LSNReviews

From: Kuang-Tsan Ken Chiang [kchiang@cnwra.swri.edu]
Sent: Tuesday, December 12, 2006 11:51 AM
To: Andy Jung
Cc: Xihua He; Yi-Ming Pan; Pavan Shukla; Lietai Yang
Subject: RE: TPA parameters Update
Attachments: TPA_Parameters_Chapter08_ENG1_overview-rev01-XH-LY-KC.xls

Andy,

I have checked and modified the parameters in the attached file. The parameters I checked include dry oxidation and fabrication related parameters. The one that was changed was the critical chloride concentration of weld. It was changed from a distribution of (0.01, 0.25) to a constant of low concentration of 0.01. This has been discussed with O. Pensado.

Let me know if you have questions.

Ken

-----Original Message-----
From: Hundal Jung [mailto:hjung@cnwra.swri.edu]
Sent: Monday, December 11, 2006 4:25 PM
To: xhe@cnwra.swri.edu; 'Yiming Pan'; 'Pavan Shukla'; 'Ken Chiang'; 'Lietai Yang'
Subject: RE: TPA parameters Update

I need all of your input for checking the key parameters. Please check and confirm your assigned parameters as soon as possible. Thanks in advance.

Andy

-----Original Message-----
From: Xihua He [mailto:xhe@cnwra.swri.edu]
Sent: Friday, December 08, 2006 2:50 PM
To: 'Hundal Jung'; 'Yiming Pan'; 'Pavan Shukla'; 'Ken Chiang'; 'Lietai Yang'
Subject: RE: TPA parameters Update

Andy,

I have checked and confirmed the parameters that have assigned to me: DS, Gal, and LOC. I also checked the parameters of ENV and MOD. I didn't confirm the parameters in ENV (Lietai, Please confirm it).

There are two parameters you need to check with Osvaldo to make sure they are correct: one is the drip shield corrosion rate (DS) and the other is the OuterOverpackErpIntercept (No. 16 in LOC).

The file with my input highlighted in blue is attached.

If there is any question, please let me know.

Thanks,

Xihua

-----Original Message-----
From: Hundal Jung [mailto:hjung@cnwra.swri.edu]
Sent: Friday, November 17, 2006 10:00 AM
To: 'Yiming Pan'; Pavan Shukla; Xihua He; Ken Chiang; Lietai Yang
Subject: TPA parameters Update

All,

AS a part of the TPA User's guide revision task, TPA parameters for EBSFAIL and DSFAIL modules will be updated. In those two modules, 85 parameters are included and each parameter has been reclassified into more specific areas (e.g., dry oxidation, localized corrosion, passivation, fabrication and so on.) for our convenience as attached excel file. To revise and update 85 parameters in ENG1, all of us in corrosion group need to participate on this revision task.
Requesting your input, general guidance is as follows;
1. Identify your assigned parameters. Two staffs are assigned for each area. First name would be a lead.
2. Check and confirm following four columns i.e., name, description, PDF type, and values(s). Any required changes in name, PDF Type and Value(s) will be requested to PA team via formal process.
3. Update the record under "Justification" column. Some parameters are needed to provide references. 4. Ensure that the data you provided is complete, accurate and up-to-date.

Based on the current schedule for TPA User's Guide revision task, I suggest to complete and respond me until December 8th (Friday), 2006. Feel free to call me if you have any questions. Thanks for your cooperation in advance.

Andy
X4238

-----Original Message-----
From: Yiming Pan [mailto:ypan@cnwra.swri.edu]
Sent: Thursday, November 09, 2006 5:43 PM
To: 'Hundal Jung'
Subject: RE: TPA parameters for completion of the TPA User's Guide

Andy,

It is a good plan. To assure all the parameters are properly reviewed, I suggest assigning two staff on each area. Please see a revision at S:\HJung, and let me know your thoughts. If agree, please provide a detailed guidance to the staff, including the assignment, how to provide comments, and by when.

Thanks,
Yiming

Properties Page

Return-path: <kchiang@cnwra.swri.edu>
Received: from SEYMORE ([129.162.200.194])
 by rogain.cnwra.swri.edu (Sun ONE Messaging Server 6.0 (built Oct 29 2003))
 with ESMTP id <0JA6000EH6T8DL20@rogain.cnwra.swri.edu>; Tue,
 12 Dec 2006 10:51:09 -0600 (CST)
Date: Tue, 12 Dec 2006 10:51:08 -0600
From: Kuang-Tsan Ken Chiang <kchiang@cnwra.swri.edu>
Subject: RE: TPA parameters Update
In-reply-to: <004801c71d73$21172d00$e7c8a281@cnwra.swri.edu>
To: 'Hundal Jung' <hjung@cnwra.swri.edu>
Cc: xhe@cnwra.swri.edu, 'Yiming Pan' <ypan@cnwra.swri.edu>,
 'Pavan Shukla' <pshukla@cnwra.swri.edu>, 'Lietai Yang' <ltyang@cnwra.swri.edu>
Reply-to: kchiang@cnwra.swri.edu
Message-id: <000001c71e0d$b9261f80$c2c8a281@cnwra.swri.edu>
Organization: CNWRA
MIME-version: 1.0
X-MIMEOLE: Produced By Microsoft MimeOLE V6.00.2800.1506
X-Mailer: Microsoft Outlook, Build 10.0.6626
Content-type: multipart/mixed;
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Importance: Normal
X-Priority: 3 (Normal)
X-MSMail-priority: Normal

Area	# of Parameters	Description	Staff assigned
DOX	1	dry oxidation	Ken/Yiming
DS	1	drip shield related	Xihua/Pavan
ENV	11	environmetal parameters (temp, pH, scale deposits, etc)	Lietai/Xihua
FAB	10	fabrication effects	Ken/Yiming
GAL	2	gavanic coupling effect	Xihua/Pavan
GEN	1	general information (safety factor,)	Andy/Yiming
LOC	21	localized corrosion of waste package	Xihua/Lietai
MOD	24	modeing parameters (corrosion potential, Butler-Volmer Eq.)	Andy/Xihua
PAS	4	passivation parameters (passive current density, activation energy)	Pavan/Ken
WPG	10	general information for waste package materials (density, equivalent weight, thickness, grain boundary thickness, etc..)	Andy/Ken
(total #)	85		

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Cha pter
1	DOX	DryOxidationConstant	Constant relating matrix and grain boundary oxygen diffusivities in metal	constant	1.0e20	The rate of dry air oxidation in Alloy 22 can be neglected if the waste package temperature is low (for example less than 400℃). Based on experimental data at high temperatures, it is assumed that dry air oxidation is a negligible process in Alloy 22.	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
1	DS	DripShieldCorrosionRate[m/yr]	Drip Shield Corrosion Rate	triangular	8.6e-8, 1.72e-7, 2.6e-7	(Xihua: Osvaldo temporarily shaved the upper end of the distribution. The revised distribution is triangular(8.6e-8, 1.72e-7, 2.6e-7) m/yr for two sides. The criterion he applied was that the distribution was symmetric.) A distribution triangular(4.3E-8, 8.6E-8, 1.7E-6) was estimated from fluoride free data reported in Brossia et al. (2001). To account for corrosion in the underside of the drip shield, the range was multiplied by a factor of 2 (i.e., there are two identi	(O. Pensado: 5/18/05) (O. Pensado: SCR626) (X. He: 12/8/06)	Y.-M. Pan	DSFAIL	ENG1	8
1	ENV	BoilingPointOfWater[C]	Boiling point of water at repository horizon (oC)	constant	97.0	Data from NIST Steam Table version 2.2 database for the elevation of the repository. [OBS] The value of 96.4 deg C for pure water not held by capillary tension is rounded up to 97 deg C to address the uncertainty of capillary tension and chemistry of the	(R. Fedors: 5/20/05) (L.Yang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
2	ENV	CriticalRelativeHumidityAqueousCorrosion	Critical RH above which aqueous corrosion may initiate	constant	0.2	This parameter controls the onset of aqueous corrosion. It represents the equilibrium relative humidity for deliquescence. The TPA model assumes that localized corrosion cannot be supported by deliquescence environments due to the presence of localized . Value was lowered from 0.3 to 0.2 because recent studied showed that aqueous corrosion can take place at lower RH (see Yang, CNWRA 2006-02(2006)]. But the effect by the amount of solution is uncertain. Need to be evaluated further.	(O. Pensado: 5/18/05) (L.Yang 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
3	ENV	CriticalRelativeHumidityHumidAirCorrosion	Critical relative humidity above which humid-air corrosion may initiate	constant	0.15	It is assumed that the rate of humid air oxidation is negligible in Alloy 22 in the base case. TPA code results are independent of the value of the parameter CriticalRelativeHumidityHumidAirCorrosion, but this parameter must not exceed the CriticalRelati. This value was lowered from 0.2 to 0.15 to be consistent with the change in CriticalRelativeHumidityAqueousCorrosion.	(O. Pensado: 5/18/05) (L.Yang 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
4	ENV	DecayingConstantRadiolysis[1/yr]	Constant controlling the exponential decay of the radiolytic potential. See Eqs. (6-8) and (6-9).	constant	7.0e-5	Value selected to avoid overflow and/or underflow in the computations. Contribution of radiolysis to uncertainty in corrosion potential should be minimal compared to other sources of uncertainty. This value has no effect on corrosion potential when DeltaPotenitalDueToRadiolysisis set to zero (see next row). Radiolysis not considered. Shoesmith and King (1999), CRWMS M&O (2001b,c) and Su and Haas (1997)	(L. Yang: 5/3/05) (L.Yang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
5	ENV	DeltaPotentialDueToRadiolysis[V]	Increase in the corrosion potential due to the presence of radiolytic species	constant	0.0	CNWRA staff currently consider that irradiation levels near the WP in the current design are not sufficiently high to increase the corrosion potential Shoesmith and King (1999), CRWMS M&O (2001b,c) and Su and Haas (1997) Radiolysis not considered	(L. Yang: 5/3/05) (L.Yang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
6	ENV	HumidAirCorrosionRate[m/yr]	Humid air corrosion rate (m/yr)	constant	2.5e-8	Constant value based on analagous information. Data for Alloy825 obtained from VanRooyen and Copson (1960). Low rate consistent with low passive dissolution rates in CNWRA 2003-01, 2004-01 and IM 06002.01.321.500. [ALOG]	(O. Pensado: 5/18/05) (L.Yang 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
7	ENV	PorosityOfScaleonWP	Porosity of the layer deposited on the WP. Porosity does not change with time	constant	1.0	Specified value used to eliminate processes associated with assumption that no seepage water contacts the waste package and then evaporates to form a scale. A value of 1.0 implies no scale deposit.	(R. Pabalan: 5/5/05)	Y.-M. Pan	EBSFAIL	ENG1	8
8	ENV	ReferencepH	pH of water	uniform	4.5, 7.0	Range is based on DOE EQ3/6 simulations of in-package chemistry presented in ANL-EBS-000050. Normal distribution is an assumption. Compare with Bechtel SAIC Company, LLC (2003d). This pH is used for in-package processes (spent fuel degradation); it is n	Ref not in list	Y.-M. Pan	EBSFAIL	ENG1	8
9	ENV	ThicknessOfWaterFilm[m]	Thickness of water film on WP surface (m)	constant	0.0	Setting this parameter equal to 0 is equivalent to assuming negligible diffusion control on the cathodic current density to determine the corrosion potential. The assumption is reasonable in the range of possible corrosion potentials. Corrosion potentia	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
10	ENV	TortuosityOfScaleonWP	Tortuosity of a porous layer scale deposited on the WP. Thickness does not change with time	constant	1.0	Specified value used to eliminate processes associated with assumption that no seepage water contacts the waste package and then evaporates to form a scale. A value of 1.0 implies no scale deposit.	(R. Pabalan: 5/5/05)	Y.-M. Pan	EBSFAIL	ENG1	8
11	ENV	WPsurfaceScaleThickness[m]	Scale deposit on WP surface	constant	0.0	Specified value used to eliminate processes associated with assumption that no seepage water contacts the waste package and then evaporates to form a scale. A value of 0.0 implies no scale deposit.	(R. Pabalan: 5/5/05)	Y.-M. Pan	EBSFAIL	ENG1	8
1	FAB	WeldInhibitingSulfateToCl	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.5	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
2	FAB	ErpInterceptWeld[mVSHE]	Erp Intercept in mV for Weld (curve fitting parameter for repassivation potential)	triangular	991.2, 1041.2, 1091.2	Central value of 1041.2 mVSHE is consistent with values reported in Dunn et al.(2003, 2005). Based on judgment from visualization of experimental data, it is considered that uncertainty in the repassivation potential is bounded by a 100 mV envelope aroun	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
3	FAB	ErpSlopeWeld[mVSHE]	Erp slope in mV for Weld (curve fitting parameter for repassivation potential)	constant	-584.2	The repassivation potential for thermally aged material conservatively bounds the repassivation potential for weld material. Empirical equations and parameter values to compute the repassivation potential are reported in Dunn et al., (2003, 2005). This	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
4	FAB	TemperatureCoefficientOfErpInterceptWeld[mVSHE/C]	Temperature coefficient of Erp intercept weld in mV/(C)	constant	-10.0	The repassivation potential for thermally aged material conservatively bounds the repassivation potential for weld material. Empirical equations and parameter values to compute the repassivation potential are reported in Dunn et al., (2003, 2005). This	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
5	FAB	TemperatureCoefficientOfErpSlopeWeld[mVSHE/C]	Temperature coefficient of Erp slope weld in mV/(C)	constant	3.7	The repassivation potential for thermally aged material conservatively bounds the repassivation potential for weld material. Empirical equations and parameter values to compute the repassivation potential are reported in Dunn et al., (2003, 2005). This	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
6	FAB	WeldCritChlorideConc[mol/L]	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.01	Dunn, D.S., D. Daruwalla, Y.-M. Pan. Effect of Fabrication Processes on Material Stability -- Characterization and Corrosion. CNWRA 2004-01. CNWRA: San Antonio, Texas; October 2003. Loguniform distribution is conservative since low values are frequently. The critical chloride concentration is change to a low constant value of 0.01. This has been discussed with O. Pensado	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
7	FAB	WeldDeltaEcritInh[mV]	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	800.0	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/20/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
8	FAB	WeldInhibitingCarbonateToCl	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.2	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
9	FAB	WeldInhibitingNitrateToCl	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.3	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
10	FAB	WPWeldThickness[m]	waste package weld thickness	constant	2.0e-2	Inner closure lid is now a fillet weld and is not a through thickness weld. The weld includes all of the fabrication welds, which are 2 cm thick. Selecting 2-cm is conservative. Parameter value is well known (probably uncertain to some extent due to st	(O. Pensado: 5/18/05) (O. Pensado: SCR626) (X. He: 12/8/06) (K.Chiang: 12/12/06)	Y.-M. Pan	EBSFAIL	ENG1	8
1	GAL	FractionalCouplingStrength	Efficiency factor, varying from 0 to 1, representing galvanic coupling between the outer and inner overpack	constant	0.0	Legacy parameter from previous versions to TPA Code Version 3. This parameter is used to compute the corrosion potential resulting from galvanic coupling. Due to its high corrosion resistance, it is reasonable to disregard galvanic coupling for Alloy 22	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
2	GAL	MeasuredGalvanicCouplePotential	Experimentally measured galvanic couple potential between inner and outer overpack	constant	0.0	Legacy parameter from previous versions to TPA Code Version 3. This parameter is used to compute the corrosion potential resulting from galvanic coupling. Due to its high corrosion resistance, it is reasonable to disregard galvanic coupling for Alloy 22	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
1	GEN	SafetyFactor	Safety factor for residual stresses	constant	1.0	Value selected so as to eliminate the underlying process. Mohanty et al. (1997)	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
1	LOC	CoefForLocCorrOfInnerOverpack	Coefficient for localized corrosion rate of inner overpack (m/yrn, n=ExponentForLocCorrOfInnerOverpack)	constant	1.0	Value chosen to eliminate the effect of the inner container as a corrosion barrier. No credit assumed for Inner 316 NG SS container. Reference: Galvanic series in handbook (Table 2, page 83). ASM International. Corrosion. Volume 13: Metals Handbook. 9th Edition. Metals Park, Ohio: ASM International. 1987. He et al. 2006 paper submitted to Electrochimica Acta	(X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
2	LOC	CoefForLocCorrOfOuterOverpack	Coefficient for localized corrosion rate of outer overpack (m/yrn, n=ExponentForLocCorrOfOuterOverpack)	constant	2.5e-4	Value chosen to have constant localized corrosion penetration rate; value supported by localized penetration rate measurements (see Figure 2-12 in CNWRA 99-003). Assumed in Mohanty et al. (1997). Conservative values. Penetration in 80 years.	(X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
3	LOC	CritChlorideConcForFirstLayer[moL/L]	Critical chloride concentration for localized corrosion of outer overpack (mol/L)	constant	0.5	Value selected to not grant any protection against corrosion by the inner overpack in the EDA II (CLST meeting 2/15/00). Most current information is in Dunn et al 2005 (CNWRA 2005-02) for Alloy 22 in the mill annealed condition (Figure 4-6) [EXP] BG: CLST meet	(X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
4	LOC	CritChlorideConcForSecondLayer[moL/L]	Critical chloride concentration for localized corrosion of inner overpack (mol/L)	constant	1.0e-10	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption. Reference: Galvanic series in handbook (Table 2, page 83). ASM International. Corrosion. Volume 13: Metals Handbook. 9th Edition. Metals Park, Ohio: ASM International. 1987. He et al. 2006 paper submitted to Electrochimica Acta	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
5	LOC	ExponentForLocCorrOfInnerOverpack	Exponent for localized corrosion rate of inner overpack	constant	1.0	Value chosen to eliminate the effect of the inner container as a corrosion barrier. No credit assumed for Inner 316 NG SS container. page 83). ASM International. Corrosion. Volume 13: Metals Handbook. 9th Edition. Metals Park, Ohio: ASM International. 1987. He et al. 2006 paper submitted to Electrochimica Acta	(X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
6	LOC	ExponentForLocCorrOfOuterOverpack	Exponent for localized corrosion rate of outer overpack	constant	1.0	Assumed constant pit penetration rate chosen to provide a constant localized corrosion penetration rate. Experimental data is needed to consider stifling effects. Current approach is conservative. Current stifling data in He et al. (CNWRA 2006-01). However, the stifling tendency is uncertain at longer time.	Update? No (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
7	LOC	FactorForDefiningChoiceOfCritPotential	Factor for defining choice of critical potential (initiation or repassivation)	constant	0.0	Repassivation potential is less than the initiation (pitting) potential. Selecting the repassivation potential (parameter value equal to zero) as the critical potential for localized corrosion is conservative. Versions 4 and later of the TPA code do not	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
8	LOC	InnerDeltaEcritInh[mV]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.0	Zero value selected to avoid any effect of inhibitors on the localized corrosion of the inner waste package (no credit is given to inner waste package protection). No credit assumed for Inner 316 NG SS container.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
9	LOC	InnerInhibitingNitrateToCl	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	1.0E+10	Arbitrarily high value selected to avoid any effect of inhibitors on the localized corrosion of the inner waste package (no credit is given to inner waste package protection). No credit assumed for Inner 316 NG SS container.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Cha pter
10	LOC	InnerOverpackErpIntercept	Inner overpack Erp intercept in mVshe	constant	-10000.0	No credit assumed for Inner 316 NG SS container. An arbitrarily large value was chosen to eliminate any protection from the inner overpack.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
11	LOC	InnerOverpackErpSlope	Inner overpack Erp slope in mV	constant	0.0	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
12	LOC	OuterDeltaEcritInh[mV]	Maximum increase in the repassivation potential due to the action of inhibitors.	constant	800.0	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
13	LOC	OuterInhibitingCarbonateToCl	Carbonate to chloride concentration ratio for computation of action of inhibitors. Below this ratio, the repassivation potential is assumed to increase linearly with the ratio up to OuterDeltaEcritInh[mV]. Above this ratio, the increase in the repassivat	constant	0.2	Parameter and value based on model described in Dunn et al. (2005, CNWRA 2005-02, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
14	LOC	OuterInhibitingNitrateToCl	Nitrate to chloride concentration ratio for computation of action of inhibitors Below this ratio, the repassivation potential is assumed to increase linearly with the ratio up to OuterDeltaEcritInh[mV]. Above this ratio, the increase in the repassivation	constant	0.1	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
15	LOC	OuterInhibitingSulfateToCl	Sulfate to chloride concentration ratio for computation of action of inhibitors. Below this ratio, the repassivation potential is assumed to increase linearly with the ratio up to OuterDeltaEcritInh[mV]. Above this ratio, the increase in the repassivati	constant	0.5	Parameter and value based on model described in Dunn et al. (2005, Equations 5-17 and 5-18) and in Dunn, Yang, Wu, and Cragnolino (2004).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
16	LOC	OuterOverpackErpIntercept	Outer overpack Erp intercept in mVSHE	triangular	1025.04, 1180.76, 1336.49	Data taken from Modeling Corrosion Processes for Alloy 22 Waste Packages, D. S. Dunn, O. Pensado, Y.-M. Pan, L.T. Yang, and X. He Paper sumitted to 29th Symposium on the Scientific Basis for Nuclear Waste Management September 12-16, 2005. Ghent, Belgium (The data is not consistent with the data in the reference. Please check with Osvaldo)	(O. Pensado: 5/24/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
17	LOC	OuterOverpackErpSlope	Outer overpack Erp slope in mV	constant	-752.034	Data taken from Modeling Corrosion Processes for Alloy 22 Waste Packages, D. S. Dunn, O. Pensado, Y.-M. Pan, L.T. Yang, and X. He Paper sumitted to 29th Symposium on the Scientific Basis for Nuclear Waste Management September 12-16, 2005. Ghent, Belgium	(O. Pensado: 5/24/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
18	LOC	TempCoefOfInnerPackErpIntercept	Temperature coefficient of inner overpack Erp intercept in mV/(C)	constant	0.0	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
19	LOC	TempCoefOfInnerPackErpSlope	Temperature coefficient of inner overpack Erp slope in mV/(C)	constant	1.0	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
20	LOC	TempCoefOfOuterPackErpIntercept	Temperature coefficient of outer overpack Erp in mV/°C	constant	-9.35026	Data taken from Modeling Corrosion Processes for Alloy 22 Waste Packages, D. S. Dunn, O. Pensado, Y.-M. Pan, L.T. Yang, and X. He Paper sumitted to 29th Symposium on the Scientific Basis for Nuclear Waste Management September 12-16, 2005. Ghent, Belgium	(O. Pensado: 5/24/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
21	LOC	TempCoefOfOuterPackErpSlope	Temperature coefficient of outer overpack Erp slope in mV/°C	constant	5.20131	Data taken from Modeling Corrosion Processes for Alloy 22 Waste Packages, D. S. Dunn, O. Pensado, Y.-M. Pan, L.T. Yang, and X. He Paper sumitted to 29th Symposium on the Scientific Basis for Nuclear Waste Management September 12-16, 2005. Ghent, Belgium	(O. Pensado: 5/24/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
1	MOD	InnerActivationEnergyReductionReactHighpH[J/mole]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	40000.0	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
2	MOD	InnerActivationEnergyReductionReactLowpH[J/mole]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	40000.0	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
3	MOD	InnerChargeTransferCoefReductionReactHighpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.0248	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
4	MOD	InnerChargeTransferCoefReductionReactLowpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.01287	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
5	MOD	InnerEffectiveReactionOrderHHighpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.01897	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
6	MOD	InnerEffectiveReactionOrderHLowpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.0256	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
7	MOD	InnerReferenceCurrReductionReactHighpH[C/(m2*yr)]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	5.51E+9	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
8	MOD	InnerReferenceCurrReductionReactLowpH[C/(m2*yr)]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	7.57E+9	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
9	MOD	InnerWPActivationEnergyforWaterReduction[J/mole]	Activation energy for water reduction reaction for WP inner overpack (J/mol)	constant	25000.0	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
10	MOD	InnerWPBetaKineticsParameterforWater	Transfer coefficient for water reduction reaction () for the WP inner overpack	constant	0.5	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
11	MOD	InnerWPRateConstantforWaterReduction[coulomb-m/m^2/yr]	Rate constant for water reduction for WP inner overpack (C/m2/yr)	constant	0.0	No credit assumed for Inner 316 NG SS container. Parameter value selected to be consistent with the no credit assumption.	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
12	MOD	OuterActivationEnergyPassiveCurrDens[J/mol]	Activation energy for Arrhenius dependence of passive current density on temperature	constant	44700.0	Effective activation energy estimated from variation of the anodic current density as a function of temperature (Pensado, Dunn, Cragnolino, and Jain, 2002).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
13	MOD	OuterActivationEnergyReductionReactHighpH[J/mole]	Activation energy for Arrhenius dependence of cathodic current density on temperature. High pH range.	constant	40000.0	Assumed value based on Calvo (1979). Value of 40000 J/mole reproduces the temperature dependence noted in the laboratory of the corrosion potential. In assigning a constant value, it is assumed that all uncertainty in the corrosion potential is due to fa	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
14	MOD	OuterActivationEnergyReductionReactLowpH[J/mole]	Activation energy for Arrhenius dependence of cathodic current density on temperature. Low pH range.	constant	40000.0	Assumed value based on Calvo (1979). Value of 40000 J/mole reproduces the temperature dependence noted in the laboratory of the corrosion potential. In assigning a constant value, it is assumed that all uncertainty in the corrosion potential is due to fa	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
15	MOD	OuterChargeTransferCoefReductionReactHighpH	Charge transfer coefficient for reduction reaction, high pH range. Parameter used to compute the corrosion potential.	constant	0.0248	Parameter estimated to match experimental corrosion potentials as function of pH (Dunn et al., 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
16	MOD	OuterChargeTransferCoefReductionReactLowpH	Charge transfer coefficient for reduction reaction, low pH range. Parameter used to compute the corrosion potential.	constant	0.01287	Parameter estimated to match experimental corrosion potentials as function of pH (Dunn et al., 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
17	MOD	OuterEffectiveReactionOrderHHighpH	Reaction order with respect to hydroxil ion (H+ or protons). Parameter used to compute the cathodic current density, used to compute the corrosion potential. High pH range.	constant	0.01897	Parameter estimated to match experimental corrosion potentials as function of pH and temperature (Dunn et al., 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
18	MOD	OuterEffectiveReactionOrderHLowpH	Reaction order with respect to hydroxil ion (H+ or protons). Parameter used to compute the cathodic current density, used to compute the corrosion potential. Low pH range.	constant	0.0256	Parameter estimated to match experimental corrosion potentials as function of pH and temperature (Dunn et al., 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
19	MOD	OuterReferenceCurrReductionReactHighpH[C/(m2*yr)]	Reference current density to compute the cathodic current density due to the main reduction reaction (e.g. oxygen reduction). This cathodic current density is used to compute the corrosion potential. High pH range.	constant	5.51e+09	Parameter estimated to match experimental corrosion potentials as function of pH and temperature (Dunn et al., 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
20	MOD	OuterReferenceCurrReductionReactLowpH[C/(m2*yr)]	Reference current density to compute the cathodic current density due to the main reduction reaction (e.g. oxygen reduction). This cathodic current density is used to compute the corrosion potnetial. Low pH range.	constant	7.57e+09	Parameter estimated to match experimental corrosion potentials as function of pH and temperature (Dunn et al., 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
21	MOD	OuterWPActivationEnergyforWaterReduction[J/mole]	Activation energy for water reduction for WP outer overpack (J/mol)	constant	25000.0	Data based on Heusler (1976). However, TPA results are independent of this parameter if OuterWPRateConstantforWaterReduction[coulomb-m/m^2/yr]=0.0. Corrosion potential computations employing this assumption produced trends consistent with experimental d	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
22	MOD	OuterWPBetaKineticsParameterforWater	Transfer coefficient for water reduction reaction () for the WP outer overpack	constant	0.0	It is assumed that the contribution of water reduction to partial cathodic current density is negligible. This assumption is reasonable in the range of possible corrosion potentials. The parameter value was selected to be consistent with this assumption	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
23	MOD	OuterWPRateConstantforWaterReduction[coulomb-m/m^2/yr]	Rate constant for water reduction for the WP outer overpack (C/m2/yr)	constant	0.0	It is assumed that the contribution of water reduction to partial cathodic current density is negligible. This assumption is reasonable in the range of possible corrosion potentials. The parameter value was selected to be consistent with this assumption	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
24	MOD	TransitionLowHighpH	Two different sets of parameters are used to compute the corrosion potential. This pH parameter defines the transition pH to select the appropriate set of parameters.	constant	6.0	Empirical data indicate the existence of a transition pH, above which corrosion potentials significantly decrease. This pH value is around 6 (Dunn et al., 2005; Dunn, Yang, Wu, and Cragnolino, 2004; Dunn, Pensado, and Cragnolino, 2005).	(O. Pensado: 5/18/05) (X. He: 12/8/06)	Y.-M. Pan	EBSFAIL	ENG1	8
1	PAS	AA_1_1[C/m2/yr]	Passive current density for WP outer overpack (C/m2/yr)	triangular	1600.0, 3200.0, 6400.0	This parameter represents an anodic current density (due to the passive dissolution of Alloy 22 in aqueous environments) at a reference temperature (RefTemperaturePassiveCurrDens[K]). This current density is used to compute the general corrosion rate as	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
2	PAS	AA_2_1[C/m2/yr]	Passive current density for WP inner overpack (C/m2/yr)	constant	1.0E4	Reasonable value of current density fo 316 SS. The accurate value is not relevant. It is assumed that localized corrosion is activated as soon as the outer container is failed by corrosion. (This value removes a non-convergence issue in the corrosion	Need Refs. O. Pensado: updated value 5/10/05	Y.-M. Pan	EBSFAIL	ENG1	8
3	PAS	InnerActivationEnergyPassiveCurrDens[J/mol]	Activation energy for Arrhenius dependence of passive current density on temperature.	constant	44700.0	No credit assumed for Inner 316 NG SS container. Same value for "Outer" container employed. Results are independent of the of the value assigned to this parameter.	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
4	PAS	RefTemperaturePassiveCurrDens[K]	Reference temperature to define Arrhenius dependence of passive current density on temperature.	constant	3.68e+02	Arbitrary reference temperature. Parameter AA_1_1 is the distribution of current densities at this reference temperature. Any other reference temperature can be selected, but the AA_1_1 parameter values must be in agreement with the reference temperatur	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
1	WPG	DensityInnerOverpack[kg/m^3]		constant	7980.0	Data is consistent with manufacturer specifications for 316L ss (see table XI.1 of ASTM G-1). [OBS]	Need description.	Y.-M. Pan	EBSFAIL	ENG1	8
2	WPG	DensityOuterOverpack[kg/m^3]	Density Outer Overpack	constant	8690.0	Data is consistent with manufacturer specifications for Alloy 22 (see ASTM B S7S or ASME SB575). ASME SB 575 [OBS] BG: refs not found but could be ASTM B575-04 or -98.	Check Refs.	Y.-M. Pan	EBSFAIL	ENG1	8
3	WPG	EquivalentWeightInnerOverpack[kg/mol]		constant	0.02494	Well-established value, given assumptions concerning oxidation states, as indicated in 0.02550 ASTM G102. [OBS]	Need description.	Y.-M. Pan	EBSFAIL	ENG1	8
4	WPG	EquivalentWeightOuterOverpack[kg/mol]		constant	0.02597	Well-established value, given assumptions concerning oxidation states, as indicated in 0.02550 ASTM G102. [OBS]	Need description.	Y.-M. Pan	EBSFAIL	ENG1	8
5	WPG	FractureToughness[MPa-m**0.5]	Fracture toughness of outer overpack material (Alloy 22)	constant	304.0	Constant value based on expert judgement. Data obtained using a correlation with limited data applicable to Ni-Cr-Mo alloys drawing from Dunn et al. (2004). Kj>300 for mill annealed, As-welded, Welded+solution annealed. Kj=150 for Welded+870C aged for 1	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8

TPA Parameters (Chapter 8, ENG1)

No	Area ID	Name	Description	PDF Type	Value(s)	Justification		Contact	TPA Section	ISI Lead	Chapter
6	WPG	GrainBoundaryThickness[micrometer]	Thickness of grain boundary used in the model for calculating coupled oxygen diffusion along grain boundaries in metal (m)	constant	7.0e-4	Legacy parameter from previous versions to TPA Code Version 3. This parameter is used to estimate the propagation rate of a dry air corrosion front. The rate of dry air oxidation in Alloy 22 can be neglected if the waste package temperature is low (for	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
7	WPG	InnerWPThickness[m]	Thickness of the inner overpack (m)	constant	0.05	Engineering specification taken from the repository design and having no significant uncertainties; current value conforms to the clearance between the drip shield bulk head and 21 PWR waste package. Information taken from ANL-XCS-ME-000001 (CRWMS M&O 200		Y.-M. Pan	EBSFAIL	ENG1	8
8	WPG	MetalGrainRadius[micrometer]	Average radius of the metal grains constituting the WP outer overpack (m)	constant	13.75	Legacy parameter from previous versions to TPA Code Version 3. This parameter is used to estimate the propagation rate of a dry air corrosion front. The rate of dry air oxidation in Alloy 22 can be neglected if the waste package temperature is low (for	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8
9	WPG	OuterWPThickness[m]	Thickness of the outer overpack (m)	constant	0.02	Engineering specification taken from the repository design and having no significant uncertainties; current value conforms to the clearance between the drip shield bulk head and 21 PWR waste package. Information taken from ANL-XCS-ME-000001 (CRWMS M&O 200		Y.-M. Pan	EBSFAIL	ENG1	8
10	WPG	YieldStrength[MPa]	Yield strength of outer overpack, Mpa	constant	310.3	Well-established value; uncertainties are expected to be insignificant. Data pertain to Alloy 22 manufacturer specifications from 1995 ASME Boiler and Pressure Vessel code.	(O. Pensado: 5/18/05)	Y.-M. Pan	EBSFAIL	ENG1	8