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From: Todd R. Zeitler

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

This memo documents the justification for a distribution of humid steel corrosion rates (parameter STEEL:HUMCORR) to be used in WIPP PA calculations. Based on the assumption that the use of increased steel corrosion rates results in higher releases, use of the revised distribution will result in "bounding" releases when the predicted amount of CO_2 in the gas phase is at or below 5 ppm. The value of 5 ppm is chosen as a reasonable expected bounding value because the maximum value from previous compliance analyses is 3.16 ppm (Brush et al. 2009, Brush and Domski 2013). In WIPP PA, steel corrosion reactions result in increased gas repository pressures. Increased gas pressures, in general, lead to increased spallings and direct brine releases (DBRs), but can also promote decreased brine saturations, which can lead to decreased DBRs.

Prior to CRA-2014 PA calculations, a value of zero was used for the humid steel corrosion rate parameter. In order to address Completeness Comment 4-C-3 received from the EPA regarding the CRA-2014, it was found that it was appropriate to construct a distribution of values for the HUMCORR parameter from the data of Roselle (2013) (Zeitler and Hansen 2015a). The data available from Roselle include corrosion rates for CO_2 concentrations of 0 and 350 ppm. For the version of the thermodynamic database used in CRA-2014 (DATA0.FM1), there was a predicted value of 3.14 ppm CO_2 in the gas phase when in equilibrium with WIPP brines (Brush and Domski 2013). A 350 ppm CO_2 concentration is two orders of magnitude higher than the predicted value, and therefore these data were considered not directly relevant to WIPP conditions. Instead of using these data directly, the 350 ppm with the 0 ppm data was 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.

Following the construction of the STEEL:HUMCORR distribution by Zeitler and Hansen (2015a), the EQ3/6 thermodynamic database was updated (DATA0.FM2) in response to the EPA's CRA-2014 Completeness Comments 3-C-3 and 3-C-4 (Domski 2015). The new database predicted a value of 0.58 ppm CO_2 in the gas phase when in equilibrium with WIPP brines (Domski and Xiong 2015). The updated value of 0.58 ppm did not change the conclusions of Zeitler and Hansen (2015a) 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 was revised to reflect the change from 3.14 ppm to 0.58 ppm

CO_2 using an identical methodology to that used by Zeitler and Hansen (2015a) (Zeitler and Hansen 2015b).

In order to avoid the necessity to construct new distributions for the STEEL:HUMCORR parameter each time that the thermodynamic database is updated, a "bounding" distribution is constructed here that provides humid steel corrosion rates for an assumed value of 5 ppm CO_2 in the gas phase when in equilibrium with WIPP brines. The new distribution is calculated using an identical methodology to that used by Zeitler and Hansen (2015a) and Zeitler and Hansen (2015b); that is, to interpolate between the 0 ppm and 350 ppm data from Roselle (2013).

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 5 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. A comparison of humid corrosion rate distributions from Zeitler and Hansen (2015a), Zeitler and Hansen (2015b), and the current work is shown in Figure 2.

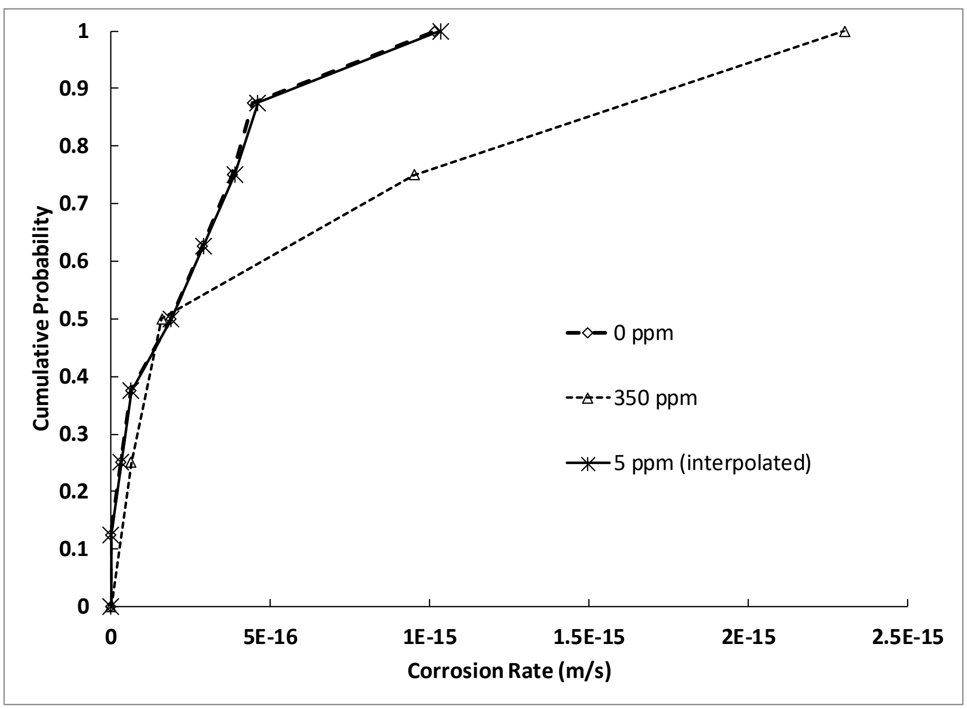

Figure 1. CDFs for the 0 ppm and 350 ppm CO_2 data sets, as well as the final interpolated CDF for 5 ppm.

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

Value (m/s)	Cumulative Probability
0	0
4.50E-19	0.125
3.22E-17	0.25
6.41E-17	0.375
1.90E-16	0.5
2.89E-16	0.625
3.89E-16	0.75
4.61E-16	0.875
1.03E-15	1

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

Mean	2.73E-16
Median	1.90E-16
St. Dev.	3.32E-16
Min.	0.00E+00
Max.	1.03E-15

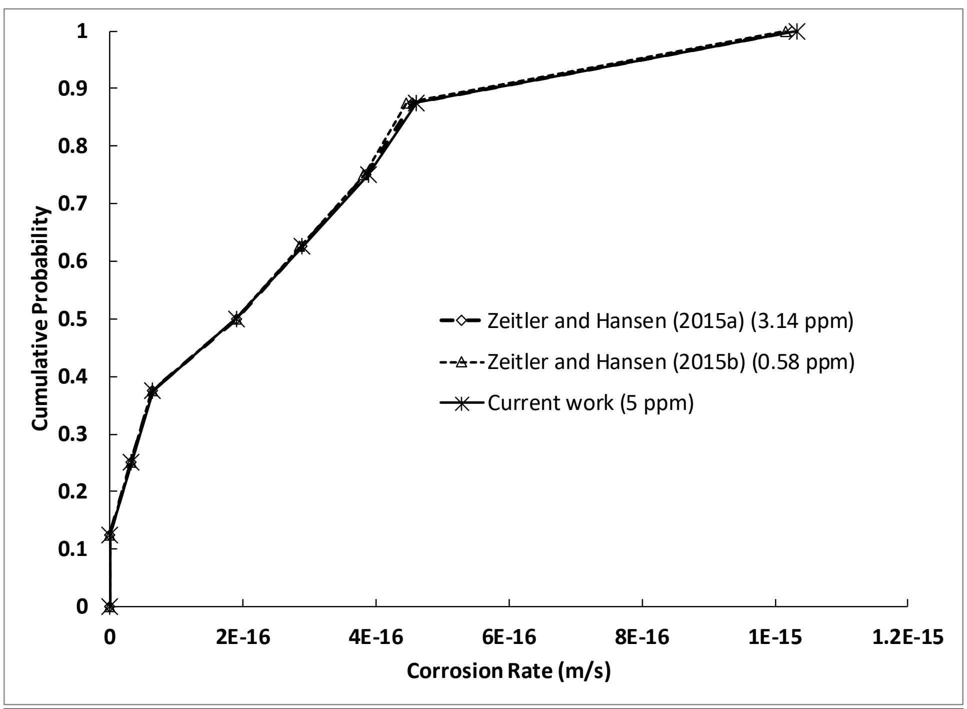

Figure 2. Comparison of CDFs for humid corrosion rates from Zeitler and Hansen (2015a) (3.14 ppm), Zeitler and Hansen (2015b) (0.58 ppm), and the current work (5 ppm).

<u>References</u>:

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.

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