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Scientific Notebook No. 460: Total-Systems Performance Assessment SR Calculation Verification (04/27/2001 through 10/12/2006)

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

20.01402.761
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* This SN will be used to record verification calculations on AOE'n TSPA. * 1

Hand check of Table 6-43 on page 266 of the TSPA-SR model report (MDL-WIS-PA-000002 Rev0).

Table 6-43. Total Carbonate Concentration Calculation Verification for the Median Value Simulation

Location	Observed pH	Calculated CO_3 Concentration (molal)	Model CO_3 Concentration (molal)
Always Drip	6.7284	0.04253	0.04253
Intermittent Drip	6.7445	0.04414	0.04414
Never Drip	6.7107	0.04084	0.04084

Table 6-38. Input Parameters for In-Package Chemistry Calculations

TSPA Parameter	Description	Parameter Value	Reference
Rel_diss_rate	Glass dissolution rate for CDSP packages	1	Data developed was applicable to CDSP packages and no glass composition correction is needed.
Ionic_Str_ CSNF_early	Ionic strength in CSNF waste packages at early times in mol/kg	Beta Distribution Min=2.757E-03 Max=2.922E-03 Mean=2.821E-03 Std Dev=5.1716E-05	CRWMS M&O 2000 [129287], Table 16
Ionic_Str_ CSNF_late	Ionic strength in CSNF waste packages at late times in mol/kg	Beta Distribution Min=2.827E-03 Max=3.943E-01 Mean=9.484E-02 Std Dev=0.13026125	CRWMS M&O 2000 [129287], Table 17
Ionic_Str_ CDSP_early	Ionic strength in CDSP waste packages at early times in mol/kg	Beta Distribution Min=2.537E-03 Max=3.479E-03 Mean=3.179E-03 Std Dev=2.764E-04	CRWMS M&O 2000 [129287], Table 18
Ionic_Str_ CDSP_late	Ionic strength in CDSP waste packages at early times in mol/kg	Beta Distribution Min=7.860-E-03 Max=1.353 Mean=3.384E-01 Std Dev=4.764E-01	CRWMS M&O 2000 [129287], Table 19
Cl	Chloride ion concentration in mol/kg	2.014E-04	CRWMS M&O 2000 [129287], Section 6.4.2
log_fO2	Log Oxygen Fugacity	-0.7	CRWMS M&O 2000 [129287], Table 20
log_fCO2	Log Carbon Dioxide Fugacity	-3.0	CRWMS M&O 2000 [129287], Table 20
Total_CO3	Total Carbonate Concentration in mol/kg	$10^{-4.47}+10^{-10.82}/10^{-pH}+10^{-21.15}/10^{-2pH}$	CRWMS M&O 2000 [129287], Table 14

DTN: MO9911SPACDP37.001 [139569]

→ for pH = 6.7284 Total_CO3 = 1.1488×10^{-4}

→ which does not agree with 0.04253 reported in Table 6-43 (See above)

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For a triangular distribution with minimum (a) = 0.0105, mean = 0.0244, and maximum (b) = 0.1942, what is the peak (c) mode

$$\text{mean} = \frac{a+b+c}{3}$$

$$3(\text{mean}) - a - b = c = 3(0.0244) - 0.0105 - 0.1942$$
$$= -0.1315$$

but $a \le c \le b$, by definition

Check calculated U solubility in Table 6-60, page 316 of TSPA-SR model report.

Table 6-60. Verification of the TSPA-SR Model Solubility Limit Calculations for U, Am, and Np

TSPA Parameter	Location	pH	Temperature (K)	CO_2 Fugacity (atm)	Manual Calculation	Model Value
Solubility_U	CSNF, Bin 4, Always Drip	6.7436	295.56	0.001	2.4630	2.4634
Solubility_U	CDSP, Bin 4, Always Drip	8.8573	295.46	0.001	1056.1	1056.2
Solubility_U_ Invert	CSNF, Bin 4, Always Drip	7.0734	298.15	0.001	3.1439	3.1440
Solubility_U_ Invert	CDSP, Bin 4, Always Drip	7.0732	298.15	0.001	3.1431	3.1430
Solubility_Np	CSNF, Bin 4, Always Drip	6.7436	Not Applicable	Not Applicable	19.599	19.598
Solubility_Np	CDSP, Bin 4, Always Drip	8.8573	Not Applicable	Not Applicable	0.1508	0.1508
Solubility_Np_ Invert	CSNF, Bin 4, Always Drip	7.0734	Not Applicable	Not Applicable	9.1713	9.1709
Solubility_Np_ Invert	CDSP, Bin 4, Always Drip	7.0732	Not Applicable	Not Applicable	9.1755	9.1757
Solubility_Am	CSNF, Bin 4, Always Drip	6.7436	Not Applicable	0.001	1.4203	1.4200
Solubility_Am	CDSP, Bin 4, Always Drip	8.8573	Not Applicable	0.001	0.2619	0.2620
Solubility_Am Invert	CSNF, Bin 4, Always Drip	7.0734	Not Applicable	0.001	0.2374	0.2374
Solubility_Am Invert	CDSP, Bin 4, Always Drip	7.0732	Not Applicable	0.001	0.2376	0.2376

Table 6-55. Solubility Limits for the Elements Considered in the TSPA-SR Model (Continued)

Description	TSPA Parameter	Parameter Value	Reference/DTN
Ra Solubility in mg/L	Not in Model	0.52	CRWMS M&O 2000 [143569], Table 19 DTN: MO0004SPASOL10.002 [151713]
Sn Solubility in mg/L	Not in Model	5.934E-03	CRWMS M&O 2000 [143569], Table 19 DTN: MO0004SPASOL10.002 [151713]
Sr Solubility in mg/L	Solubility_Sr	8.76E04	CRWMS M&O 2000 [143569], Table 19 DTN: MO0004SPASOL10.002 [151713]
Tc Solubility in mg/L	Solubility_Tc	9.89E04	CRWMS M&O 2000 [143569], Table 19 DTN: MO0004SPASOL10.002 [151713]
Th Solubility in mg/L	Solubility_Th	2.32	CRWMS M&O 2000 [143569], Table 19 DTN: MO0004SPASOL10.002 [151713]
Logarithm of U Solubility in mg/L. This equation is not applicable for temperatures above 90°C	Log_Sol_U_a	$7.9946-2.6963pH+0.4292pH^2-1.6286\log f_{CO_2}+0.0095T+0.4161pH\times\log f_{CO_2}-0.0051pH\times T-0.0022\log f_{CO_2}\times T$	CRWMS M&O 2000 [143569], Table 18 DTN: MO0004SPASOL10.002 [151713]
Zr Solubiliity in mg/L	Not in model	6.20E-05	CRWMS M&O 2000 [143569], Table 18 DTN: MO0004SPASOL10.002 [151713]

From 6-55 above

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$$\log(Sol_U) = 7.9946 - 2.6963pH + 0.4292pH^2 - 1.6286\log f_{CO_2} + 0.0095T + 0.4161pH \times \log f_{CO_2} - 0.0051pH \times T - 0.0022\log f_{CO_2} \times T$$

Term

1 : $-2.6963 \times 6.7436 = -18.1828$

2 : $0.4292 \times (6.7436)^2 = 19.5184$

3 : $-1.6286 \times \log_{10}(0.001) = 4.8858$

4 : $0.0095 \times (295.56\ K) = 2.8078$

5 : $0.4161 \times (6.7436) \times \log_{10}(0.001) = -8.4180$

6: $-0.0051 \times (6.7436) \times (295.56) = -10.1650$

7: $-0.0022 \times \log_{10}(0.001\ \text{atm}) \times (295.56) = 19.5070$ 1.9507

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$\log(Sol\,U) = 8.7613 = 17.9477 = 0.391465$

$10^{(\log(Sol\,U))} = 2.4630 = 10^{(0.391465)}$

→ Which agrees with manual calculation in Table 6-60

The calculations in 6-60 check, but these are not the same as provided in the DOE "hand calc" spreadsheet which is affixed to page 5 of this SN (opposite). For CSNF the pH = 3.4454 (vs. 6.7436) and T = 298.928 K (vs 295.56 K). The solubility of U = 8894.97 ~~mol~~ mg/L

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Check hand calculations in Table 6-101 on Page 422 of the TSPA-SR model report. (for Kd_Vol_Irr) → Page 6

Table 6-101. Comparison of Abstraction Prescribed Input Parameter Values for Volcanic_Properties to those Selected for Median Value Simulation

TSPA-SR Model Parameter	Model Equation (if applicable)	Model Value	Abstraction Value or Calculated Value
Kd_Vol_Rev	KDRN10_Median	0.05 m^3/kg	0.05 m^3/kg
Volcanic_MatrixPorosity	Direct input	0.19	0.19
Volcanic_Density	Direct input	1940 kg/m^3	1940 kg/m^3
Fracture_Perimeter	Direct input	2.0 m	2.0 m
Fracture_Area	((10^(FPVO_Median*1{m-1}))*(10^(FISVO_Median*1{m-1})))*1 m^2	0.020893 m^2	0.020893 m^2
Coating_Thickness	Direct input	0.0001 m	0.0001 m
Coating_Porosity	Direct input	0.01	0.01
Kd_Vol_Irr	((10^CORVO_Median-1)*Fracture_Area/Fracture_Perimeter/Coating_Thickness-Coating_Porosity)/Volcanic_Density	8.67924 m^3/kg	8.67926 m^3/kg
Dispersivity	(10^(LDISP_Median*1{m-1}))*1 m	100 m	100m

Am Coefficients	A	B	C	D	E	G	H
	58.0335	-18.9422	1.4744	-6.0032	-0.7005	0.1162	0.1146

Global:

fCO2	0.001
Time (yrs)	100,000
Bin 4	
Temp_CSNF_WP	*295.927887*
Temp_CDSP_WP	295.774109
Temp_CSNF_Inv	298.15
Temp_CDSP_Inv	298.15
Environment: Always Drip	
pH_CSNF	3.4454
pH_CDSP	8.8802
pH_Invert (CSNF)	7.0607
pH_Invert (CDSP)	7.0508
Solubility_U (CSNF)	8894.97456
Solubility_U (CDSP)	1158.8833
Solubility_Np (CSNF)	38943.0377
Solubility_Np (CDSP)	0.14309684
Solubility_Am (CSNF)	2.4709E+21
Solubility_Am (CDSP)	0.29200901
Solubility_U_Invert (CSNF)	3.04737253
Solubility_U_Invert (CDSP)	3.04778459
Solubility_Np_Invert (CSNF)	9.66339715
Solubility_Np_Invert (CDSP)	9.66117233
Solubility_Am_Invert (CSNF)	0.2636994
Solubility_Am_Invert (CDSP)	0.26357584
Environment: Intermittent Drip	
pH_CSNF	6.9003
pH_CDSP	5.0199
pH_Invert (CSNF)	7.0507
pH_Invert (CDSP)	7.0508
Solubility_U (CSNF)	2.80381534
Solubility_U (CDSP)	12.1391558
Solubility_Np (CSNF)	13.6624891
Solubility_Np (CDSP)	1037.36078
Solubility_Am (CSNF)	0.56585567
Solubility_Am (CDSP)	157635892
Solubility_U_Invert (CSNF)	3.04737253
Solubility_U_Invert (CDSP)	3.04778459
Solubility_Np_Invert (CSNF)	9.66339715
Solubility_Np_Invert (CDSP)	9.66117233
Solubility_Am_Invert (CSNF)	0.2636994
Solubility_Am_Invert (CDSP)	0.26357584
Environment: No Drip	
pH_CSNF	6.8896
pH_CDSP	8.8893
pH_Invert (CSNF)	7.0507
pH_Invert (CDSP)	7.0508
Solubility_U (CSNF)	2.77189084
Solubility_U (CDSP)	1212.8851
Solubility_Np (CSNF)	14.0032818
Solubility_Np (CDSP)	0.14012966
Solubility_Am (CSNF)	0.60011885
Solubility_Am (CDSP)	0.30510729
Solubility_U_Invert (CSNF)	3.04737253
Solubility_U_Invert (CDSP)	3.04778459
Solubility_Np_Invert (CSNF)	9.66339715
Solubility_Np_Invert (CDSP)	9.66117233
Solubility_Am_Invert (CSNF)	0.2636994
Solubility_Am_Invert (CDSP)	0.26357584

$$Kd_Val_Irr = ((10^{Corva_med} - 1)\, Frac_{Area} / Frac_{Perim} / Coat_{Thick} - Coat_{Poros}) / \rho_{Volcanic}$$

$Frac_{Area} = 0.020893\ m^2$ $\rho_{Volcanic} = 1940\ kg/m^3$

$Frac_{Perim} = 2.0\ m$

$Coat_{Thick} = 0.0001\ m$

$Coat_{Poros} = 0.01$

Table 6-99. Comparison of Abstraction Prescribed Input Parameter Values to those Selected for Median Value Simulation

CORVO	Cumulative Distribution			Probability Level	Value	
		2.21		0	0.025308	
				0.039	0.04139	
				0.08125	0.77815	
				0.2605	2	
				0.7605	2.4472	
				1	2.9031	

Attached above is a portion of Table 6-99 on page 419. The median value of CORVO is found by linear interpolation

$$\frac{Corva_med - 2}{2.4472 - 2} = \frac{0.5 - 0.2605}{0.7605 - 0.2605}$$

$Corva_med = 2.2142$ (4 sig. figs)

$Kd_Val_Irr = 8.7641$

Using a rounded value of $Corva_med = 2.21$

$Kd_Val_Irr = 8.67926$ (5 sig figs)

GW 4/30/2001

Notes from PA/QA discussion via telephone 5/9/2001

Background: 2 issues: inconsistency and QA controls. Described a lot of action being taken by DOE: further review, review of documentation, care in providing hand calculations to NRC to be sure that DOE knows what's going on. (needs to go through Tim Gunter)

Archeum:

1.1 Early should be Late, but the model correctly implements the eqns. Documentation error.

1.2 Error... incorrect exponent in GoldSim file as well as in the document, but the effect was conservative ... lead to greater release.

2.1 Incorrect documentation, but model uses the number correctly. Documentation error.

3.1 Excel calculation is not the hand calculation ... suggests that the documentation of the hand calc. is missing?

4.1 As above, the actual chemistries are different ...
Per Sarvanjan: they have no separate documentation of the hand calculation.

4.2 Uses pH outside accepted range, true! Leads to large U solubility, very conservative results. Will lead to a revised AMR.

5.1 Table 6-133 in incorrect. Error

6.1 The non-convergence errors result in mass being added ... not clear if this is a in not conservative.

7.1

8.1 Typo only. Correct value used in code. Looked at nominal case scenario file SR00_005JM4.gsm has the correct probability. Documentation error.

Beckman:

GW 5/9/2001

In this entry I will attempt to develop a dimensionless group (Π using Buckingham approach) that expresses the relative importance of radionuclides in the HLW inventory, which consider the following factors: for radionuclide x.

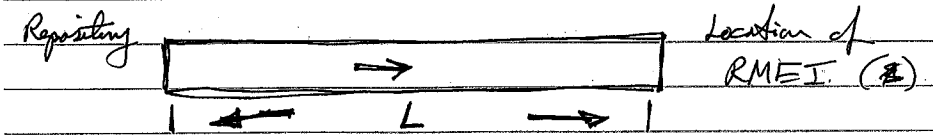
- Initial inventory: I_x, $[I_x] = Ci$ or Bq could be on a per waste package basis
- Half-life: T_x, $[T_x] = yr$
- Solubility of primary species of x: S_x, $[S_x] = kg/m^3$
- Retardation Coefficient; Rd_x: $[Rd_x] = \phi$
- Unretarded Travel time; T_{t_x}: $[T_{t_x}] = yr$
- Dose Conversion Factor, DCF_x: $[DCF] = rem/Ci$ or Sv/Bq
- Dilution Volume, V_D: $[V_D] = m^3$

Kernel for 1-D Advection-dispersion with sorption and decay

$$\frac{\exp(-\mu t)}{Rd} \frac{L}{2\sqrt{\pi D (t/Rd)^3}} \exp\left\{-\frac{(L - V(t/Rd))^2}{4 D t/Rd}\right\}$$

μ: decay rate $[\mu] = 1/t$
D: dispersion coef. $[D] = L^2/t$
L: location at which conc is measured $[L] = L$
V: transport velocity $[V] = L/t$

The basic idea for pipe flow-type transport with sorption and decay is as follows



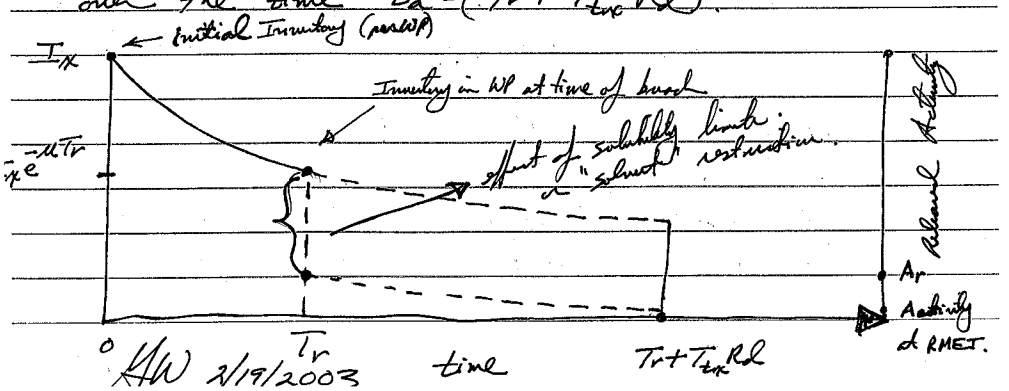
Unretarded travel time, $T_{tx} = L/v$

Travel time for retarded nuclide, $T = T_{tx} R_d$

Reduction in activity resulting from decay depends on the time of release from the repository, T_r, and the retarded travel time.

$$A_x(t_a) = I_x \exp\{-\mu(T_r + T_{tx} R_d)\}$$

Activity of radionuclide x at RMEI location at first arrival t_a = initial activity times decay over the time $t_a = (T_r + T_{tx} R_d)$.



GW 2/19/2003

This scientific notebook is closed. No further entries will be made. None of the results shown in this SN have been used in official reports.* All results are therefore preliminary.

Gordon Wittmeyer
10/3/2006

* Reference is made to this SN (460) in a Aug 21, 2001 letter from Gordon Wittmeyer to James Firth
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