p 17.

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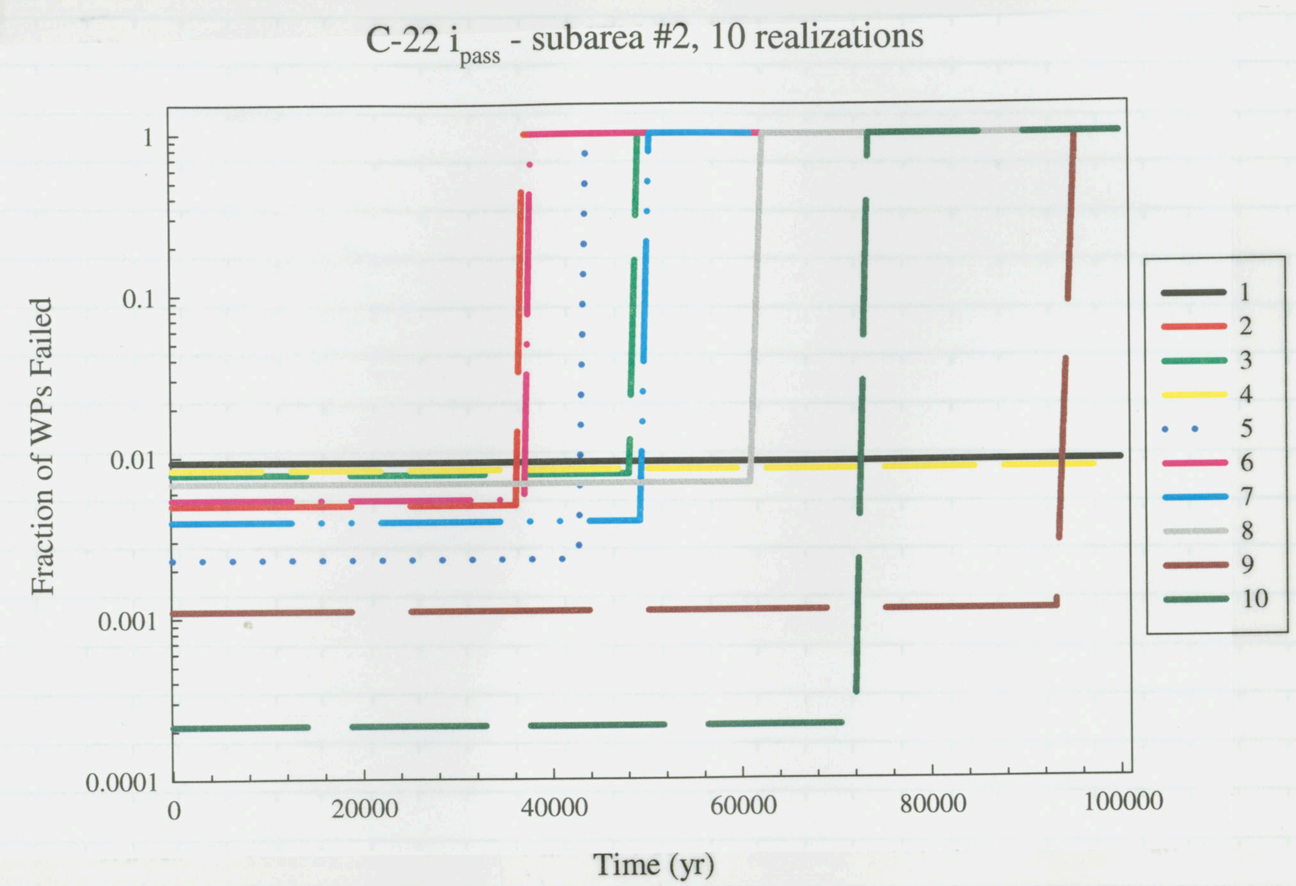
10 realizations, 100 kyr, subarea analysis
→ sub area #1 not plotted as no sig diff was observed in other subareas.



files: \C-22_100kyr
subarea analysis.JNB - sigma plot
totdose, tpa, wpsfail, ebsfail, rlt

→ continue for next several pages to p24.

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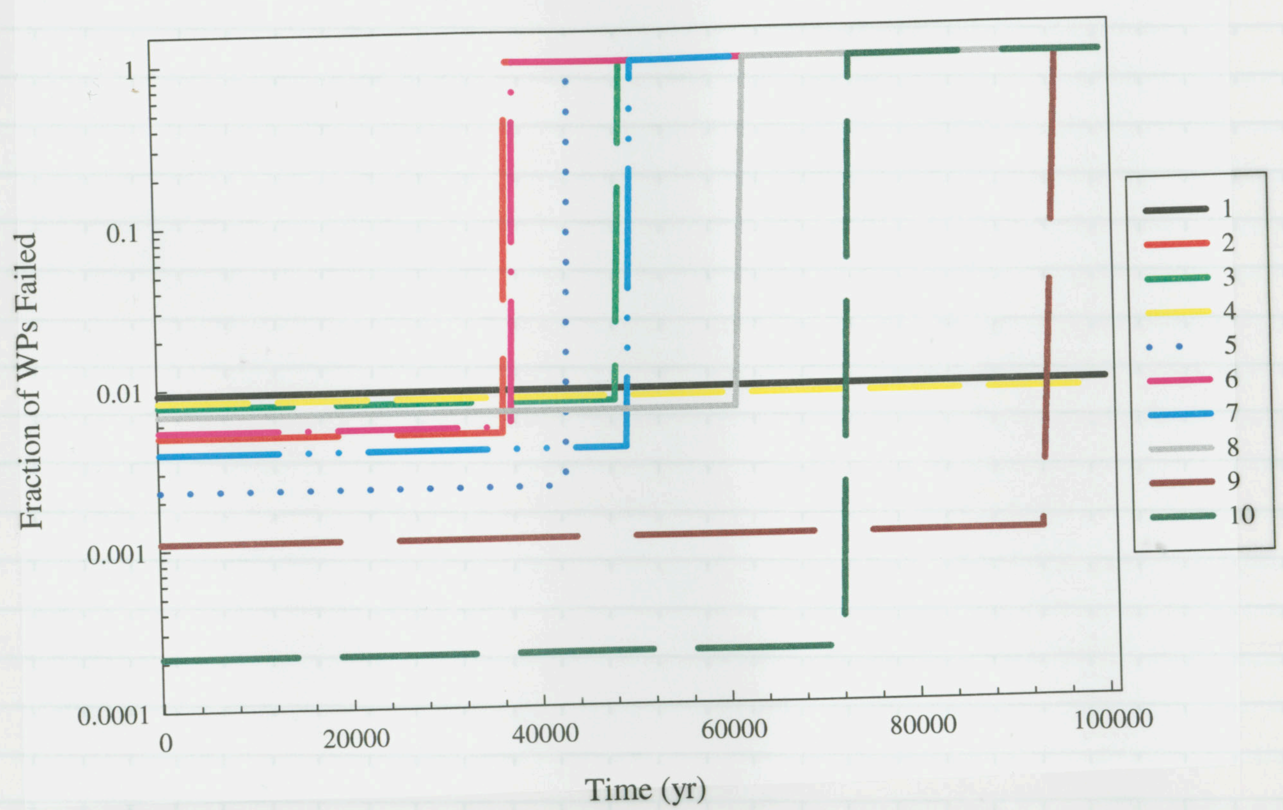
C-22 i_{pass} - subarea #3, 10 realizations



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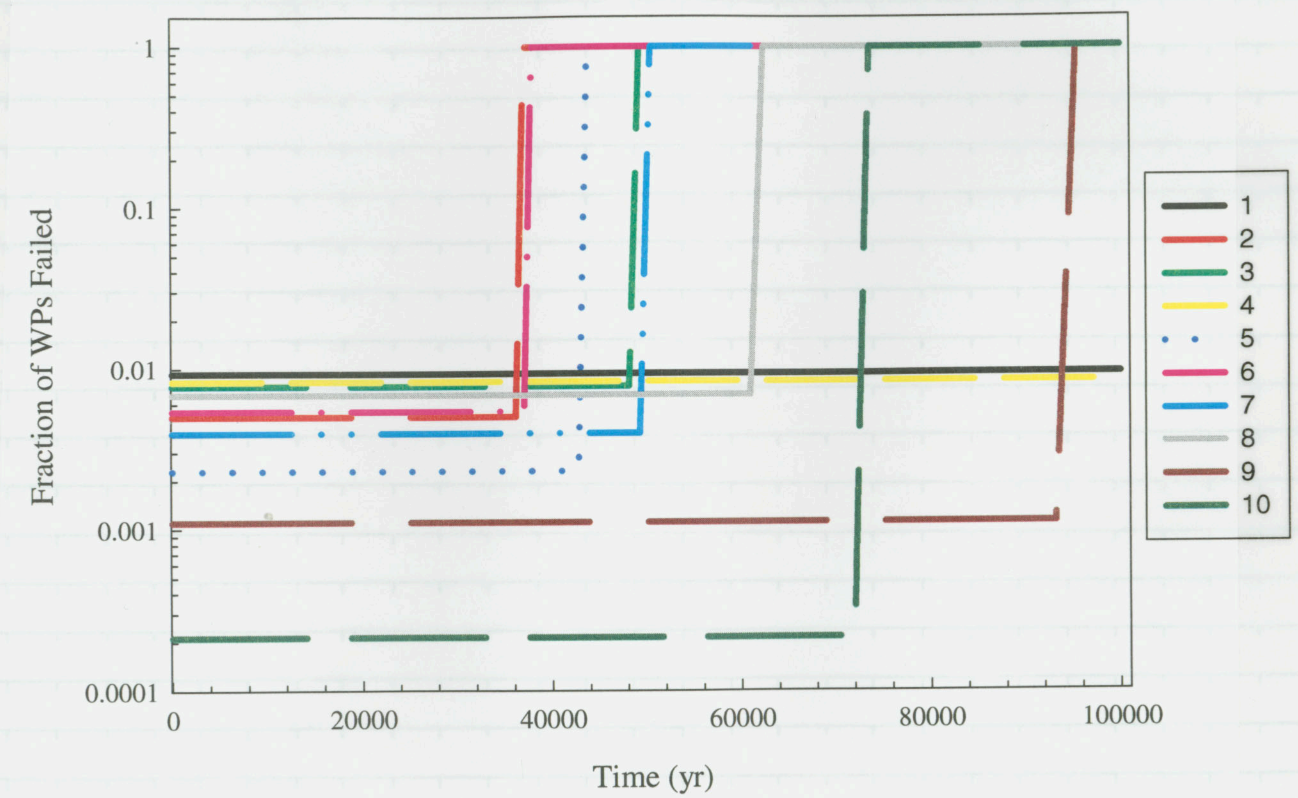
C-22 i_{pass} - subarea #4, 10 realizations



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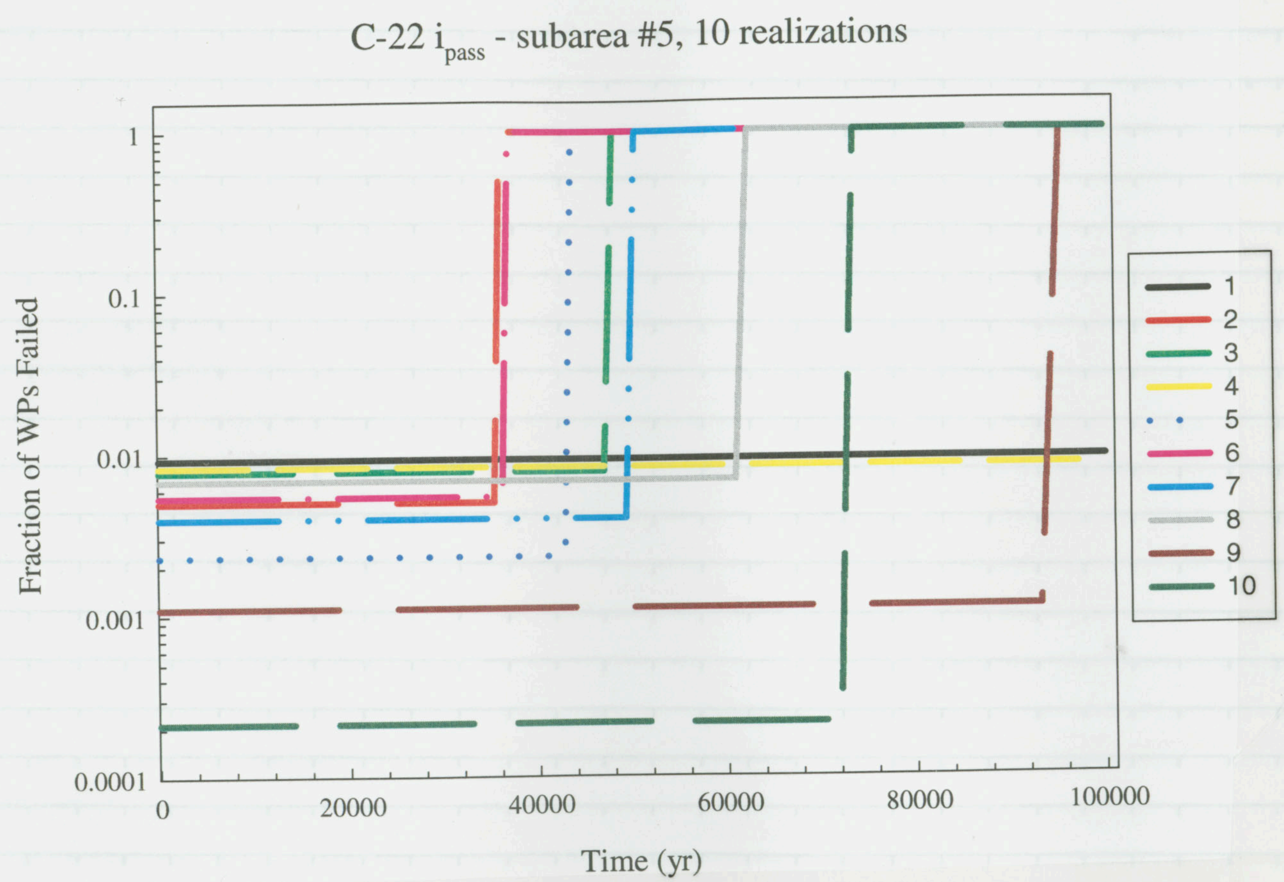

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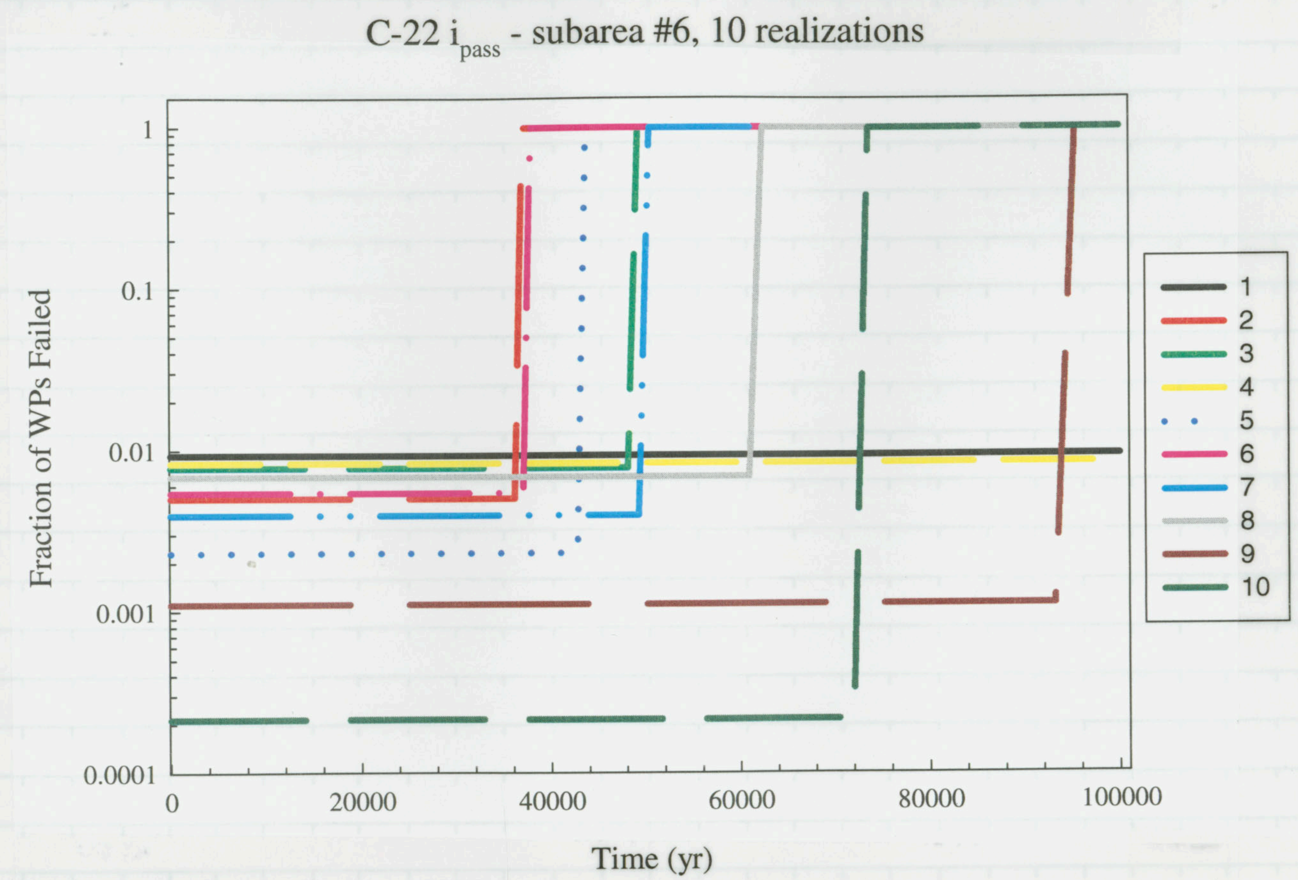

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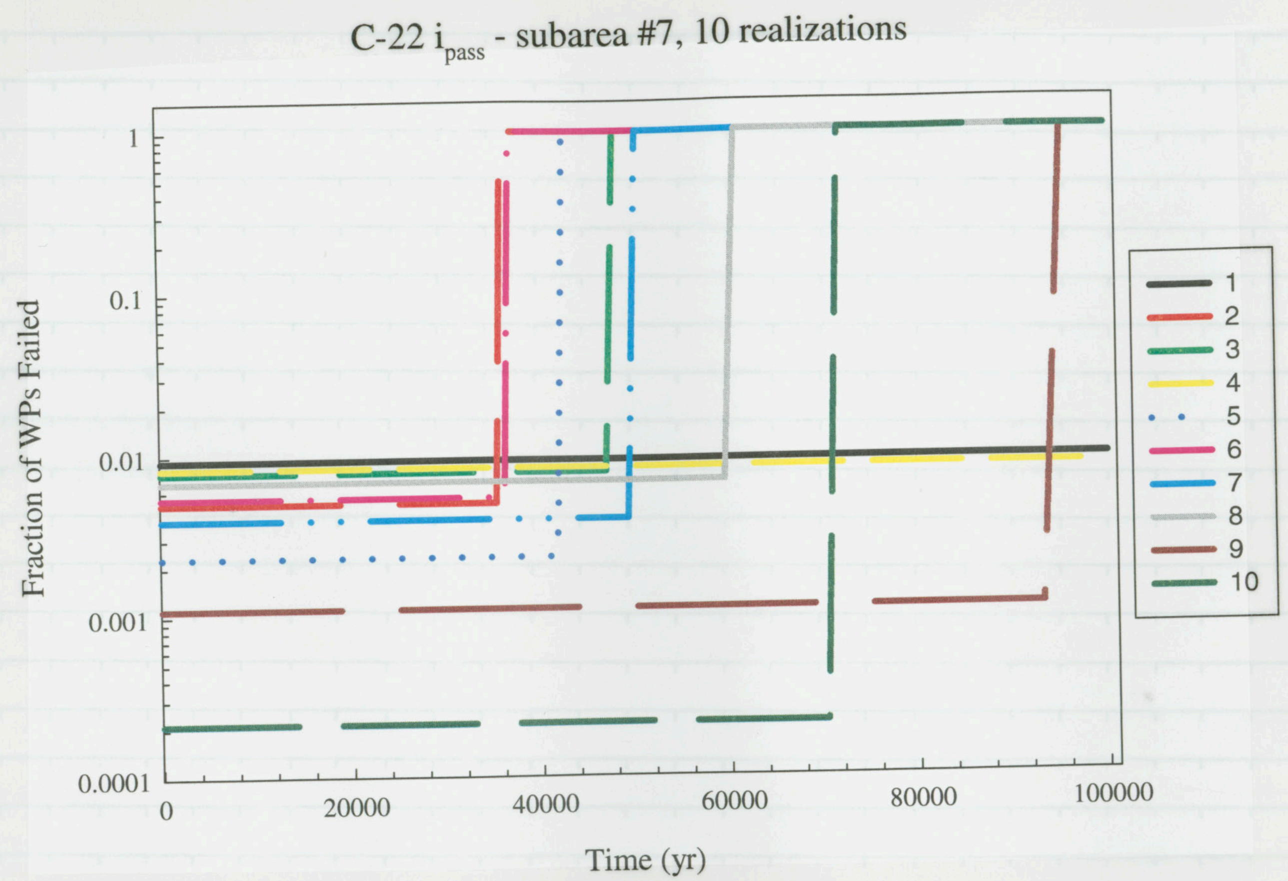

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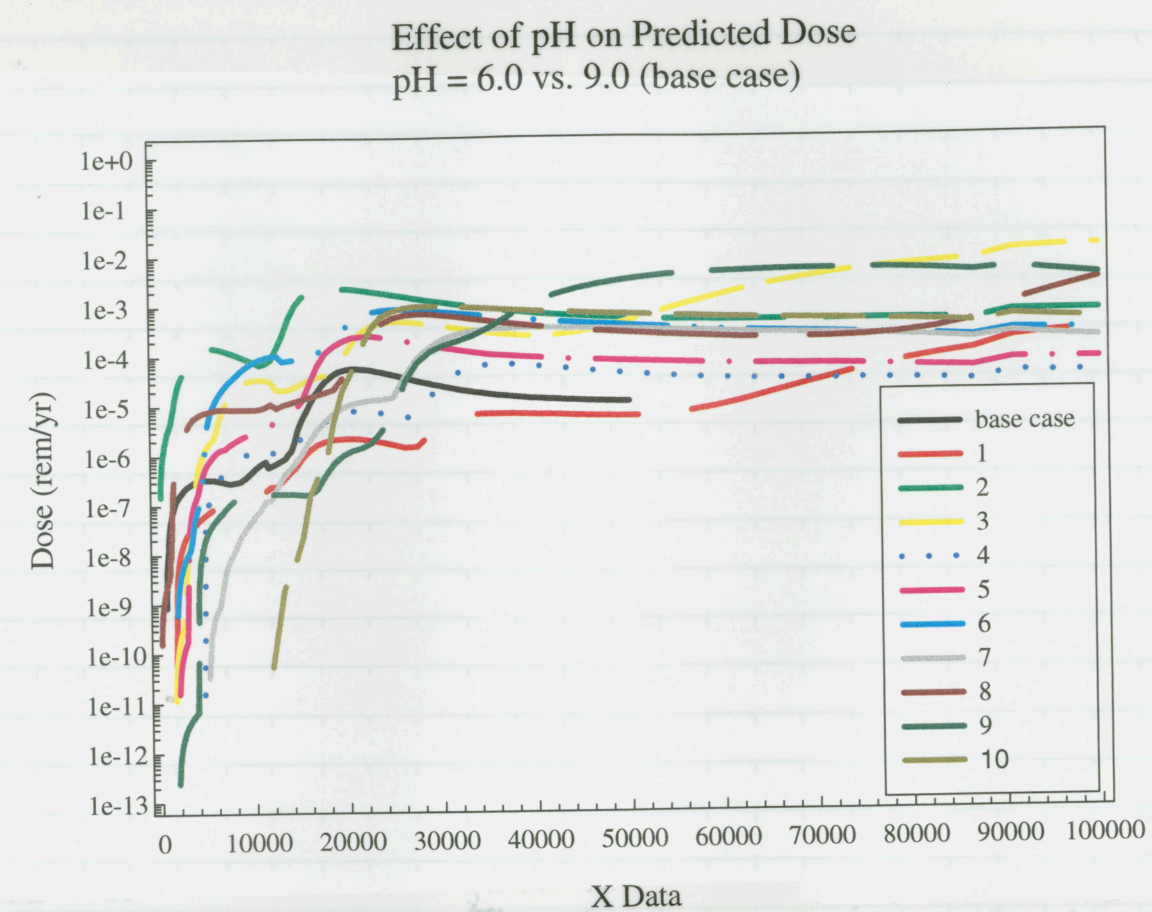
Effect of pH on Dose - 10 realizations



files: \ pH
pH dose . JNB - Sigma Plot
totdose, tpa, wpsfail

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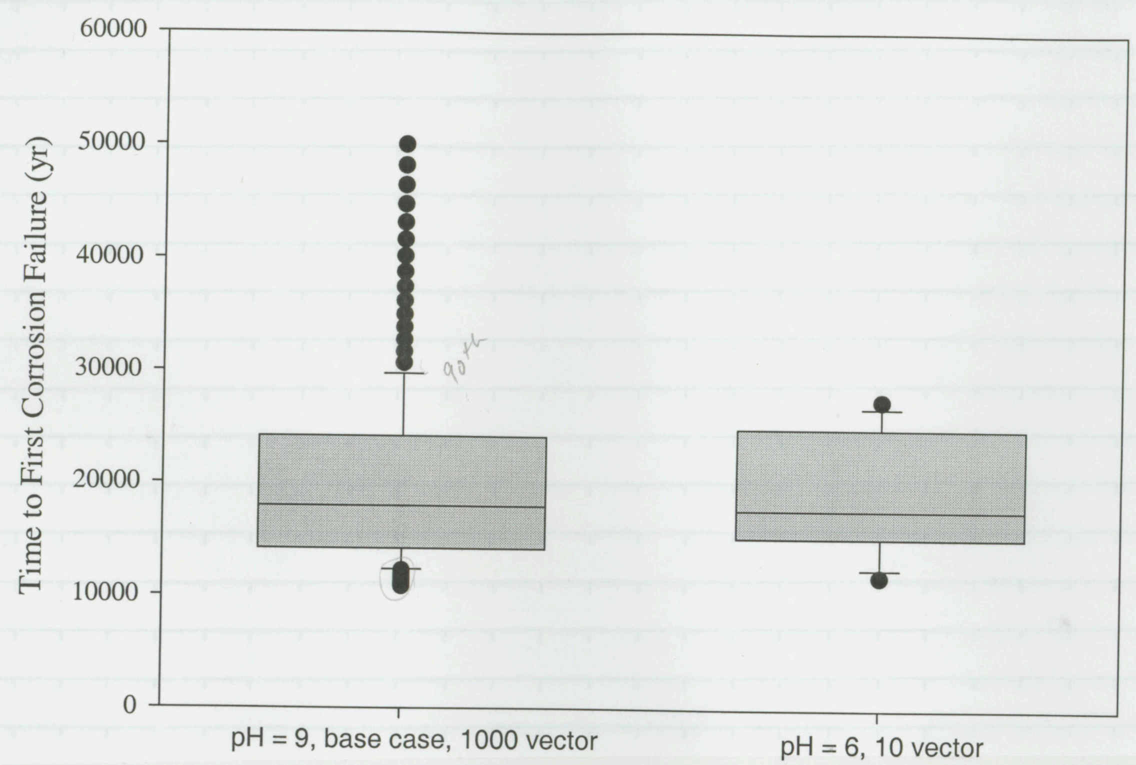
Distribution on time to 1st corrosion failure
-Effect of pH



files: \ pH
pH wp. JNB – Sigma Plot
others – same as p25

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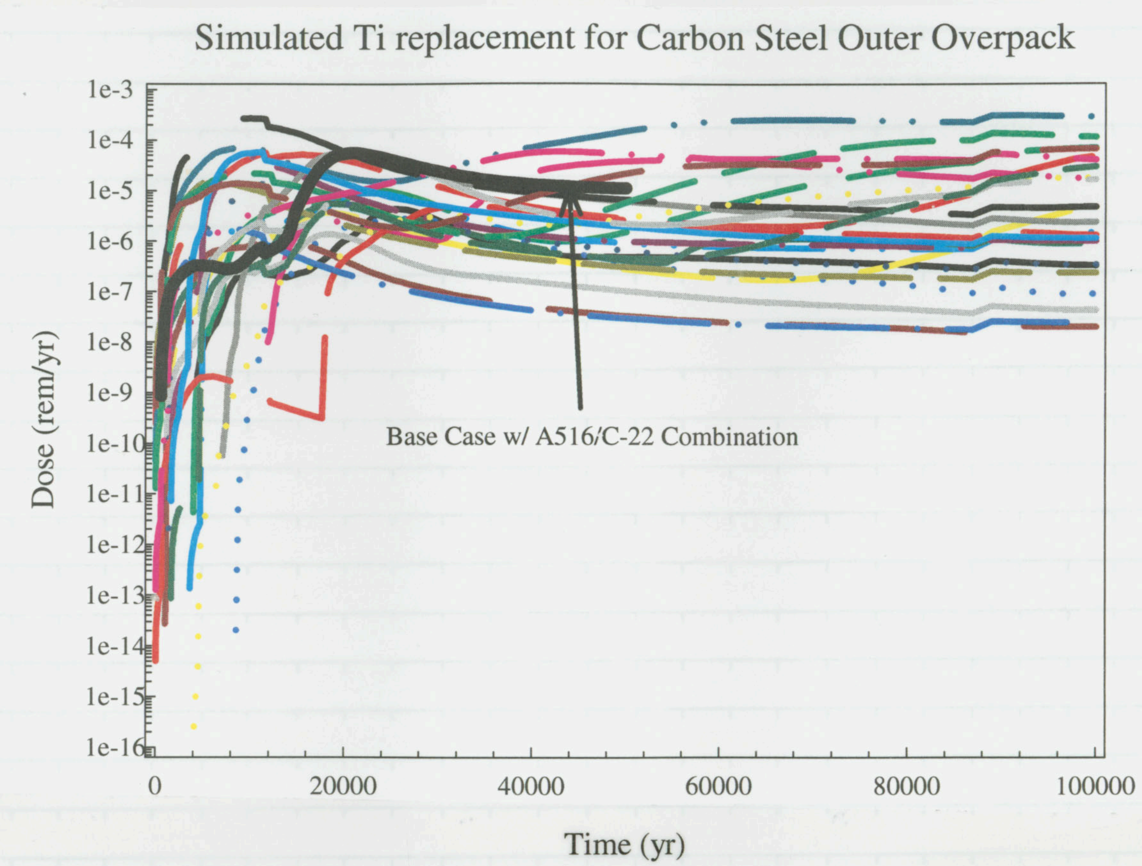
Ti simulation – 100 kyr 25 realizations
- high doses may be a result of mechanical failures
- noticed more frequent seismic failures as mech. props not changed



files: \ Ti_simulation
Ti1 100kyr 25runs.JNB – Sigma Plot
totdose.res
ipstaul.res) – Ti1
tpa.inp

$t^{Ti} = 0.02$ outer
$t^{C22} = 0.05$ inner
$E_{rp}^{Ti} = 1240$ mV$_{SHE}$, coefs = 0
$i_{pass}^{Ti} = 3.15 \times 10^{2}$ c/m^{2}yr $\Rightarrow 10^{-9}$ A/cm^2
Humid Air $CR^{Ti} = 1.16 \times 10^{-8}$ m/yr
$[Cl^-]_{crit}^{Ti} = 6$ M

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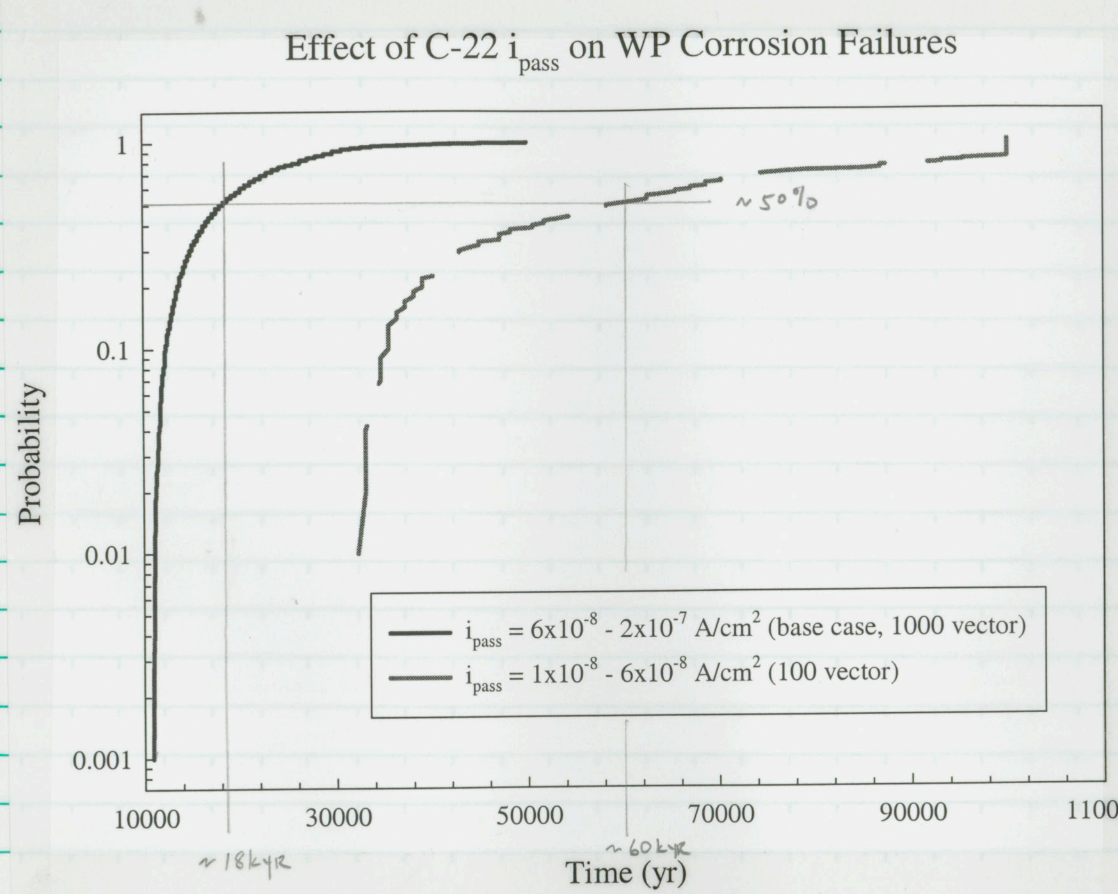
re plot of p 18.



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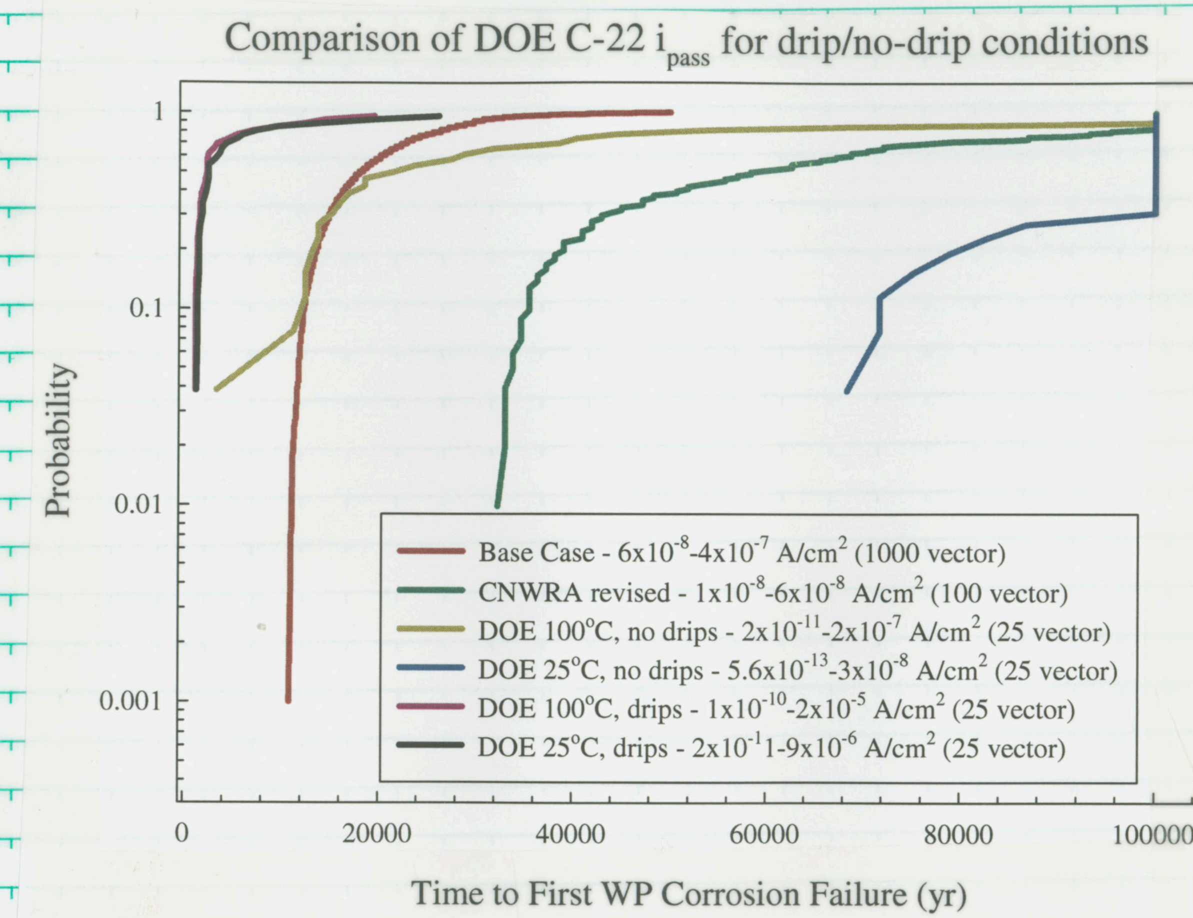
Comparison of DOE C-22 ipass cases at 100°C ; 25°C for dripping and no-dripping



12/8/98 CSB

the DOE values used are off – conversion from mm/yr to A/cm² was off by a factor of 10x based on calculations supplied by Darrell Dunn. Re work shows that:

$$\text{mm}/\text{YR} \rightarrow \text{A}/\text{cm}^2 \Rightarrow 1\ \frac{\text{mm}}{\text{YR}} = 1.08 \times 10^{-4}\ \text{A}/\text{cm}^2$$

no drip

100°C: 2×10^{-8} mm/YR – 2×10^{-4} (see p34) ⇒ $i \simeq 2 \times 10^{-12} - 2 \times 10^{-8}$ A/cm², so current densities used are a factor of 10x too large

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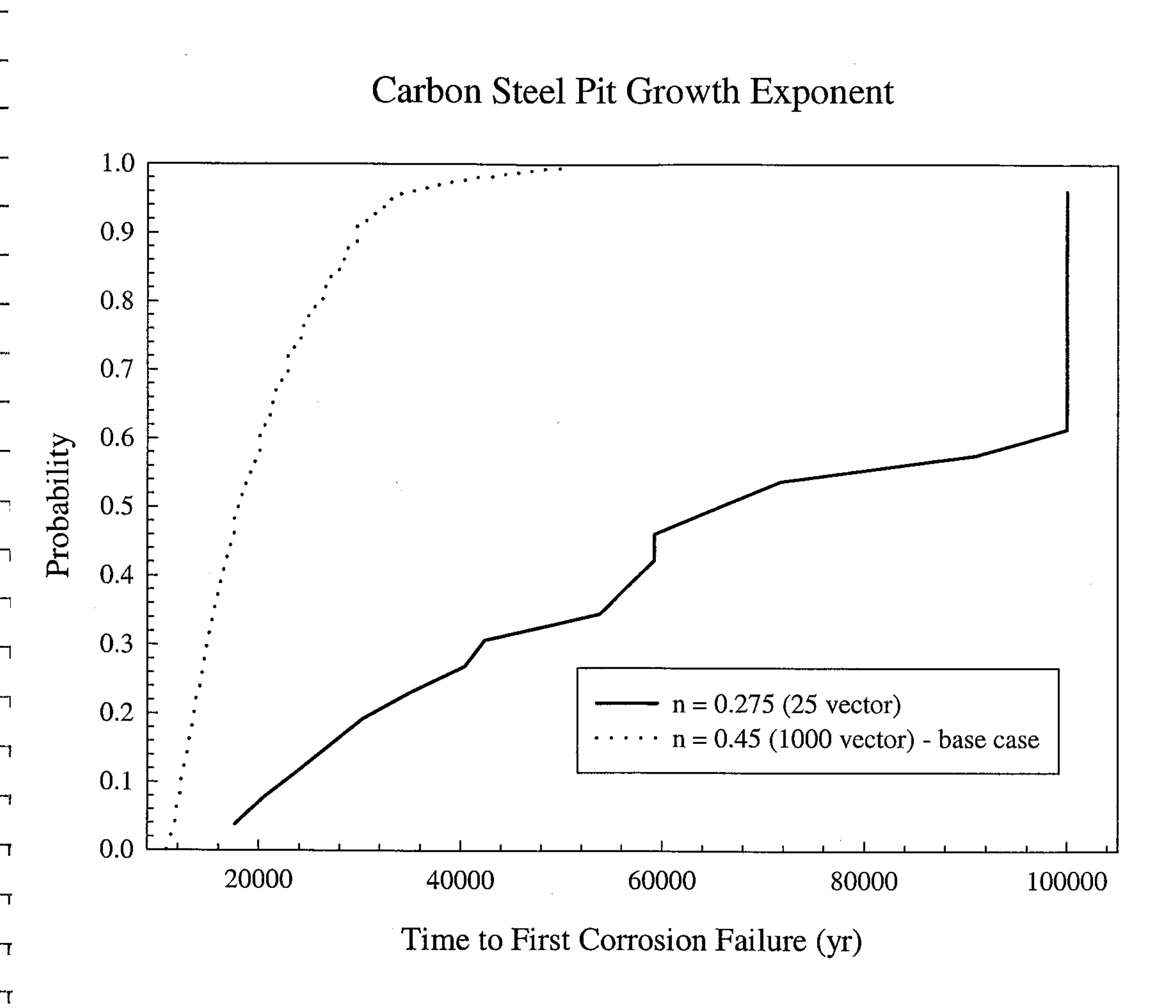
25 vector carbon steel pit growth exponent (n)

→ n = 0.275, C-22 ipass = base case



totdose, tpa, wpsfail_n0275_25 runs

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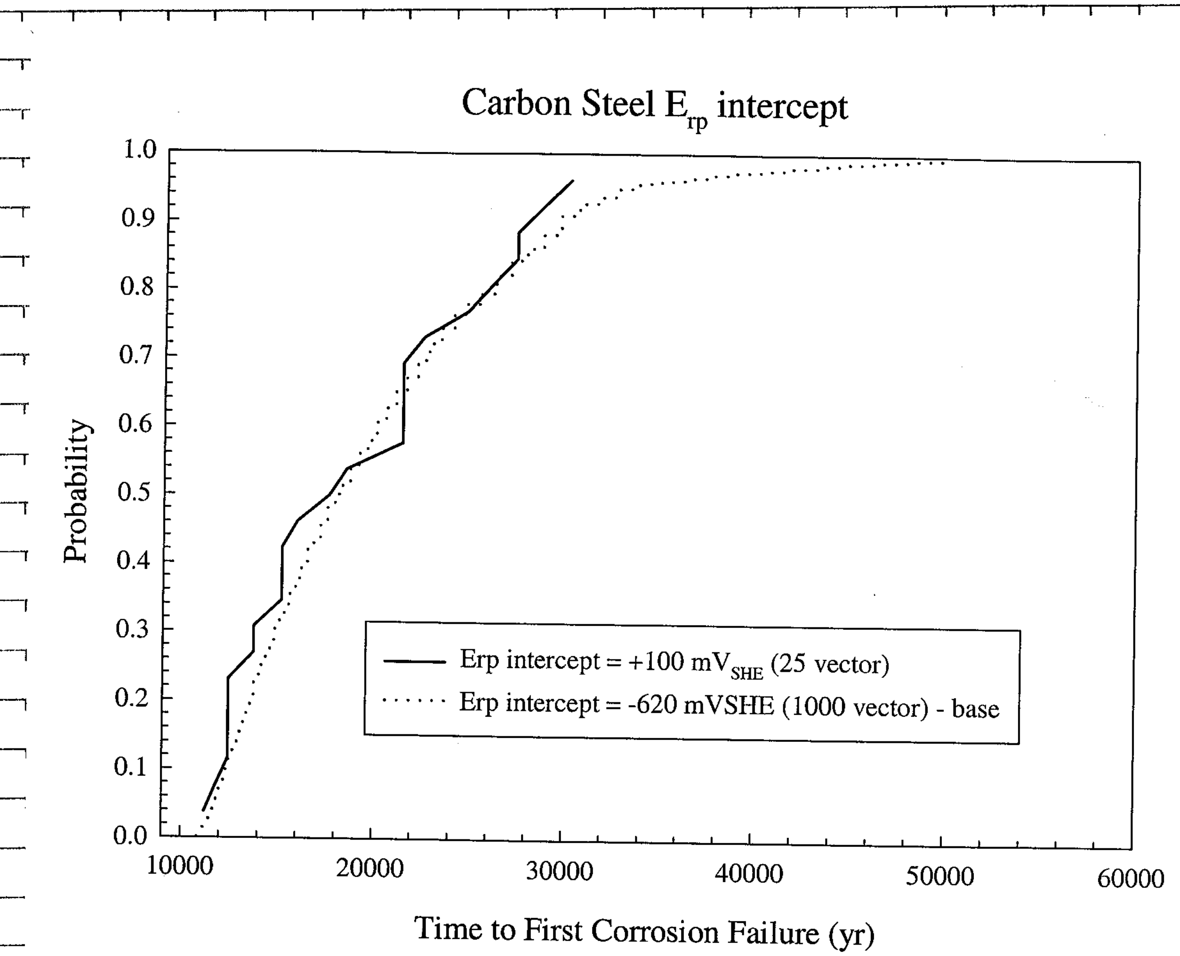

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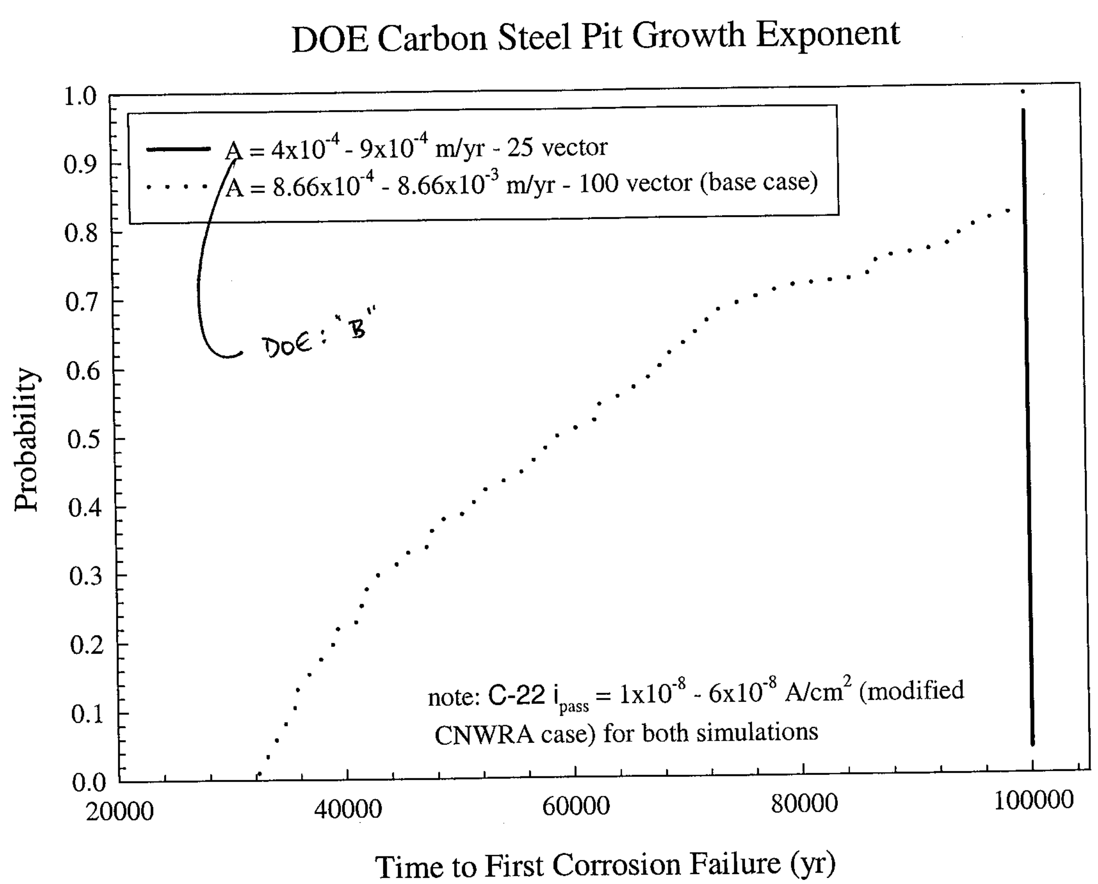

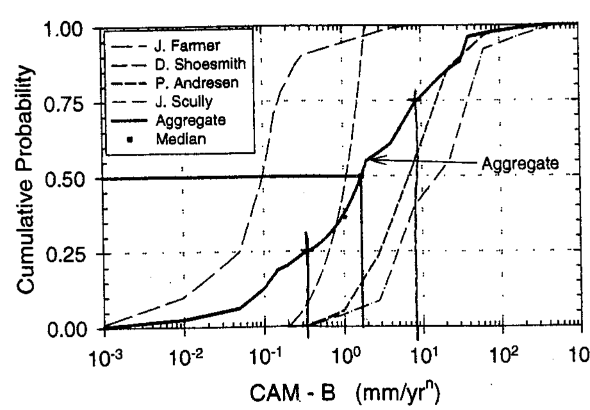

Figure 5-20. Cumulative distribution function of corrosion rate term in high pH CAM localized corrosion model.

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chapter 5, TSPA-VA
Tech. Bases Doc
B00000000-01717-
4301-00005 Rev 00
p F5-13

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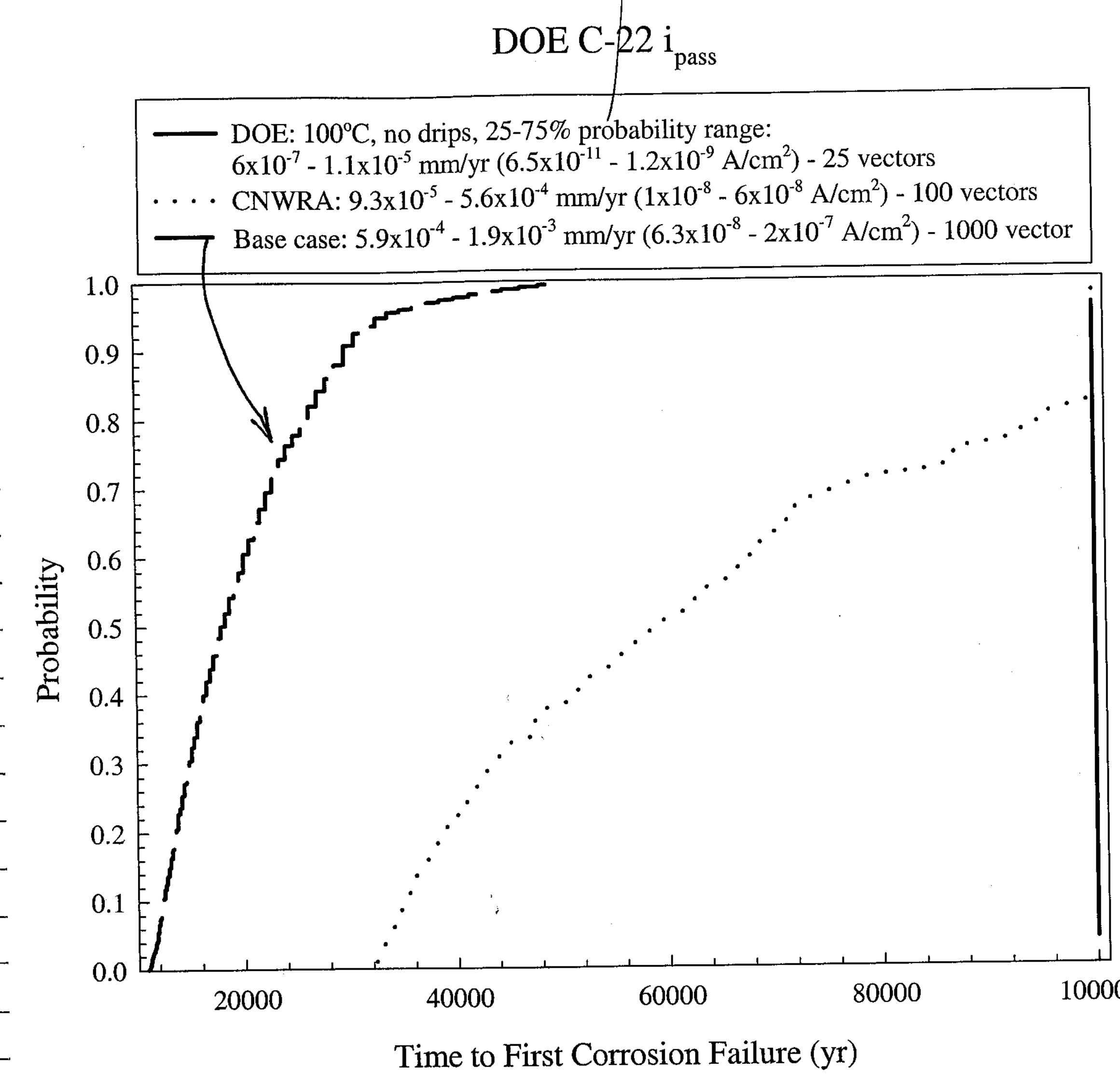
see p 34



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From Page No. 33 — DOE C-22 ipass / General Corrosion rates

no Dripping

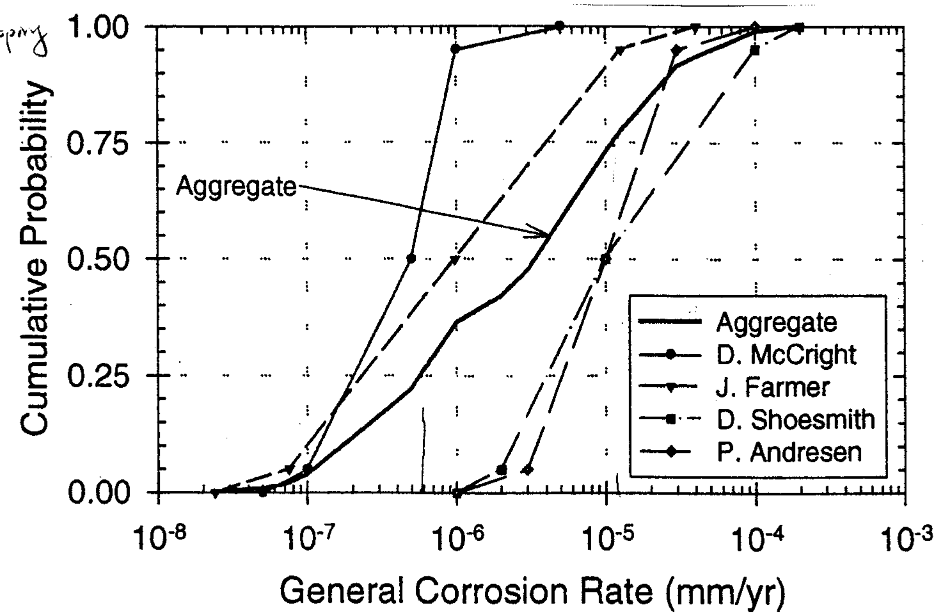

Figure 5-23. The cumulative distribution functions for the general corrosion rate of Alloy 22 at 100°C in the absence of dripping from the Waste Package Degradation Expert Elicitation (Pendleton 1998).

Dripping

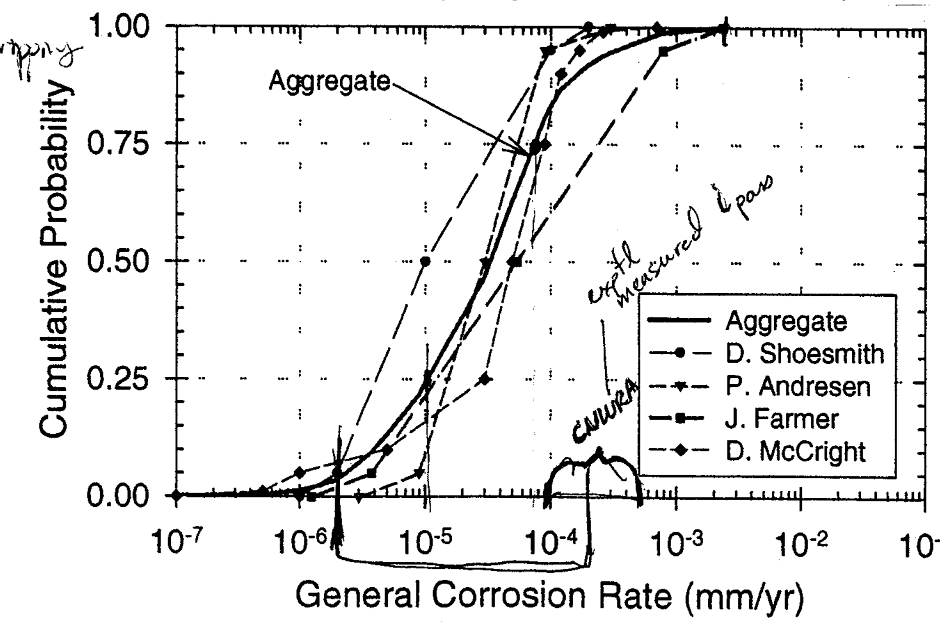

Figure 5-30. The cumulative distribution functions for the general corrosion rate of Alloy 22 at 100°C in the pH = 3 to 10, 340mV SHE dripping environment from the Waste Package Degradation Expert Elicitation (Pendleton 1998).

from B00000000-01717-4301-00005 Rev 00
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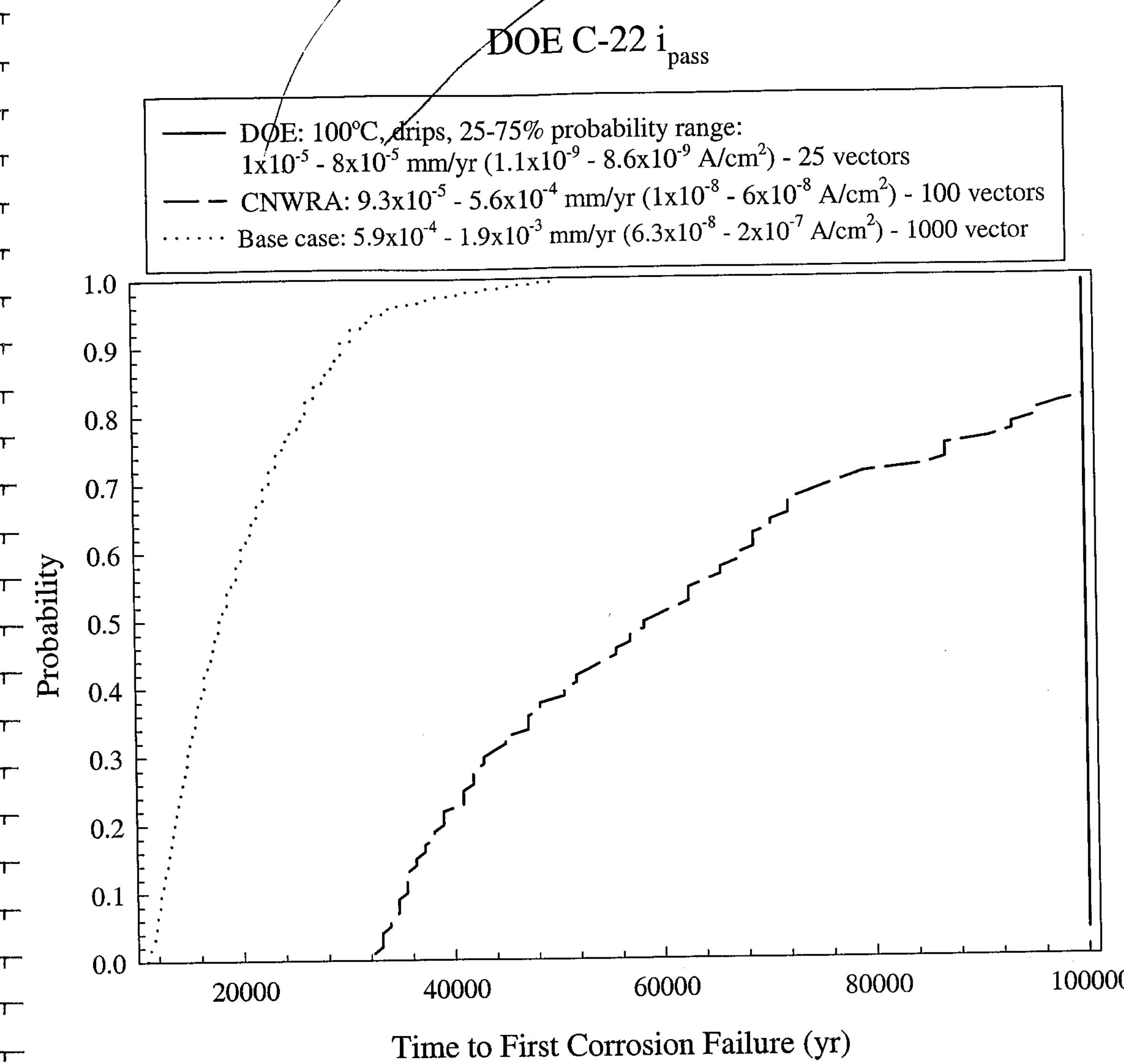
DOE ipass 25-75% probability value simulations
100 °C w/ dripping - values from p34 (Fig F5-30)
C CSB 12/16/98

3.40e2 2.12e3 C/m²·yR



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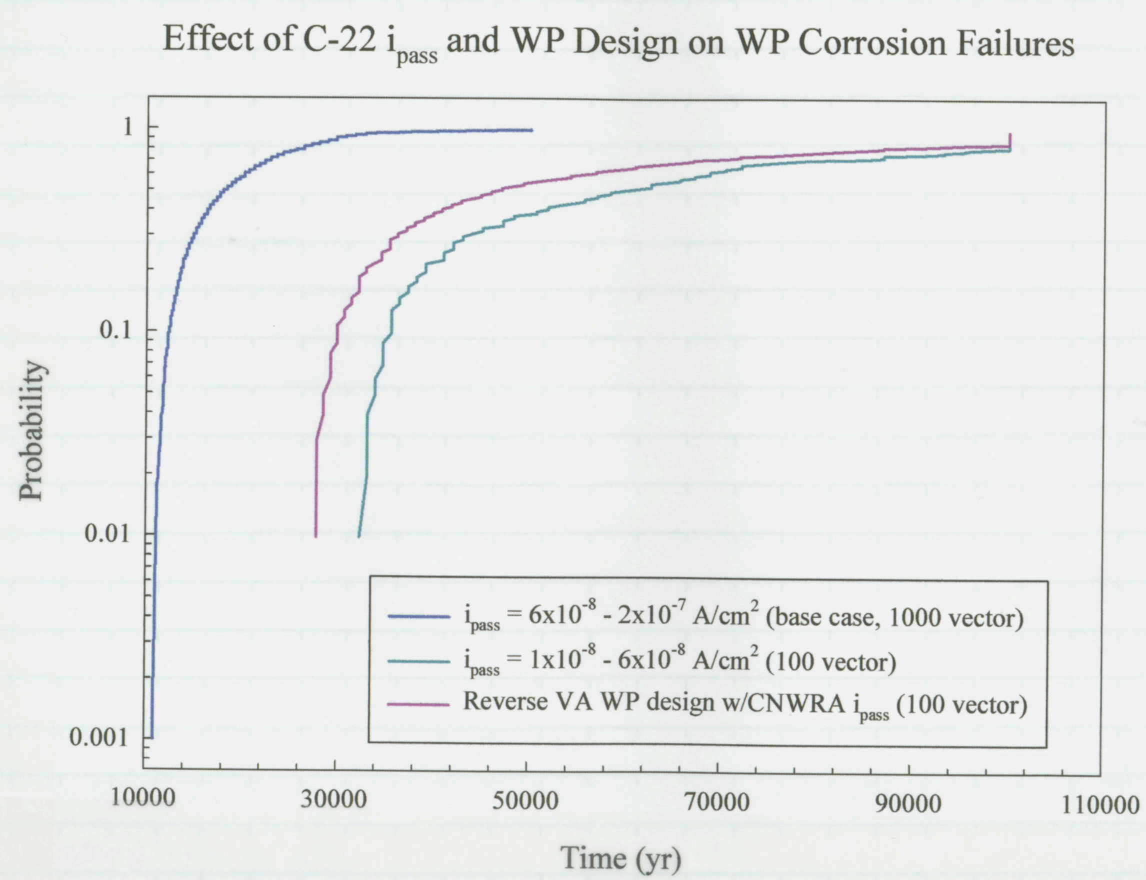
Simulated Reverse VA WP 4/2/99

C-22 thickness = 0.02

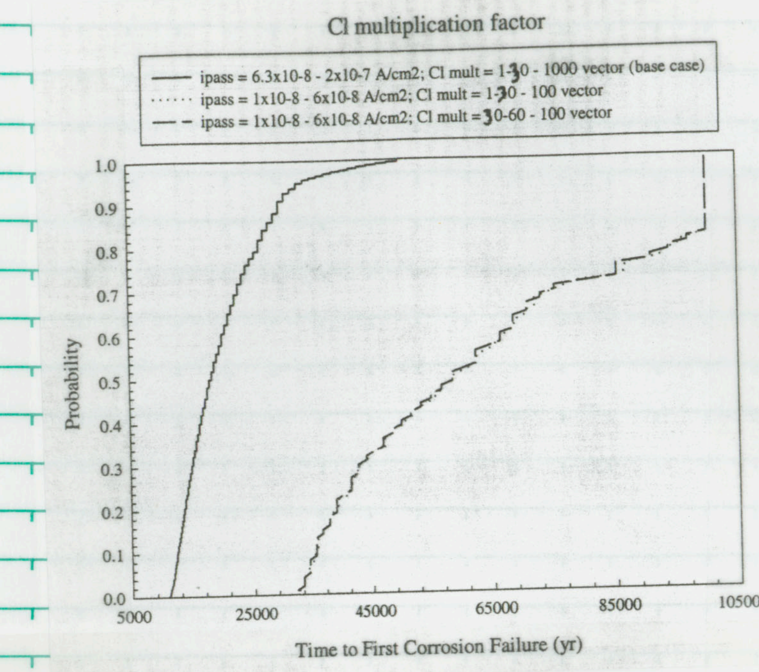
A516 thickness = 0.05

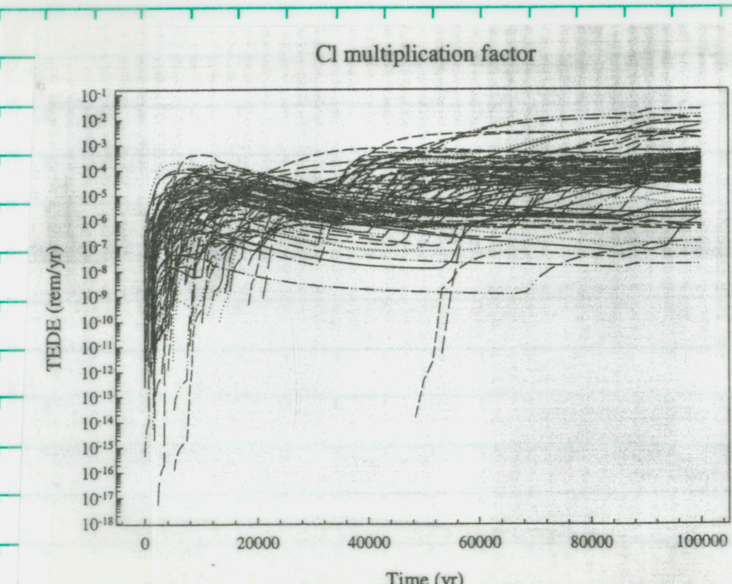
in TPA 3.2 code, parameters for C-22 and A516 swapped



SB 4/2/99

Effect of Cl mult on WP fail time & dose





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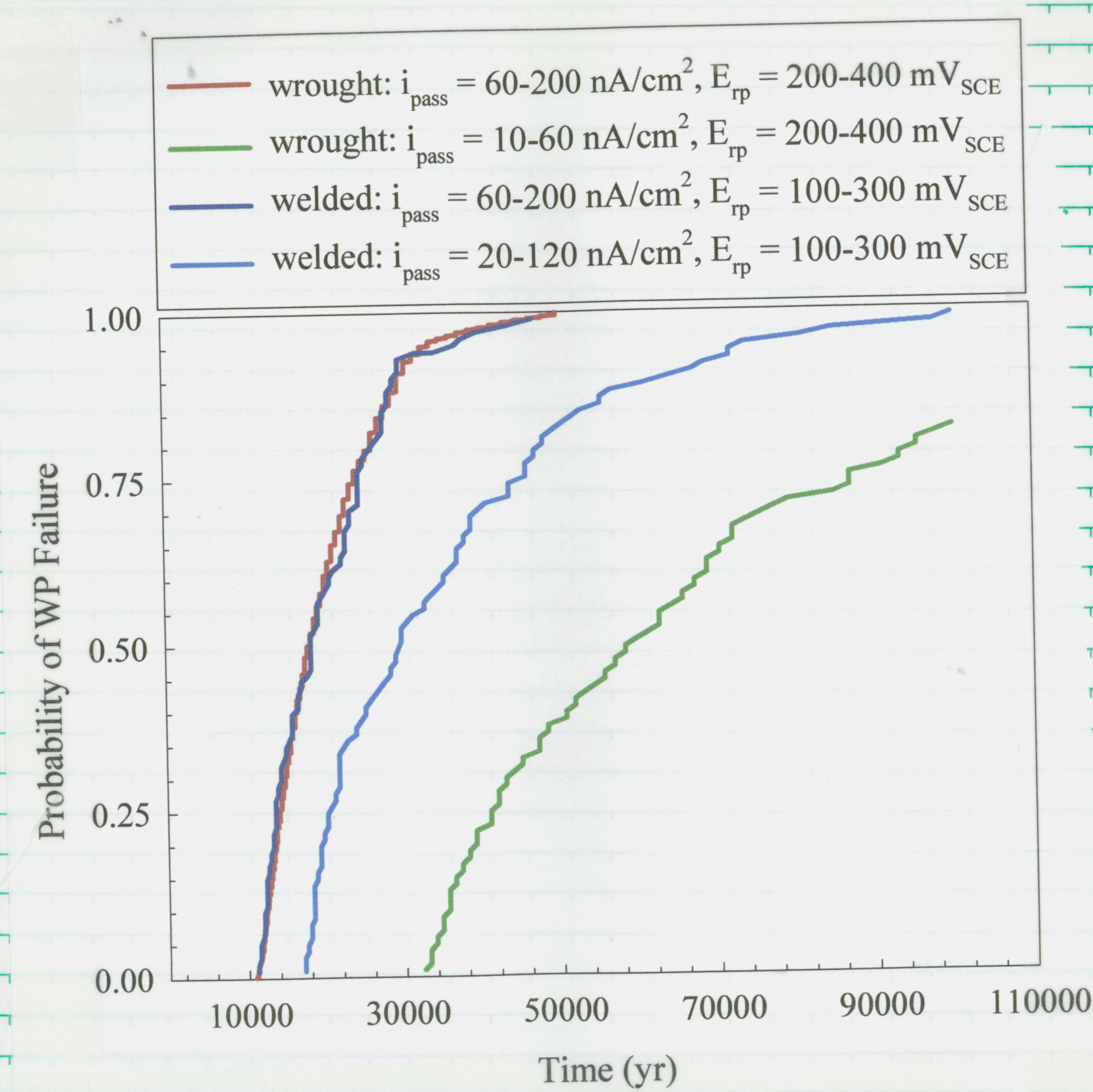
Effect of using CNWRA generated data for properties/parameters for welded C-22:



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Conversion Calculations

C-22 1/3

	wt %	at wt	ρ	EW	z
Ni	57.8	58.71	8.90	29.355	+2
Cr	21.4	51.996	7.19	17.332	+3
Mo	13.6	95.94	10.20	15.99	+6
Fe	3.80	55.847	7.86	27.924	+2
W	3.0	183.85	19.3	30.64	+6

$\rho = 8.69 \frac{g}{cm^3}$ (NACE Corrosion Engineer's Handbook page 79)

$$\text{At\% Ni} = \frac{0.578(58.71)}{0.578(58.71) + 0.214(51.996) + 0.136(95.94) + 0.038(55.847) + 0.03(183.85)}$$

$$= \frac{33.93438}{65.74705}$$

$$\boxed{= 0.516}$$

$$\text{At\% Cr} = \frac{0.214(51.996)}{65.74705}$$

$$\boxed{= 0.169}$$

$$\text{At\% Mo} = \frac{0.136(95.94)}{65.74705}$$

$$\boxed{= 0.198}$$

$$\text{At\% Fe} = \frac{0.038(55.847)}{65.74705}$$

$$\boxed{= 0.032}$$

$$\text{At\% W} = \frac{0.030(183.85)}{65.74705}$$

$$\boxed{= 0.084}$$

Equivalent Wt = EW

$$= 0.516(29.355) + 0.169(17.332) + 0.198(15.99) + 0.032(27.924) + 0.084(30.64)$$

$$\boxed{= 24.71 \text{ g/equiv}}$$

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$\rho = 8.69 \; g/cm^3$

$E.W. = 24.71 \; g/equiv.$

$F = 96481 \; C/equiv$

$\frac{A}{cm^2} = \frac{C}{cm^2 \cdot s}$

To convert A/cm^2 to $mm/yr \implies$

$$\frac{A}{cm^2} \Big| \frac{1}{\rho} \Big| EW \Big| \frac{1}{F} \Rightarrow \frac{C}{cm^2 \cdot s} \Big| \frac{cm^3}{g} \Big| \frac{g}{equiv} \Big| \frac{equiv}{C} \Rightarrow [cm/s]$$

$$\frac{1\,A}{cm^2} = \frac{1\,C}{cm^2 \cdot s} \Big| \frac{cm^3}{8.69\,g} \Big| \frac{24.71\,g}{equiv} \Big| \frac{equiv}{96481\,C}$$

$$= \underline{2.95 \times 10^{-5} \; cm/s}$$

to $\frac{mm}{yr}$ $\quad \frac{cm}{s} \Rightarrow \frac{cm}{s} \Big| \frac{10\,mm}{cm} \Big| \frac{3600\,s}{hr} \Big| \frac{24\,hr}{d} \Big| \frac{365\,d}{YR}$

$$1 \frac{cm}{s} = \underline{3.15 \times 10^{8} \frac{mm}{YR}}$$

so

$$1 \; A/cm^2 = 2.95 \times 10^{-5} \frac{cm}{s} \Big| \frac{3.15 \times 10^{8} \; mm/YR}{\frac{cm}{s}}$$

$$\boxed{= 9283 \; \frac{mm}{YR}}$$

$$\boxed{1 \frac{mm}{YR} = 1.08 \times 10^{-4} A/cm^2}$$

Convert from A/cm^2 to $C/m^2 \cdot yr$

$$\frac{A}{cm^2} = \frac{C}{cm^2 \cdot s} \Rightarrow \frac{C}{cm^2 \cdot s} \Big| \left(\frac{100\,cm}{m}\right)^2 \Big| \frac{3600\,s}{hr} \Big| \frac{24\,hr}{d} \Big| \frac{365\,d}{YR}$$

$$\boxed{1 \; A/cm^2 = 3.15 \times 10^{11} \frac{C}{m^2\,YR}}$$

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$$10^{-5} \frac{mm}{YR} \Rightarrow 10^{-5} \left[1.08 \times 10^{-4} \frac{A}{cm^2} / \frac{mm}{YR} \right]$$

$$= \underline{1.08 \times 10^{-9} A/cm^2}$$

$$\hookrightarrow 1.08 \times 10^{-9} A/cm^2 \Big| 3.15 \times 10^{11} = \underline{\underline{3.4 \times 10^{2} \; C/m^2 \cdot YR}}$$

$$mm/YR \underset{9283}{\overset{1.08 \times 10^{-4}}{\rightleftarrows}} A/cm^2 \underset{3.17 \times 10^{-12}}{\overset{3.15 \times 10^{11}}{\rightleftarrows}} C/m^2 \cdot YR$$

mm/YR	A/cm²	C/m²·YR
10^{-10}	1.08×10^{-14}	3.4×10^{-3}
10^{-8}	1.08×10^{-12}	3.4×10^{-1}
10^{-6}	1.08×10^{-10}	3.4×10^{1}
10^{-4}	1.08×10^{-8}	3.4×10^{3}
10^{-2}	1.08×10^{-6}	3.4×10^{5}
10^{0}	1.08×10^{-4}	3.4×10^{7}
10^{2}	1.08×10^{-2}	3.4×10^{9}

- base case

C/m²·YR	A/cm²	mm/YR
2×10^{4}	6.3×10^{-8}	5.9×10^{-4}
6.3×10^{4}	2×10^{-7}	1.9×10^{-3}

> modified base case

A/cm²	mm/YR	C/m²·YR
1×10^{-8}	9.3×10^{-5}	3.15×10^{3}
6×10^{-8}	5.6×10^{-4}	1.89×10^{4}

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TPA Test Plan and Results for SCR 294

Test name: Evaluation of New WP Corrosion Parameters and Overall Performance of TPA 4.0 on WP Corrosion

Anticipated start date: March 13, 2000

Anticipated completion date: March 21, 2000

Amount of your time available to perform this test: 20 hrs

Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50): 25/75

Output files to be checked: corrode.out/wpsfail.res

Input files to be checked for proper data transfer to the program: ebsfail.inp/tpa.inp

Disposition of documentation (storage medium, physical location, and access method):

Documentation contained in Scientific Notebook #298 in addition to zip disk electronic file storage in notebook.

Functional Test Descriptions:
Parameters Examined:

tpa.inp name	tpanames.dbs name	name in this analysis
CoefForLocCorrOfInnerOverpack	IO-CofLC	A_{C22}
ExponentForLocCorrOfInnerOverpack	IO-ExpLC	n_{C22}
DensityOuterOverpack	OO-Densy	316 density
DensityInnerOverpack	IO-Densy	C22 density
EquivalentWeightOuterOverpack	OO-EqWei	EW_{316}
EquivalentWeightInnerOverpack	IO-EqWei	EW_{C22}
AA_2_1	AA_2_1	C22 passive current density
CoefForLocCorrOfOuterOverpack	OO-CofLC	A_{316}
ExponentForLocCorrOfOuterOverpack	OO-ExpLC	n_{316}

- Hand Calculations: Hand calculations using an Excel spreadsheet were performed to analyze the output from process level modeling of failt.e. The parameters examined were the EW and density for both 316 stainless steel (SS) and alloy C22. The predicted time to failure and remaining thickness at 100,000 yr (if no failure had occurred) were calculated. Several assumptions were made in these calculations: (1) the initial humid-air corrosion/dry period was neglected for simplicity, (2) the

corrosion rate current density (i) in Equation 1 (EW is Equivalent Weight, F is Faraday's constant, and ρ is density), was determined based on the calculating the corrosion rate from the basecase time

$$CR = \frac{iEW}{F\rho} \qquad (1)$$

to failure and using the basecase parameters and was assumed to be constant for all simulations. This second assumption also allowed for a check of the Excel spreadsheet to ensure that it was performing properly.

- Process-level tests: The parameters examined were the EW and density for both 316SS and alloy C22. Each parameter was examined at 5 different levels: basecase, and 1/10, 1/2, 2x, and 10x of the basecase value. The predicted time to failure and remaining thickness at 100,000 yr (if no failure had occurred) were determined. For these simulations, only the corresponding material was analyzed. That is, for analysis of 316SS the thickness of the alloy C22 barrier was set to zero. Similarly the thickness of the 316SS was set to zero for the alloy C22 analyses.

- System-level tests: The analyses performed were aimed at examining the new corrosion parameters inserted into TPA 4.0 (EW and density for 316SS and alloy C22), parameters associated with localized corrosion (A and n from Equation 2, where D is the pit depth, A is a multiplication factor and t is time) which were already present but applied to carbon steel, and to gage the performance of TPA 4.0 as compared to TPA 3.2 from a WP corrosion perspective. For the analysis of A and n for alloy C22, the localized corrosion parameters associated with calculation of E_{rp} as

$$D = At^{n} \qquad (2)$$

well as the critical chloride concentration were assigned the values observed for alloy 625 to ensure that localized corrosion of alloy C22 would take place. In addition, given the long WP lifetimes expected with alloy C22, the simulations were run out to 100,000 y and each simulation consisted of 100 vectors.

Reasonableness Test Description: The results from the simulations were compared to hand calculations as well as to the direction of expected change (increasing or decreasing time to WP corrosion failures) to determine reasonableness.

Final Checklist (completed during testing):
- Did the modification substantially change the results?
No. There did not appear to be a significant change in the results from the modifications.

- Were TPA 3.3 and TPA 4.0beta compared using corresponding mean values in tpa.inp?
No, but TPA 3.2 and TPA 4.0beta were compared using identical parameters. No significant differences observed.

- Which nuclides were monitored to determine reasonableness of results in term of dose?
No radionuclides were monitored, only WP corrosion was examined in this test.

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Results of Test Plan:

System-level tests:
Overall the modifications to the TPA 4.0 code as compared to TPA 3.2 were implemented correctly without significant effects on the functionality of the code. All the system level results are shown in the accompanying figures in the form of the probability of a WP corrosion failure as a function of time. As can be seen, there was no significant difference between the results obtained for the TPA 4.0 and TPA 3.2 basecase. When the EW for 316SS was increased, a decrease in time to corrosion failure would have been expected. No change was observed and was attributed to the likelihood that corrosion failure of 316 was dominated by localized corrosion rather than passive dissolution (where EW would influence the results). Similar results were found for changes in the density of 316SS. Changes in the localized corrosion propagation parameters for 316SS did result in noticeable changes in predicted performance and the changes were in accordance with what was expected (i.e., increasing A resulted in a decrease in time to WP corrosion failure and increasing n resulted in delaying WP corrosion failure).

Examination of the corrosion parameters for alloy C22 yielded similar results. For further comparison of TPA 4.0 to TPA 3.2, the passive dissolution rate was modified to reflect the values measured in CNWRA experimental work (lower than that used in the TPA basecase). Only a slight deviation was noticed in comparing the two versions. This deviation is likely caused by the observation that the values used in the TPA 4.0 basecase for EW of 316SS and alloy C22 were reversed. That is, the value for EW for alloy C22 was lower than it should have been as the EW was assumed to be that of 316 and vise-versa. The net effect is that the EW for alloy C22 used in TPA 4.0 would cause an increase in the time to WP corrosion failure as was observed. This was further confirmed when EW was examined in which an increase in EW resulted in a decrease in the time to WP corrosion failure. Decreasing the density of alloy C22 by a factor of 10 also resulted in a significant decrease in time to first WP corrosion failure. When the localized corrosion parameters associated with Erp and the critical chloride concentration for alloy C22 were assigned the values used for alloy 625, a significant change in predicted performance was observed (similar to what has been seen with TPA 3.2). When the localized corrosion propagation terms (A and n) where then varied, the expected results were observed.

Summary of Observations from System-level tests:
Given the simplifying assumptions that went into these analyses and the observation that the changes made to various parameters had the appropriate effect on the end result of predicted WP corrosion performance, it appears that the modifications made to TPA 4.0 are satisfactory and have been correctly implemented.

Process-level tests:
Lastly, to examine the failt.e module, a series of simulations were run to calculate the corrosion rate and thus the effective time to failure for each of the WP barrier component materials considering the new EW and density parameters. When examining 316SS, the alloy C22 thickness was set to zero and the corrosion rates/time to failure from the code were compared to those determined through a simple hand calculation (see tables below). Based on the simplifying assumptions as outlined above, the hand calculations and the simulations agreed well (< 6% difference). The only exception to this were cases in which the time to failure was very short in which case the initial humid air corrosion/dry period would play a more significant role in determining the time to failure which was not considered in the hand calculations.

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Similar results were observed when examining alloy C22 with the 316SS thickness set to zero. In this case, however, the time to failure was not always used as in some simulations it was > 100,000 y (the end of the simulation). In these instances, the remaining thickness determined from the simulation and the hand calculation were compared. Again there was some deviation between the results, with the calculated thickness always being larger than the thickness determined from the simulation. At most the differences between these was 21 %.

Summary of Observations from Process-level tests:
Given the simplifying assumptions that went into these analyses and calculations and the observation that the changes made to various parameters had the appropriate effect on the end result of predicted WP corrosion performance, it appears that the modifications made to failt.e are satisfactory and have been correctly implemented.

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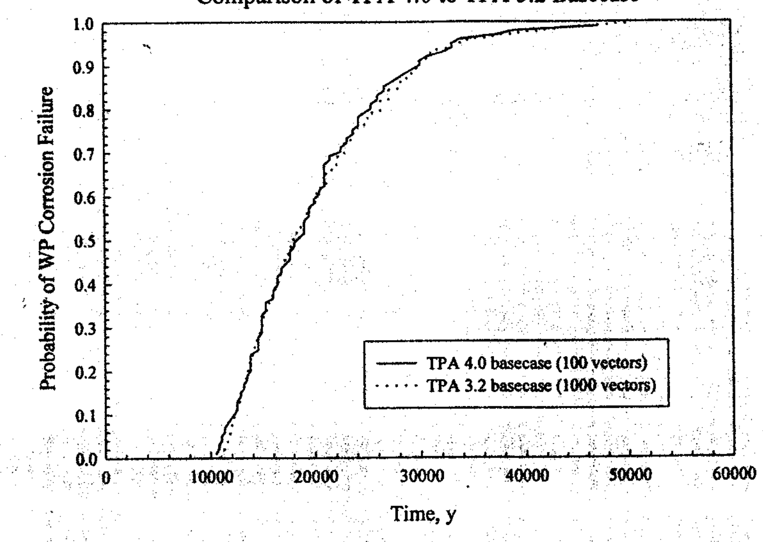
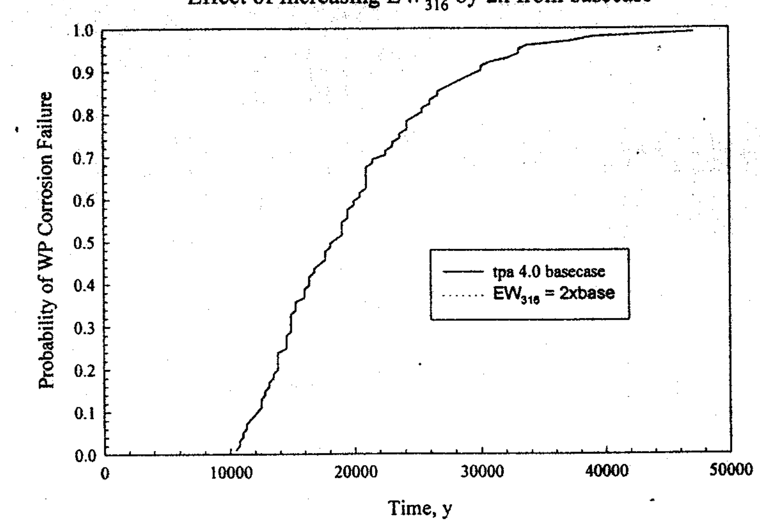
Comparison of TPA 4.0 to TPA 3.2 Basecase



Effect of Increasing EW_{316} by 2x from basecase



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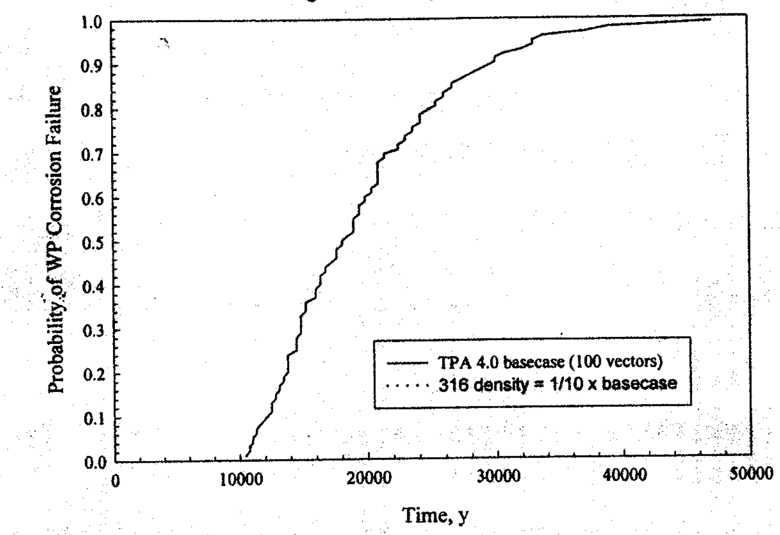
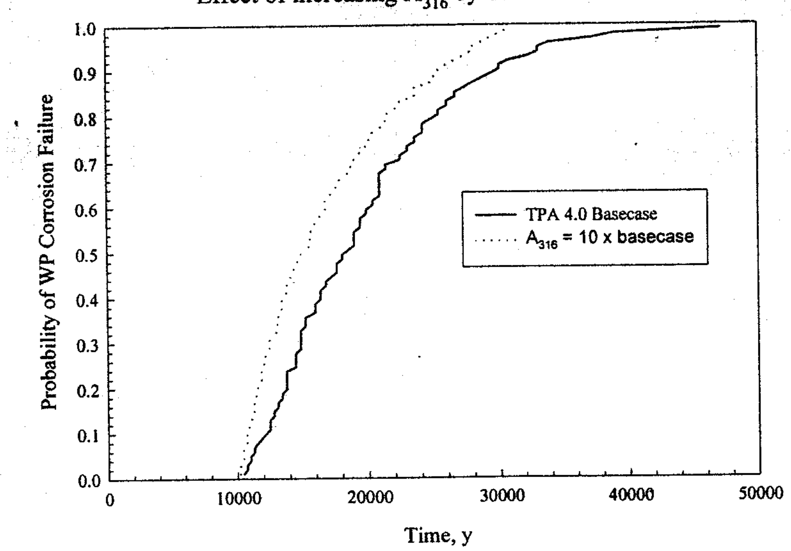
Effect of decreasing 316 density by a factor of 1/10 of basecase



Effect of increasing A_{316} by 10x from basecase



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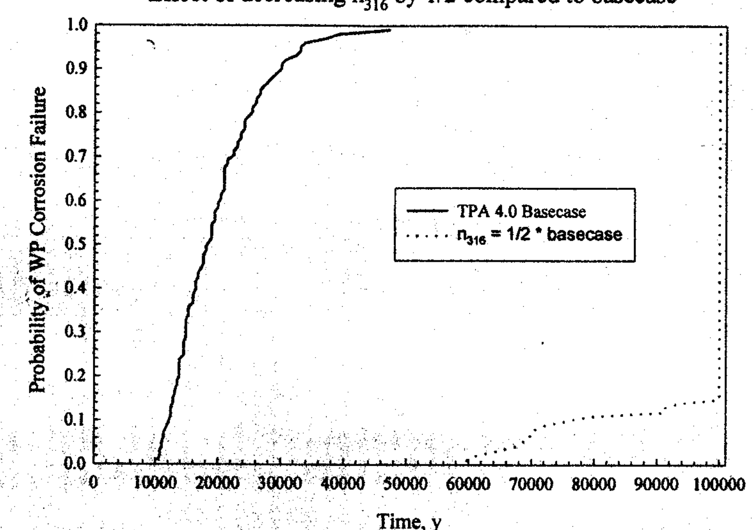
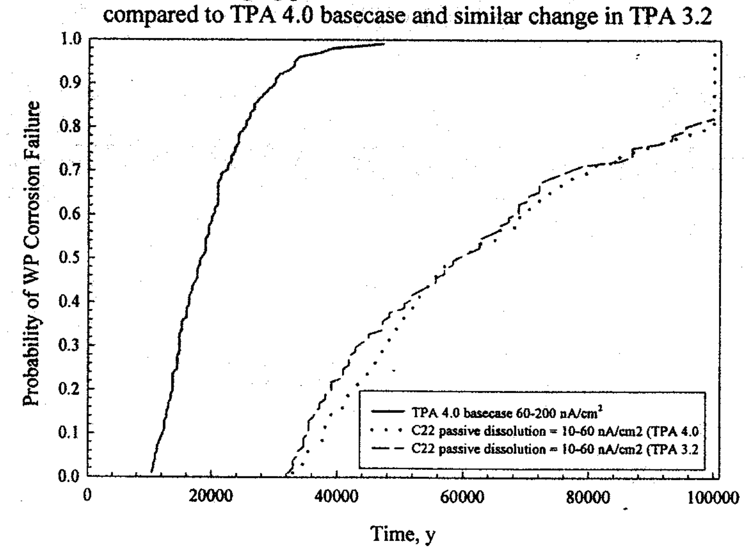
Effect of decreasing n_{316} by 1/2 compared to basecase



Effect of changing passive dissolution rate of C22 in TPA 4.0 compared to TPA 4.0 basecase and similar change in TPA 3.2



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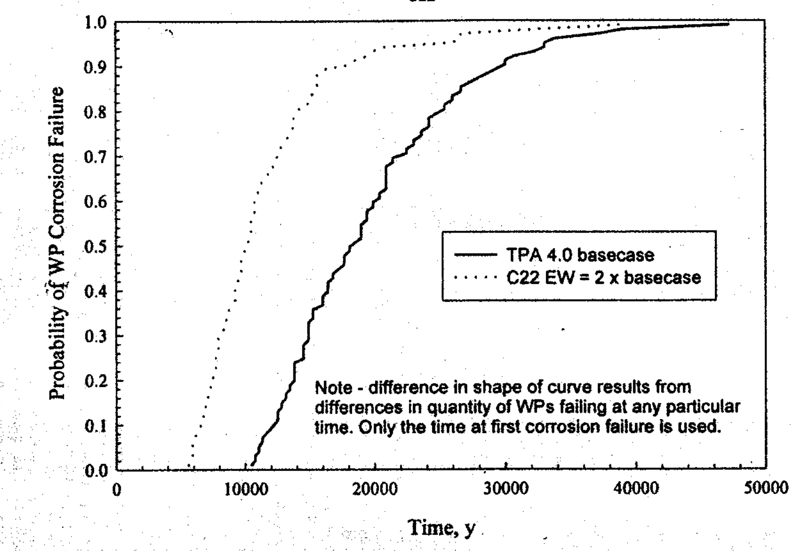
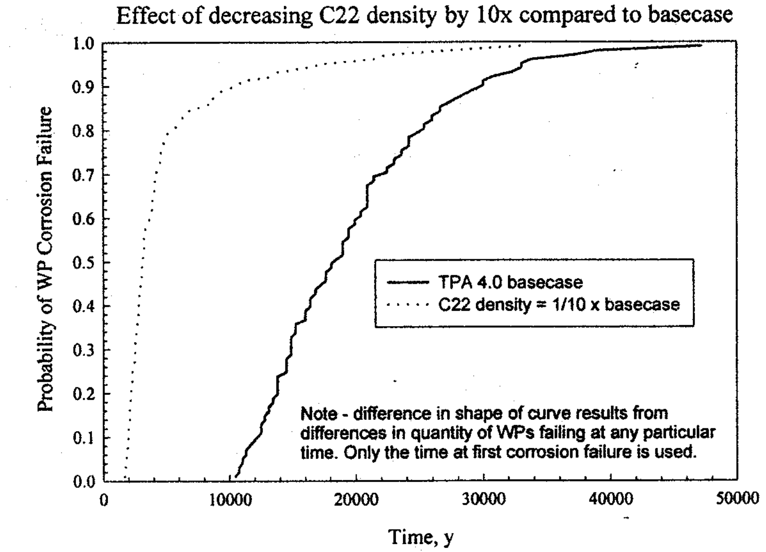
Effect of increasing EW_{C22} by 2x compared to basecase



Effect of decreasing C22 density by 10x compared to basecase



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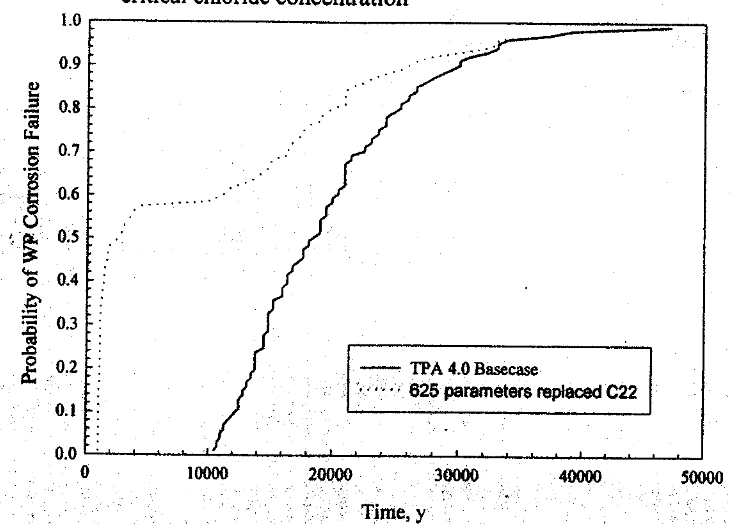
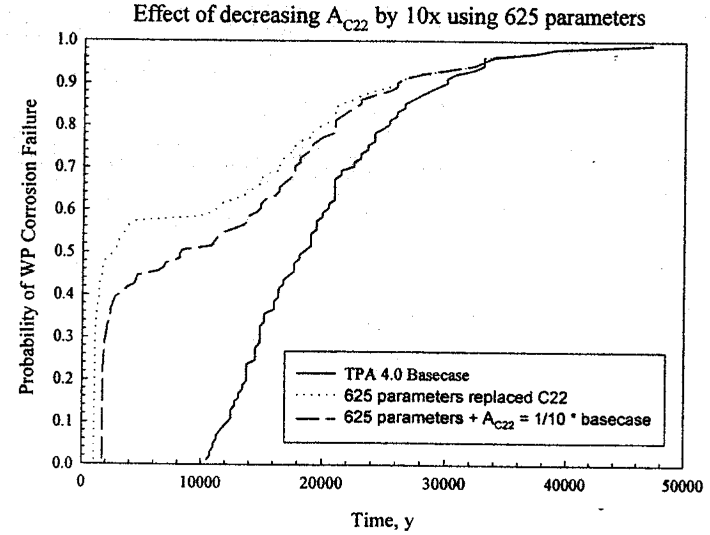
Replacement of 625 parameters for C22:
E_{rp} (including slope, temperature dependence, intercepts)
critical chloride concentration



Effect of decreasing A_{C22} by 10x using 625 parameters



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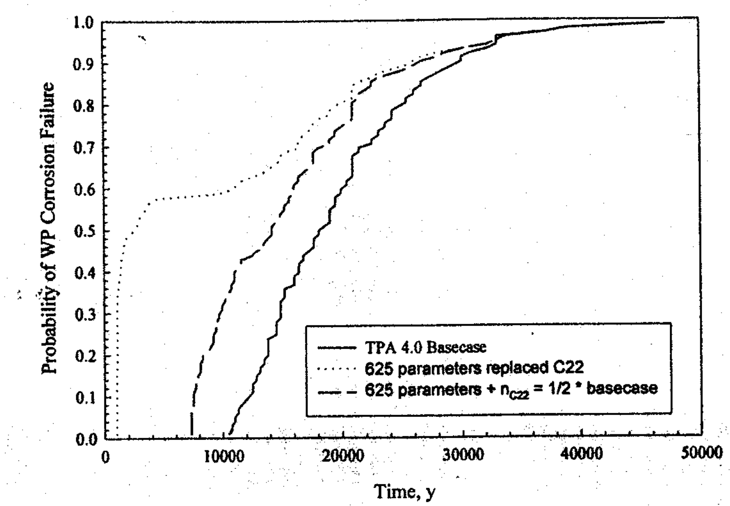
Effect of decreasing n_{C22} by 2x using 625 parameters



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316 Analysis

Case	EW	density	I,	CR	time to failure (0.1m) yrs	failt.e time to failure yrs	% difference
EW1	2.79E-02	7.86E+03	9.57E-03	3.52E-13	8995.73	8995.73	0.000
EW2	2.79E-03	7.86E+03	9.57E-03	3.52E-14	89957.3	84897.32	-5.960
EW3	1.40E-02	7.86E+03	9.57E-03	1.76E-13	17991.46	17659.68	-1.879
EW4	5.59E-02	7.86E+03	9.57E-03	7.05E-13	4497.865	4741.63	5.141
EW5	2.79E-01	7.86E+03	9.57E-03	3.52E-12	899.573	1390.75	35.317
p1	2.79E-02	7.86E+03	9.57E-03	3.52E-13	8995.73	8995.73	0.000
p2	2.79E-02	7.86E+02	9.57E-03	3.52E-12	899.573	1390.75	35.317
p3	2.79E-02	3.93E+03	9.57E-03	7.05E-13	4497.865	4741.63	5.141
p4	2.79E-02	1.57E+04	9.57E-03	1.76E-13	17991.46	17659.68	-1.879
p5	2.79E-02	7.86E+04	9.57E-03	3.52E-14	89957.3	84897.32	-5.960

note: assumed the same value for all runs based on basecase; also cannot account for initial dry/humid corrosion period in calculation

C22 Analysis 0.2 m

Case	EW	density	i (A/m²)	CR (m/s)	time to failure (yr)	failt.e ttf (yr)	% diff	thickness at 100kyr (m)	failt.e thickness at 100kyr (m)	%diff
EW1	2.55E-02	8.14E+03	2.84E-04	9.22E-15	68749.77999	68749.78	0.00	-0.0091	0.0000	#DIV/0!
EW2	2.55E-03	8.14E+03	2.84E-04	9.22E-16	687497.7999	100000	-588	0.0171	0.0151	-13.18
EW3	1.28E-02	8.14E+03	2.84E-04	4.61E-15	137499.56	100000	-37.50	0.0055	0.0045	-21.05
EW4	5.11E-02	8.14E+03	2.84E-04	1.84E-14	34374.89	34658.61	0.82	-0.0382	0.0000	#DIV/0!
EW5	2.54E-01	8.14E+03	2.84E-04	9.18E-14	6907.484189	7308.63	5.49	-0.2695	0.0000	#DIV/0!
p1	2.55E-02	8.14E+03	2.84E-04	9.22E-15	68749.77999	68749.78	0.00	-0.0091	0.0000	#DIV/0!
p2	2.55E-02	8.14E+02	2.84E-04	9.22E-14	6874.977999	7308.63	5.93	-0.2709	0.0000	#DIV/0!
p3	2.55E-02	4.07E+03	2.84E-04	1.84E-14	34374.89	34658.61	0.82	-0.0382	0.0000	#DIV/0!
p4	2.55E-02	1.63E+04	2.84E-04	4.61E-15	137499.56	100000	-37.50	0.0055	0.0045	-21.05
p5	2.55E-02	8.14E+04	2.84E-04	9.22E-16	687497.7999	100000	-588	0.0171	0.0151	-13.18

note: assumed the same value for all runs based on basecase; also cannot account for initial dry/humid corrosion period in calculation

11

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Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by SB	3/13/00

TITLE
Project No.
Book No.

From Page No.

Ti Calculations:

$1 A/cm^2 \Rightarrow \frac{1\,A}{cm^2} \left| \frac{1\,cm^3}{4.51\,g} \right| \frac{47.86\,g}{4\,equiv} \left| \frac{1\,equiv}{96481\,C} \right. = 2.75 \times 10^{-5}\,cm/s$

$\frac{1\,cm}{s} \left| \frac{10\,mm}{cm} \right| \frac{3600\,s}{h} \left| \frac{24\,h}{d} \right| \frac{365\,d}{y} \Rightarrow 1 A/cm^2 = 8671.8\,mm/y$

$1 \times 10^{-8}\,A/cm^2 = 8.7 \times 10^{-5}\,mm/y \Rightarrow$ 172,974 yr to 15mm failure

$5 \times 10^{-7}\,A/cm^2 = 4.3 \times 10^{-3}\,mm/y \Rightarrow$ 3,459 yr to 15mm failure

To Page No.

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by SB	8/9/2000

From Page No.____

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

SCIENTIFIC NOTEBOOK REVIEW CHECKLIST RECORD

Scientific Notebook No.: 298

Accomplished

Yes ✓	1. Initial entries per QAP-001
Yes ✓	2. Dating of entries
No ✓	3. Corrections (crossed out, one line through w/initials/date)
No ✓	4. White out not used — incorrect, page tear not white out. SB 8/16/2000
Yes ✓	5. Page number visible on original notebook
Yes ✓	6. In process entries per QAP-001
N/A ✓	7. Figure numbers present
Yes ✓	8. Text visible
N/A ✓	9. Electronic Scientific Notebook changes initialed and dated
No ✓	10. Permanent ink or type only — small note, not entry in notebook SB 8/16/2000
Yes ✓	11. Signing of entries (not required on each page)
N/A ✓	12. Statement at the end of electronic Scientific Notebook print outs—"No original text removed"
N/A ✓	13. Electronic media in the scientific notebook properly labeled

Discrepancies have been identified. Yes X No ______

Checker: [signature] Date: 8/16/00

The discrepancies identified in this Scientific Notebook Review Checklist have been addressed by:

CSB [signature] 8/16/2000

Signature Date

CNWRA Form QAP-01 (8/2000)

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by SB [signature]	8/16/2000

From Page No.____

Copy of pages 42 - 54 sent to QA

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by SB [signature]	8/8/2000

Project No.______
Book No.______
TITLE Cl Mult / Multiflo Cl effects on WP

From Page No.____

```
Alloy 22 TPA 4.1a Cl

**        ***>>>  EBSFAIL   <<<***
**
constant
OuterWPThickness[m]
0.02
**
constant
InnerWPThickness[m]
0.00
**0.05
**
constant
MetalGrainRadius[micrometer]
13.75
**
constant
GrainBoundaryThickness[micrometer]
7.0e-4
**
constant
[illegible]Constant
[illegible]
**
constant
CriticalRelativeHumidityHumidAirCorro
sion
0.55
**
normal
CriticalRelativeHumidityAqueousCorros
ion
0.6, 0.65
**
uniform
ThicknessOfWaterFilm[m]
0.001, 0.003
**
constant
BoilingPointOfWater[C]
97.0
**
constant
OuterOverpackErpIntercept
[illegible]
**2006.0
**
constant
TempCoefOfOuterPackErpIntercept
-13.2
**-15.2
**
constant
OuterOverpackErpSlope
-362.7
**-590.7
```

```
**
constant
TempCoefOfOuterPackErpSlope
2.3
**4.3
**
constant
InnerOverpackErpIntercept
-10000.0
**48.5, 148.5   >>> 625 <<<
**
constant
TempCoefOfInnerPackErpIntercept
0.0
**
constant
InnerOverpackErpSlope
0.0
**-160.8   >>> 625 <<<
**
constant
TempCoefOfInnerPackErpSlope
0.0
**
constant
OuterWPBetaKineticsParameterforOxygen
0.75
**
constant
OuterWPBetaKineticsParameterforWater
0.5
**
constant
InnerWPBetaKineticsParameterforOxygen
0.75
**
constant
InnerWPBetaKineticsParameterforWater
0.5
**
constant
OuterWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
OuterWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
OuterWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
**
constant
```

To Page No. 68

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by SB	1/4/01

TITLE______
Project No.______
Book No.______

From Page No.____

```
OuterWPActivationEnergyforWaterReduct
ion[J/mole]
25000.0
**
constant
InnerWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
InnerWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
InnerWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
**
constant
InnerWPActivationEnergyforWaterReduct
ion[J/mole]
[illegible]
**
[illegible]
AA_1_1[C/m2/yr]
1.6e3, 1.7e4
**
constant
AA_2_1[C/m2/yr]
1e10
**
constant
MeasuredGalvanicCouplePotential
0.0
**
constant
CoefForLocCorrOfOuterOverpack
2.5e-4
**
constant
ExponetForLocCorrOfOuterOverpack
1.0
**OPR
constant
CoefForLocCorrOfInnerOverpack
1.0
**
constant
ExponentForLocCorrOfInnerOverpack
1.0
**ENDOPR
constant
HumidAirCorrosionRate[m/yr]
1.0e-15
**
**OPR deleted parameter 1/10/2000
```

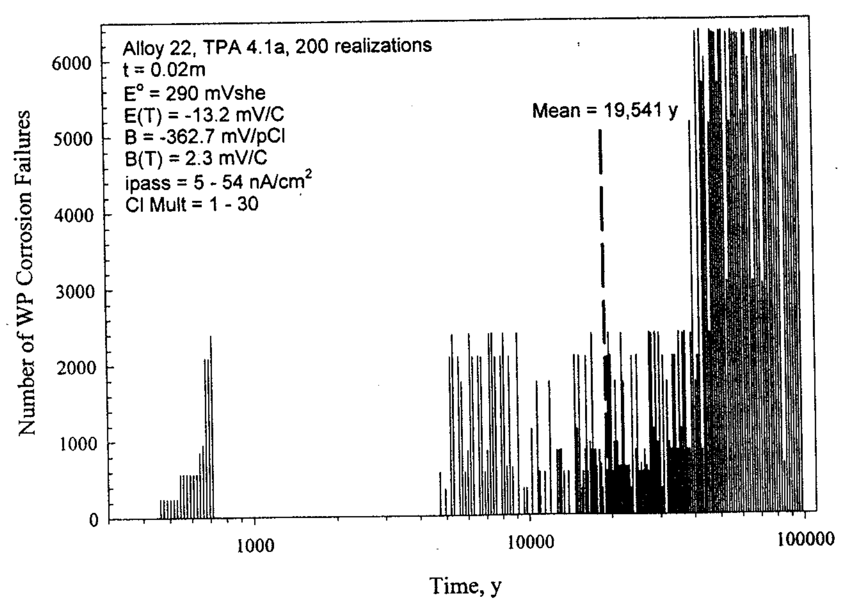
```
**constant
**LocalizedCorrRateOfInnerOverpack[m/
yr]
**2.5e-4
**ENDOPR
**
constant
FractionalCouplingStrength
0.0
**
constant
FactorForDefiningChoiceOfCritPotentia
l
0.0
**
constant
CritChlorideConcForFirstLayer[mol/L]
1.0
**0.5
**
constant
[illegible]ChlorideConcForSecondLayer[mol/L]
[illegible]e-10
**3.0e-2  >>> 625 <<<
**
uniform
ChlorideMultFactor
1.0, 30.0
**
**OPR
constant
ChlorideMultFactorIntactDripShield
1.0
**
lognormal
DripShieldFailureTime[yr]
1, 20
**3700.0, 27300.0
**ENDOPR
constant
ReferencepH
9.0
**
constant
WPsurfaceScaleThickness[m]
0.0
**
constant
TortuosityOfScaleonWP
1.0
**
constant
PorosityOfScaleonWP
1.0
**
constant
YieldStrength[MPa]
```

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by SB	1/4/01

From Page No.

```
370.0
**
constant
SafetyFactor
1.4
**
constant
FractureToughness[MPa-m**0.5]
1.0e7
**
**OPR
constant
DensityOuterOverpack[kg/m^3]
8690.0
**
constant
DensityInnerOverpack[kg/m^3]
7700.0
**
constant
EquivalentWeightOuterOverpack[kg/mol]
0.02597
**
constant
EquivalentWeightInnerOverpack[kg/mol]
0.02494
**
constant
DeltaPotentialDueToRadiolysis[V]
0.0
**
constant
DecayingConstantRadiolysis[1/yr]
7.0e-5
**ENDOPR
```



To Page No.______

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		Recorded by [signature]	1/4/01

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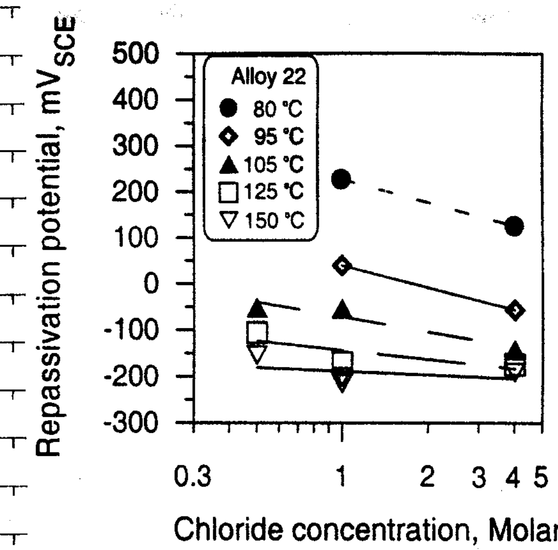
Determination of E^0 for Alloy 22

MRS 2000 paper

CORROSION PROCESSES AFFECTING THE PERFORMANCE OF ALLOY 22 AS A HIGH-LEVEL RADIOACTIVE WASTE CONTAINER MATERIAL

G.A. Cragnolino, [redacted] Y.-M. Pan, and O. Pensado
Center for Nuclear Waste Regulatory Analyses (CNWRA)
Southwest Research Institute
6220 Culebra Road, San Antonio, TX, 78238-5166, USA
gcragno@swri.edu



regression equation in paper:

$E^0(T) = +1300 - 13.1\,T$ (mVsce)

$B(T) = -362.7 + 2.3\,T$

$E^0 = 1300 + 242$ (convert to she) $- 13.1\,(95°C)$

$= 297.5$ mVshe ~ 290 mVshe

To Page No.______

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	1/04/01

From Page No.____

```
Alloy 22 TPA4.1a lowClmult
**        ***>>>  EBSFAIL   <<<***
**
constant
OuterWPThickness[m]
0.02
**
constant
InnerWPThickness[m]
0.00
**0.05
**
constant
MetalGrainRadius[micrometer]
13.75
**
constant
GrainBoundaryThickness[micrometer]
7.0e-4
**
constant
DryOxidationConstant
9999
**
constant
CriticalRelativeHumidityHumidAirCorro
sion
0.55
**
normal
CriticalRelativeHumidityAqueousCorros
ion
0.6, 0.65
**
uniform
ThicknessOfWaterFilm[m]
0.001, 0.003
**
constant
BoilingPointOfWater[C]
97.0
**
constant
OuterOverpackErpIntercept
290
**2006.0
**
constant
TempCoefOfOuterPackErpIntercept
-13.2
**-15.2
**
constant
OuterOverpackErpSlope
-362.7
**-590.7
**
constant
TempCoefOfOuterPackErpSlope
2.3
**4.3
**
constant
InnerOverpackErpIntercept
-10000.0
**48.5, 148.5  >>> 625 <<<
**
constant
TempCoefOfInnerPackErpIntercept
0.0
**
constant
InnerOverpackErpSlope
0.0
**-160.8   >>> 625 <<<
**
constant
TempCoefOfInnerPackErpSlope
0.0
**
constant
OuterWPBetaKineticsParameterforOxygen
0.75
**
constant
OuterWPBetaKineticsParameterforWater
0.5
**
constant
InnerWPBetaKineticsParameterforOxygen
0.75
**
constant
InnerWPBetaKineticsParameterforWater
0.5
**
constant
OuterWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
OuterWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
OuterWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
**
constant
OuterWPActivationEnergyforWaterReduct
ion[J/mole]
```

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	01/04/01

From Page No.____

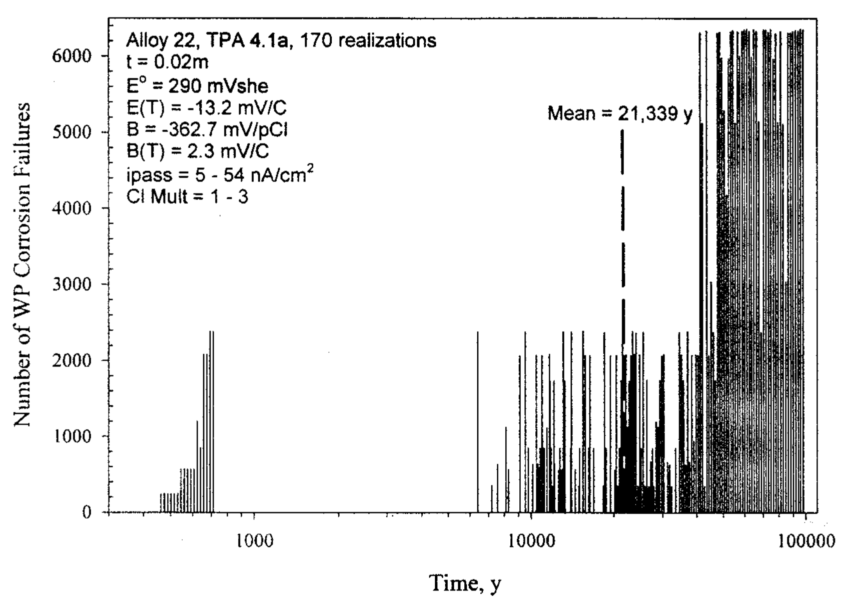
```
25000.0
**
constant
InnerWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
InnerWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
InnerWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
**
constant
InnerWPActivationEnergyforWaterReduct
ion[J/mole]
25000.0
**
normal
AA_1_1[C/m2/yr]
1.6e3, 1.7e4
**
constant
AA_2_1[C/m2/yr]
1e10
**
constant
MeasuredGalvanicCouplePotential
0.0
**
constant
CoefForLocCorrOfOuterOverpack
2.5e-4
**
constant
ExponetForLocCorrOfOuterOverpack
1.0
**OPR
constant
CoefForLocCorrOfInnerOverpack
1.0
**
constant
ExponentForLocCorrOfInnerOverpack
1.0
**ENDOPR
constant
HumidAirCorrosionRate[m/yr]
1.0e-15
**
**OPR deleted parameter 1/10/2000
**constant
**LocalizedCorrRateOfInnerOverpack[m/
yr]
**2.5e-4
**ENDOPR
**
constant
FractionalCouplingStrength
0.0
**
constant
FactorForDefiningChoiceOfCritPotentia
l
0.0
**
constant
CritChlorideConcForFirstLayer[mol/L]
1.0
**0.5
**
constant
CritChlorideConcForSecondLayer[mol/L]
1.0e-10
**3.0e-2  >>> 625 <<<
**
uniform
ChlorideMultFactor
1.0, 3.0
**
**OPR
constant
ChlorideMultFactorIntactDripShield
1.0
**
lognormal
DripShieldFailureTime[yr]
1, 20
**3700.0, 27300.0
**ENDOPR
constant
ReferencepH
9.0
**
constant
WPsurfaceScaleThickness[m]
0.0
**
constant
TortuosityOfScaleonWP
1.0
**
constant
PorosityOfScaleonWP
1.0
**
constant
YieldStrength[MPa]
370.0
```

To Page No.____

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	01/04/01

From Page No.

```
**
constant
SafetyFactor
1.4
**
constant
FractureToughness[MPa-m**0.5]
1.0e7
**
**OPR
constant
DensityOuterOverpack[kg/m^3]
8690.0
**
constant
DensityInnerOverpack[kg/m^3]
7700.0
**
constant
EquivalentWeightOuterOverpack[kg/mol]
0.02597
**
constant
EquivalentWeightInnerOverpack[kg/mol]
0.02494
**
constant
DeltaPotentialDueToRadiolysis[V]
0.0
**
constant
DecayingConstantRadiolysis[1/yr]
7.0e-5
**ENDOPR
```



To Page No.______

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	01/04/01

From Page No.

```
Alloy 625 TPA4.1a Cl
**          ***>>>  EBSFAIL   <<<***
**
constant
OuterWPThickness[m]
0.02
**
constant
InnerWPThickness[m]
0.00
**0.05
**
constant
MetalGrainRadius[micrometer]
13.75
**
constant
GrainBoundaryThickness[micrometer]
7.0e-4
**
constant
DryOxidationConstant
9999
**
constant
CriticalRelativeHumidityHumidAirCorro
sion
0.55
**
normal
CriticalRelativeHumidityAqueousCorros
ion
0.6, 0.65
**
uniform
ThicknessOfWaterFilm[m]
0.001, 0.003
**
constant
BoilingPointOfWater[C]
97.0
**
constant
OuterOverpackErpIntercept
98.5
**290
**2006.0
**
constant
TempCoefOfOuterPackErpIntercept
0.0
**-13.2
**-15.2
**
constant
OuterOverpackErpSlope
-160.8
```

```
**-362.7
**-590.7
**
constant
TempCoefOfOuterPackErpSlope
0.0
**2.3
**4.3
**
constant
InnerOverpackErpIntercept
-10000.0
**48.5, 148.5  >>> 625 <<<
**
constant
TempCoefOfInnerPackErpIntercept
0.0
**
constant
InnerOverpackErpSlope
0.0
**-160.8   >>> 625 <<<
**
constant
TempCoefOfInnerPackErpSlope
0.0
**
constant
OuterWPBetaKineticsParameterforOxygen
0.75
**
constant
OuterWPBetaKineticsParameterforWater
0.5
**
constant
InnerWPBetaKineticsParameterforOxygen
0.75
**
constant
InnerWPBetaKineticsParameterforWater
0.5
**
constant
OuterWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
OuterWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
OuterWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
```

To Page No.______

Witnessed & Understood by me,	Date	Invented by	Date
		Recorded by [signature]	01/04/01

From Page No.

```
**
constant
OuterWPActivationEnergyforWaterReduct
ion[J/mole]
25000.0
**
constant
InnerWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
InnerWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
InnerWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
**
constant
InnerWPActivationEnergyforWaterReduct
ion[J/mole]
25000.0
**
normal
AA_1_1[C/m2/yr]
1.6e3, 1.7e4
**
constant
AA_2_1[C/m2/yr]
1e10
**
constant
MeasuredGalvanicCouplePotential
0.0
**
constant
CoefForLocCorrOfOuterOverpack
2.5e-4
**
constant
ExponetForLocCorrOfOuterOverpack
1.0
**OPR
constant
CoefForLocCorrOfInnerOverpack
1.0
**
constant
ExponentForLocCorrOfInnerOverpack
1.0
**ENDOPR
constant
HumidAirCorrosionRate[m/yr]
1.0e-15
```

```
**
**OPR deleted parameter 1/10/2000
**constant
**LocalizedCorrRateOfInnerOverpack[m/
yr]
**2.5e-4
**ENDOPR
**
constant
FractionalCouplingStrength
0.0
**
constant
FactorForDefiningChoiceOfCritPotentia
l
0.0
**
constant
CritChlorideConcForFirstLayer[mol/L]
3.0e-2
**1.0
**0.5
**
constant
CritChlorideConcForSecondLayer[mol/L]
1.0e-10
**3.0e-2  >>> 625 <<<
**
uniform
ChlorideMultFactor
1.0, 30.0
**
**OPR
constant
ChlorideMultFactorIntactDripShield
1.0
**
lognormal
DripShieldFailureTime[yr]
1, 20
**3700.0, 27300.0
**ENDOPR
constant
ReferencepH
9.0
**
constant
WPsurfaceScaleThickness[m]
0.0
**
constant
TortuosityOfScaleonWP
1.0
**
constant
PorosityOfScaleonWP
1.0
```

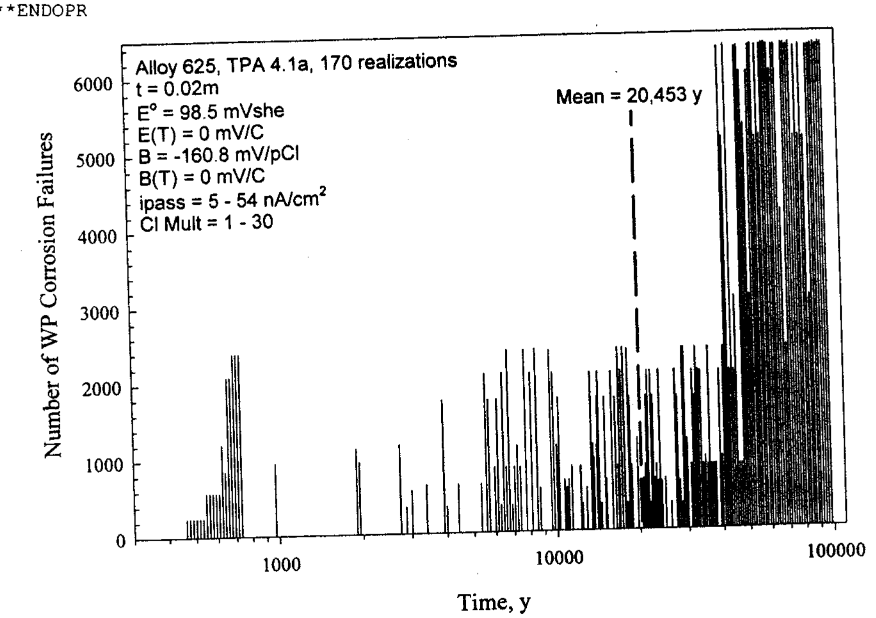
To Page No.

Witnessed & Understood by me, | Date | Invented by | Date

Recorded by [signature] 01/04/01

From Page No.

```
**
constant
YieldStrength[MPa]
370.0
**
constant
SafetyFactor
1.4
**
constant
FractureToughness[MPa-m**0.5]
1.0e7
**
**OPR
constant
DensityOuterOverpack[kg/m^3]
8690.0
**
constant
DensityInnerOverpack[kg/m^3]
7700.0
**
constant
EquivalentWeightOuterOverpack[kg/mol]
0.02597
**
constant
EquivalentWeightInnerOverpack[kg/mol]
0.02494
**
constant
DeltaPotentialDueToRadiolysis[V]
0.0
**
constant
DecayingConstantRadiolysis[1/yr]
7.0e-5
**ENDOPR
```



To Page No.

Witnessed & Understood by me, | Date | Invented by | Date

Recorded by [signature] 01/04/01

Project No.

Book No. TITLE

From Page No.

```
Alloy 625 TPA4.1a lowClmult
**          ***>>>  EBSFAIL   <<<***
**
constant
OuterWPThickness[m]
0.02
**
constant
InnerWPThickness[m]
0.00
**0.05
**
constant
MetalGrainRadius[micrometer]
13.75
**
constant
GrainBoundaryThickness[micrometer]
7.0e-4
**
constant
DryOxidationConstant
9999
**
constant
CriticalRelativeHumidityHumidAirCorro
sion
0.55
**
normal
CriticalRelativeHumidityAqueousCorros
ion
0.6, 0.65
**
uniform
ThicknessOfWaterFilm[m]
0.001, 0.003
**
constant
BoilingPointOfWater[C]
97.0
**
constant
OuterOverpackErpIntercept
98.5
**290
**2006.0
**
constant
TempCoefOfOuterPackErpIntercept
0.0
**-13.2
**-15.2
**
constant
OuterOverpackErpSlope
-160.8
**-362.7
**-590.7
**
constant
TempCoefOfOuterPackErpSlope
0.0
**2.3
**4.3
**
constant
InnerOverpackErpIntercept
-10000.0
**48.5, 148.5  >>> 625 <<<
**
constant
TempCoefOfInnerPackErpIntercept
0.0
**
constant
InnerOverpackErpSlope
0.0
**-160.8    >>> 625 <<<
**
constant
TempCoefOfInnerPackErpSlope
0.0
**
constant
OuterWPBetaKineticsParameterforOxygen
0.75
**
constant
OuterWPBetaKineticsParameterforWater
0.5
**
constant
InnerWPBetaKineticsParameterforOxygen
0.75
**
constant
InnerWPBetaKineticsParameterforWater
0.5
**
constant
OuterWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
OuterWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
OuterWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
```

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```
**
constant
OuterWPActivationEnergyforWaterReduct
ion[J/mole]
25000.0
**
constant
InnerWPRateConstantforOxygenReduction
[coulomb-m/mole/yr]
3.0e10
**
constant
InnerWPRateConstantforWaterReduction[
coulomb-m/m^2/yr]
3.2
**
constant
InnerWPActivationEnergyforOxygenReduc
tion[J/mole]
40000.0
**
constant
InnerWPActivationEnergyforWaterReduct
ion[J/mole]
25000.0
**
normal
AA_1_1[C/m2/yr]
1.6e3, 1.7e4
**
constant
AA_2_1[C/m2/yr]
1e10
**
constant
MeasuredGalvanicCouplePotential
0.0
**
constant
CoefForLocCorrOfOuterOverpack
2.5e-4
**
constant
ExponetForLocCorrOfOuterOverpack
1.0
**OPR
constant
CoefForLocCorrOfInnerOverpack
1.0
**
constant
ExponentForLocCorrOfInnerOverpack
1.0
**ENDOPR
constant
HumidAirCorrosionRate[m/yr]
1.0e-15
**
**OPR deleted parameter 1/10/2000
**constant
**LocalizedCorrRateOfInnerOverpack[m/
yr]
**2.5e-4
**ENDOPR
**
constant
FractionalCouplingStrength
0.0
**
constant
FactorForDefiningChoiceOfCritPotentia
l
0.0
**
constant
CritChlorideConcForFirstLayer[mol/L]
3.0e-2
**1.0
**0.5
**
constant
CritChlorideConcForSecondLayer[mol/L]
1.0e-10
**3.0e-2  >>> 625 <<<
**
uniform
ChlorideMultFactor
1.0, 3.0
**
**OPR
constant
ChlorideMultFactorIntactDripShield
1.0
**
lognormal
DripShieldFailureTime[yr]
1, 20
**3700.0, 27300.0
**ENDOPR
constant
ReferencepH
9.0
**
constant
WPsurfaceScaleThickness[m]
0.0
**
constant
TortuosityOfScaleonWP
1.0
**
constant
PorosityOfScaleonWP
1.0
```

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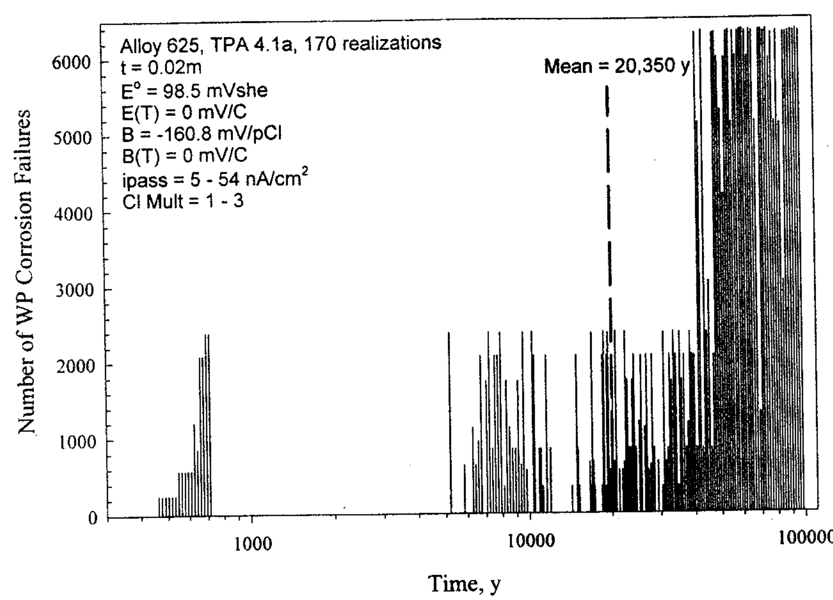
```
**
constant
YieldStrength[MPa]
370.0
**
constant
SafetyFactor
1.4
**
constant
FractureToughness[MPa-m**0.5]
1.0e7
**
**OPR
constant
DensityOuterOverpack[kg/m^3]
8690.0
**
constant
DensityInnerOverpack[kg/m^3]
7700.0
**
constant
EquivalentWeightOuterOverpack[kg/mol]
0.02597
**
constant
EquivalentWeightInnerOverpack[kg/mol]
0.02494
**
constant
DeltaPotentialDueToRadiolysis[V]
0.0
**
constant
DecayingConstantRadiolysis[1/yr]
7.0e-5
```



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mean failure time ~ 20 kyrs

from page 41,

$5\ nA/cm^2 = 4.64 \times 10^{-5}\ mm/y \Rightarrow 430,895$ yrs to failure

$54\ nA/cm^2 = 5.01 \times 10^{-4}\ mm/y \Rightarrow 39,920$ yrs to failure

seems to indicate that some failures by localized corrosion occur

SB 1/4/01

Alternative E^{o}'s to try

E^{o} @ 25°C = 1300 + 242 − 13.1(25) = 1214 mVshe

E^{o} @ 50°C = 1300 + 242 − 13.1(50) = 887 mVshe

E^{o} @ 75°C = 1300 + 242 − 13.1(75) = 567 mVshe

Default E^{o} in TPA 4.1a ~ 2000

→ misinterpretation of E^{o} in code? should E^{o} for code be 1300 + 242 = 1542 ?

⇒ try base case E^{o} (2000)

E^{o} = 1542

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Zr-4 passive current density conversion

$10^{-8}\,A/cm^2 \Rightarrow$

$$\frac{10^{-8}\,A}{cm^2}\left|\frac{1}{\rho}\right|EW\left|\frac{1}{F}\right|\frac{10\,mm}{cm}\left|\frac{3600\,s}{hr}\right|\frac{24\,hr}{d}\left|\frac{365\,d}{yR}\right.$$

$$\Rightarrow 10^{-8}\,A/cm^2\left|\frac{1\,cm^3}{6.52\,g}\right|\frac{91.22\,g}{4\,e^-}\left|\frac{1}{96481}\right|10\,|\,3600\,|\,24\,|\,365$$

$\Rightarrow 1.143 \times 10^{-4}$ mm/yR

SB 7/30/01

$\cancel{10^{-6}}$ 10^{-7} $\Rightarrow 1.143 \times 10^{-3}$ mm/yR

$1\,A/cm^2 = 3.15 \times 10^{11}\ C/m^2 \cdot yR$

$10^{-8} = 3{,}150$
$10^{-7} = 31{,}500$ $\Big\}\ C/m^2 \cdot yR$

Based on 0.6 mm thickness, general corrosion failure times range from 525 to 5249 yRS

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$\underbrace{A/cm^2\ \cancel{9}\,5 \times 10^{-9}}$ $= 1{,}575$ $C/m^2 \cdot yR$

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β change for ORR on Zr   assumes $\alpha = \beta$

① $b = \frac{2.3RT}{F(1+\beta)} = 0.04$ for   ② $b = \frac{2.3RT}{F\beta} = .120$

$\alpha = 1+\beta$

charge transfer rds   electrodic desorption

③ $b = 15$ mV/dec for recombination rds (Gileadi, p 174 Electrode Kinetics for Chemists... VCH pubs, 1993)

case ①   case ②

$\alpha = 3/2 = 1+\beta$ $\alpha = 1/2 = \beta$
$\beta = 1/2$

case ③

$b = \frac{2.3RT}{F\alpha}$ (assume $\alpha = \beta$) ; 25°C = 298K

$= 0.015 \Rightarrow \alpha = \frac{2.3(8.3144)(298)}{96481\ (0.015)}$

$\alpha = 3.94$

---

try $\beta = 0.5$ in code, see what Ecorr is predicted
compare w/ measured values; modify β to get higher OCP.

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instead of β, change ΔE for radiolysis to 0.3V

nominal ocp ~ 0.225 Vshe   ~ −0.017 Vsce

ocp for oxidized avg ~ 0.25 Vsce

0.492 − 0.225
= 0.267 ~ 0.3

→ slow ipass to 5×10^{-9} – 10^{-8} A/cm^2
→ slow LC rate by changing coef from 1.0 to 0.1 to slow Lc to see across multiple time steps
⇒ Lc occurred too quickly failing in 1 step.

→ incorrect change

n = 0.5 – diffn limited
A = 2.5×10^{-5} m/yr rate @ pit base

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I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

4/8/03

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