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To: Records Center

From: Todd R. Zeitler and Clifford Hansen

Subject: Updated calculation of the cumulative distribution for STEEL:HUMCORR

In the response to the EPA's CRA-2014 Completeness Comments 3-C-3 and 3-C-4, the EQ3/6 thermodynamic database was updated (DATA0.FM2) and the new baseline solubilities were calculated (Domski 2015 and Domski and Xiong 2015). The new analysis report differs from that of Brush and Domski (2013) by the use of an updated thermodynamic database for EQ3/6, Version 8.0a (Wolery and Jarek 2003; Wolery 2008; Wolery et al. 2010; Xiong 2011).

Whereas the previous version of the database predicted a value of 3.14 ppm CO_2 in the gas phase when in equilibrium with WIPP brines (Brush and Domski 2013), the current version predicts a value of 0.58 ppm (Domski and Xiong 2015). Previously, the STEEL:HUMCORR parameter was revised to include data from Roselle (2013), assuming a predicted value of 3.14 ppm CO_2 in the gas phase (Zeitler and Hansen 2015). The updated value of 0.58 ppm does not change the conclusions of Zeitler and Hansen (2015) to use 0 ppm and 350 ppm CO_2 data from Roselle (2013) in deriving a distribution for STEEL:HUMCORR. However, the distribution for STEEL:HUMCORR does need to be revised to reflect the change from 3.14 ppm to 0.58 ppm CO_2.

Based on the data from corrosion experiments performed by Roselle (2013), a cumulative distribution for the STEEL:HUMCORR (humid corrosion rate for steel) has been constructed, as described below. Although Roselle proposed to maintain the HUMCORR parameter at a value of zero, in order to address a comment received from the EPA regarding the CRA-2014, we found that it was appropriate to construct a distribution of values for the HUMCORR parameter from Roselle's data.

Because there is a predicted value of 0.58 ppm CO_2 in the gas phase when in equilibrium with WIPP brines (Domski and Xiong 2015), corrosion rates based solely on 0 ppm CO_2 experiments may not completely reflect iron corrosion under WIPP conditions. Therefore it is appropriate to also consider data from corrosion experiments performed under conditions with nonzero CO_2 concentrations. The data available from Roselle (2013) include corrosion rates for CO_2 concentrations of 0 and 350 ppm. A 350 ppm CO_2 concentration is two orders of magnitude higher than the predicted value, and therefore these data are not directly relevant to WIPP conditions. Instead of using these data directly the 350 ppm with the 0 ppm data is used to construct a distribution for the STEEL:HUMCORR parameter via interpolation between the two data sets, rather than by aggregating the two sets of data.

The humid corrosion rate data in Roselle (2013) comprises 16 data points, 8 for samples tested at 0 ppm carbon dioxide (CO_2) and 8 for samples tested at 350 ppm CO_2. The 350 ppm CO_2 data set was reduced to four samples by excluding nonphysical, negative corrosion rates. Each data set was initially considered

separately. The corrosion rates from Table A-1 of Roselle (2013) were converted from units of μm/yr to m/s and sorted in ascending order, with appropriate percentiles assigned to each corrosion rate, resulting in two empirical cumulative distribution functions (CDFs) (see attached Excel spreadsheet for the detailed calculations). For completeness, a value of 0 m/s was assigned to the zeroth percentile for each CDF. In order to combine the CDFs, a common set of percentiles was constructed over the range 0-100 by linearly interpolating the 350 ppm data between existing data points. Finally, a CDF representative of corrosion rates at 0.58 ppm CO_2 was formed by linearly interpolating between quantiles (Figure 1). The result is a CDF that can be used as a cumulative distribution to describe the STEEL:HUMCORR parameter (Table 1). Statistics for the CDF are shown in Table 2.

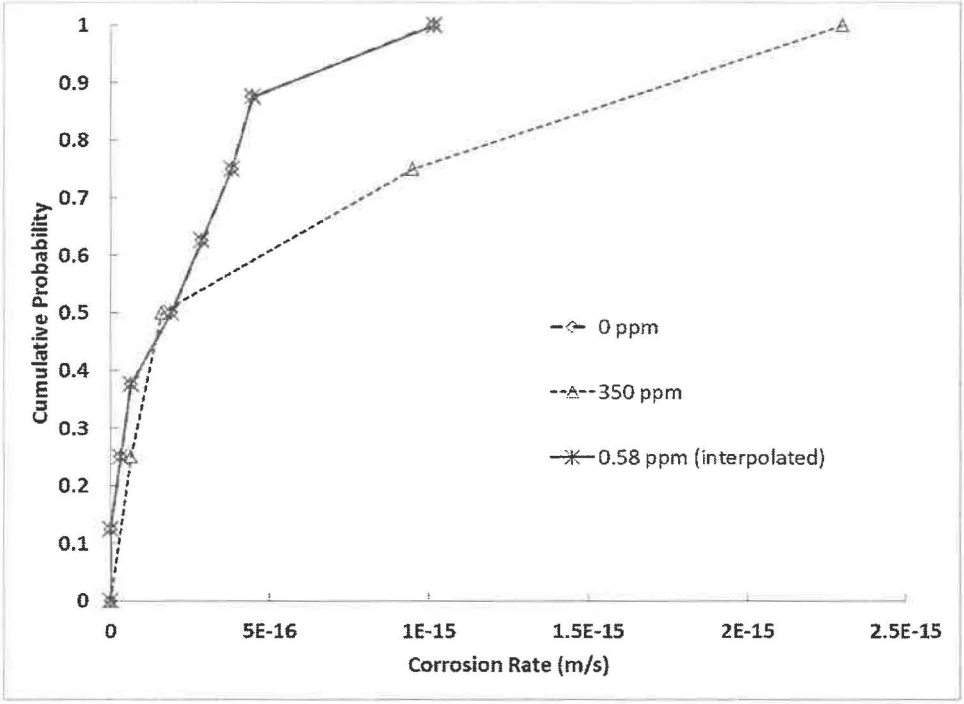

Figure 1. CDFs for the 0 ppm and 350 ppm CO_2 data sets, as well as the final interpolated CDF for 0.58 ppm.

Table 1. CDF data for the STEEL:HUMCORR parameter that describes iron corrosion rates.

Value (m/s)	Cumulative Probability
0	0
5.22E-20	0.125
3.18E-17	0.25
6.35E-17	0.375
1.90E-16	0.5
2.86E-16	0.625
3.81E-16	0.75
4.46E-16	0.875
1.02E-15	1

Table 2. Statistics for the CDF of STEEL:HUMCORR.

Mean	2.68E-16
Median	1.90E-16
St. Dev.	3.27E-16
Min.	0.00E+00
Max.	1.02E-15

References:

Domski, P., Y.-L. Xiong. 2015. Prediction of Baseline Actinide Solubilities with an Updated EQ3/6 Thermodynamic Database (DATA0.FM2) in Response to EPA Completeness Comment 3-C-3 for CRA 2014. ERMS 565032. Sandia National Laboratories, Carlsbad, NM.

Domski, P.S. 2015. "Memo AP-173, EQ3/6 Database Update: DATA0.FM2" Memorandum to WIPP Records, October 27, 2015. Carlsbad, NM : Sandia National Laboratories. ERMS 564914.

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Wolery, T.J., Y.-L. Xiong, and J.J. Long, 2010. "Verification and Validation Plan/Validation Document for EQ3/6 Version 8.0a for Actinide Chemistry, Document Version 8.10." Carlsbad, NM: Sandia National Laboratories. ERMS 550239.

Xiong, Y.-L, 2011b. "WIPP Verification and Validation Plan/Validation Document for EQ3/6 Verison 8.0a for Actinide Chemistry, revision 1. Supersedes ERMS 550239." May 12, 2011. Carlsbad, NM. Sandia National Laboratories. ERMS 555358.

Zeitler, T.R. and C. Hansen. 2015. Cumulative distribution for STEEL:HUMCORR. ERMS 565009. Sandia National Laboratories, Carlsbad, NM.

µm/m	seconds in a year
1.00E+06	3.1536E+07

0 ppm "humid" CO_2 experiments with non-negative corrosion rates

Test ID	µm/m	m/s
Fe-Atm-0000-6-1	0.012	3.81E-16
Fe-Atm-0000-6-2	0.006	1.90E-16
Fe-Atm-0000-12-1	0.009	2.85E-16
Fe-Atm-0000-12-2	0.032	1.01E-15
Fe-Atm-0000-18-2	0.002	6.34E-17
Fe-Atm-0000-18-3	0	0.00E+00
Fe-Atm-0000-24-1	0.014	4.44E-16
Fe-Atm-0000-24-2	0.001	3.17E-17

Empirical CDF

Percentile	Value
0	0
12.5	0.00E+00
25	3.17E-17
37.5	6.34E-17
50	1.90E-16
62.5	2.85E-16
75	3.81E-16
87.5	4.44E-16
100	1.01E-15

Interpolated CDF @ 0 ppm

Value	Percentile
0	0
0.00E+00	12.5
3.17E-17	25
6.34E-17	37.5
1.90E-16	50
2.85E-16	62.5
3.81E-16	75
4.44E-16	87.5
1.01E-15	100

350 ppm "humid" CO_2 experiments with non negative corrosion rates

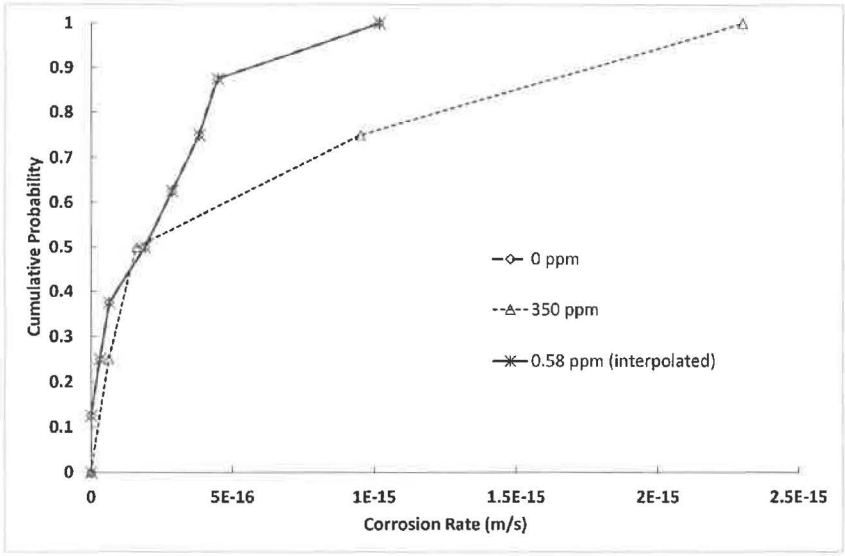
Test ID	µm/m	m/s
Fe-Atm-0350-6-2	0.005	1.59E-16
Fe-Atm-0350-12-1	0.03	9.51E-16
Fe-Atm-0350-12-2	0.072	2.28E-15
Fe-Atm-0350-18-3	0.002	6.34E-17

Empirical CDF

Percentile	Value	
0	0	0
25	6.30E-17	0.25
50	1.60E-16	0.5
75	9.50E-16	0.75
100	2.30E-15	1

Interpolated CDF @ 350 ppm

Value	Percentile
0	0
3.15E-17	12.5
6.30E-17	25
1.12E-16	37.5
1.60E-16	50
5.55E-16	62.5
9.50E-16	75
1.63E-15	87.5
2.30E-15	100



CO_2 fugacity (ppm) 0.58

Interpolated CDF @ 0.58 ppm

Value (m/s)	Cumulative Probability	Percentile
0	0	0
5.22E-20	0.125	12.5
3.18E-17	0.25	25
6.35E-17	0.375	37.5
1.90E-16	0.5	50
2.86E-16	0.625	62.5
3.81E-16	0.75	75
4.46E-16	0.875	87.5
1.02E-15	1	100

Mean	2.68E-16
Median	1.90E-16
St. Dev.	3.27E-16
Min.	0.00E+00
Max.	1.02E-15