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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

AP-175
Revision 0

Analysis Plan for Determination of Hydrogen and Iron from Steel Corrosion Products in WIPP-Relevant Conditions

Task 4.4.2.2.1

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Table of Contents

1 Introduction and Objectives 3
1.1 Introduction 3
1.2 Objectives 11
2 Approach 11
3 Software List 12
4 Tasks 12
4.1 Task 1 – Determination of STOIFX parameter value for Gas Generation Rate Calculations 12
4.2 Task 2 – Application of Results 12
5 Special Considerations 12
6 Applicable Procedures 12
7 References 13

1 *Introduction and Objectives*

1.1 Introduction

The Waste Isolation Pilot Plant (WIPP), located in the Chihuahuan Desert of southeastern New Mexico, is a geologic repository licensed to permanently dispose of defense-generated transuranic waste. Project facilities include disposal rooms excavated at a depth of 2,150 feet below the surface in the Salado salt formation. Within the WIPP repository, a significant quantity of iron (Fe) and other Fe-base metal/alloys (i.e. stainless steel and lead-lined waste containers and drums) are being emplaced. Currently, it is estimated that the WIPP will contain over 49,000 metric tons of iron (Van Soest 2012) when all the waste is emplaced.

Two waste characteristics that are of significance to performance assessment (PA) calculations are cellulose, plastic, and rubber (CPR) material and steel (iron). For the latter, iron has the potential to impact several aspects of the repository's chemical environment, such as:

a.) the redox conditions after repository closure,
b.) consumption of microbially produced carbon dioxide (CO_2)
c.) the formation of actinide/organic ligand complexes
d.) hydrogen gas generation due to corrosion of metals

The interaction of steel in the WIPP with repository brines has been shown to result in the formation of H_2 gas depending on the corrosion rate of steel and the type of corrosion products formed. This production of H_2 gas during the anoxic corrosion of steel is a concern for deep geologic disposal. The concern arises when progressive corrosion occurs in that the H_2 partial pressure influences the porosity of the waste repository, playing a significant role in transport of radionuclides from the repository. Accordingly, it is crucial to be able to accurately quantify the corrosion rate of steel and, thereby, the release rate of H_2 gas over time in the repository.

1.1.1 Corrosion Rate for Steel

Experimentally, there are a variety of ways to quantify the corrosion rate of steel. One method is to directly measure the rate of release of H_2 gas and from those measurements calculate the metal corrosion rates. This method avoids many of the pitfalls associated with alternate ways of determining corrosion rates and allows a direct determination of a critical parameter in steel corrosion, namely, H_2 gas production. Telander and Westerman (1993, 1997) determined steel corrosion rates under WIPP-relevant conditions by quantifying the rate of H_2 gas release by application of the ideal gas law. The studies included corrosion of low-carbon steel waste packaging materials in synthetic brines, representative of intergranular Salado brines at the repository horizon, under anoxic conditions. From these data, Wang and Brush (Wang and Brush 1996a) provided estimates of gas-generation parameters for the long-term WIPP PA.

Another method of quantifying the corrosion rate is by measuring the weight loss associated with the corrosion of steel. Roselle (2013) conducted experiments with mixed gases (N_2 and CO_2), but did not directly determine the corrosion rate unlike Telander and Westerman. Instead of quantifying the rate of H_2 gas generation, he determined the corrosion rate for the different brine types by measuring the iron coupon mass loss data results from both fully immersed and partially submerged coupons for each brine type under WIPP relevant conditions.

These WIPP experiments (Telander and Westerman, 1993, 1997; Roselle 2013) investigated gas generation from corrosion under a wide range of possible conditions in the repository. In

general, after the available O_2 is consumed in the closed repository, the most plausible corrosion mechanism of steel (Wang and Brush 1996a) exposed to WIPP brines and/or humid WIPP conditions is represented by:

$$Fe + 2H_2O \rightarrow Fe(OH)_2 + H_2 \quad (1)$$

In relatively low ionic strength solutions, Fe(II) hydroxide transforms into Fe(III) magnetite via the following reaction:

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2 \quad (2)$$

When normalized to 1 mole of Fe and linearly weighted by the factors x and 1-x ($0 \leq x \leq 1$), reactions (1) and (2) become

$$Fe + \left(\frac{4+2x}{3}\right) H_2O = \left(\frac{4-x}{3}\right) H_2 + xFe(OH)_2 + \left(\frac{1-x}{3}\right) Fe_3O_4 \quad (3)$$

where x and (1-x) are the fractions of Fe consumed in the reactions (1) and (2), respectively.

Although magnetite (Fe_3O_4) has been observed to form as a corrosion product in low-Mg anoxic brines (Haberman and Frydrych 1988) and at elevated temperatures (Telander and Westerman 1997), there is no evidence that it will form at WIPP repository temperatures. If Fe_3O_4 were to form as seen in reaction (2), H_2 would be produced (on a mole basis) in excess of the amount of Fe consumed. However, anoxic corrosion experiments (Telander and Westerman 1993) did not indicate the production of H_2 in excess of the amount of Fe consumed, which implies that Reaction (1) represents corrosion. Roselle (2013) also determined the average corrosion rates with the assumption that Reaction (1) was the predominant overall reaction.

Furthermore, researchers have noted that after $Fe(OH)_2$ is formed it can be transformed by two different reaction paths as shown in Reaction (4) and (5).

$$3Fe(OH)_2 \rightarrow Fe_3O_4 + H_2 + H_2O \quad (4)$$

$$2Fe(OH)_2 + Cl^- + H^+ \rightarrow Fe(II)_2(OH)_3Cl(cr) + H_2O \quad (5)$$

In Reaction (5) iron hydroxide reacts to form $Fe(II)_2(OH)_3Cl(cr)$, which is the pure iron end-member of hibbingite $(Fe(II),Mg)_2(OH)_3Cl(s)$. The solubility controlling phase, Fe-hibbingite, will control the solubility of iron, leading to a predicted solubility on the order of ~10^{-3} M for pH between 8.5 and ~9 (Nemer et al. 2011). This is because in environments where there are relatively high concentrations of chloride, like that of the WIPP brines (e.g., 6.40 m Cl^- in GWB, and 5.27 m Cl^- in ERDA-6; Xiong and Lord 2008), the reaction shown as Reaction (5) is favored over the reaction shown as Reaction (4). It should be noted that in the case of Reaction (5), there is no hydrogen gas produced.

Another example of the importance of accurately identifying corrosion phases can be found in consideration of iron coupons reacted with CO_2-bearing solutions:

$$Fe + H_2O + CO_2 \rightarrow FeCO_3 + H_2 \quad (6)$$

For decades, it was assumed that Reaction (6) described the stoichiometric relationship between Fe metal reacted and H_2 gas produced. However, beginning in the 1990's investigators (e.g., Refait et al. 1998, Génin et al. 2001, Ruby et al. 2003 and Simon et al. 2003) documented the existence of a new form of secondary corrosion product called "green rust", and the

carbonate-rich form has the formula: $[Fe(III)_2Fe(II)_4(OH)_{12}CO_3 \cdot 2H_2O]$. The net reaction for the generation of carbonated green rust is then:

$$6\ Fe + CO_2 + 15\ H_2O \rightarrow Fe(III)_2Fe(II)_4(OH)_{12}CO_3 \cdot 2H_2O + 7\ H_2 \quad (7)$$

The study conducted by Roselle's steel coupons did show formation of several phases dependent on the partial pressure of CO_2 (P_{CO2}). Scanning electron microscope (SEM) analysis with energy dispersive spectroscopy (EDS) showed the presence of a green Fe (±Mg) chlorhydroxide phase (Reaction 5) at P_{CO2} values <1500 ppm. At higher P_{CO2} the dominant corrosion product was a Fe-Mg-Ca hydroxicarbonate phase (Reaction 7). In general, his experiments showed corrosion rates increasing as a function of increasing CO_2 concentrations. In the analysis work, Roselle (2013) expanded his conclusions saying: "It is possible that other corrosion products (e.g., green rust, hibbingite, etc.) may also form (Nemer et al., 2011)." The presence of these possible corrosion products was never determined or characterization completed on Roselle's corrosion coupons.

Nemer et al. (2011) supported the statement "that other corrosion products may also form" by concluding that when low-carbon steel interacts with chloride-rich anoxic brine, the phase $Fe(II)_2(OH)_3Cl(cr)$ is likely to buffer the oxygen fugacity in the repository and is also expected to be a likely corrosion product in addition to some transient green rust containing sulfate. The anoxic corrosion of iron in chloride-rich brines to form the pure-iron end member of hibbingite, the likely final product, can be expressed as the following overall reaction,

$$2Fe(cr) + 3H_2O(l) + Cl^- + H^+ = Fe(II)_2(OH)_3Cl(cr) + 2H_2(g) \quad (8)$$

Using $Fe(OH)_2$ as the predominant and most likely corrosion product in the absence of O_2, Roselle calculated the corrosion rates from the mass loss data according to the following formula (NACE, 2000):

$$rate = \frac{W \times 87.6}{SA \times t \times \rho} \times 1000 \quad (9)$$

Where *rate* is the corrosion rate in μm/yr, *W* the mass loss (mg), *SA* the exposed surface area of the coupon (cm^2), *t* the exposure duration (hours), *ρ* the metal density (g/cm^3) and 1,000 converts the rate from mm/yr to μm/yr. A metal density of 7.872 g/cm^3 was used for the steel respectively (MatWeb, 2009). Roselle's calculated corrosion rates are provided below in Table 1 as a function of time for each CO_2 concentration and brine type and in Table 2 as average corrosion rates for steel averaged over all time segments.

Table 1. Average Corrosion Rates (µm/Yr) For Steel Samples (Roselle 2013)

Brine	Exposure Duration (months)			
	6	12	18	24
0 ppm CO_2 Concentration				
GWB	0.080 ± 0.07	0.186 ± 0.03	0.098 ± 0.01	0.201 ± 0.02
GWB Org	0.140 ± 0.09	0.188 ± 0.04	0.112 ± 0.01	0.149 ± 0.03
ERDA-6	0.075 ± 0.04	0.247 ± 0.03	0.189 ± 0.02	0.480 ± 0.04
ERDA-6 Org	0.189 ± 0.11	0.126 ± 0.02	0.116 ± 0.02	0.481 ± 0.07
Humid	0.009 ± 0.00	0.021 ± 0.02	0.001 ± 0.00	0.008 ± 0.01
350 ppm CO_2 Concentration				
GWB	0.189 ± 0.04	0.218 ± 0.02	0.120 ± 0.02	0.231 ± 0.05
GWB Org	0.200 ± 0.01	0.232 ± 0.03	0.144 ± 0.03	0.126 ± 0.01
ERDA-6	0.021 ± 0.02	0.176 ± 0.03	0.182 ± 0.05	0.989 ± 0.20
ERDA-6 Org	0.022 ± 0.03	0.180 ± 0.05	0.129 ± 0.02	0.444 ± 0.16
Humid	0.005 ± 0.0	0.051 ± 0.03	0.001 ± 0.0	0.000 ± 0.0
1500 ppm CO_2 Concentration				
GWB	0.239 ± 0.04	0.166 ± 0.05	0.180 ± 0.01	0.289 ± 0.08
GWB Org	0.259 ± 0.06	0.221 ± 0.03	0.160 ± 0.01	0.220 ± 0.06
ERDA-6	0.530 ± 0.03	0.577 ± 0.14	0.427 ± 0.09	0.499 ± 0.08
ERDA-6 Org	0.258 ± 0.07	0.206 ± 0.04	0.338 ± 0.06	0.427 ± 0.12
Humid	0.000 ± 0.0	0.000 ± 0.0	0.014 ± 0.00	0.009 ± 0.00
3500 ppm CO_2 Concentration				
GWB	0.397 ± 0.03	0.312 ± 0.01	0.246 ± 0.01	0.316 ± 0.05
GWB Org	0.388 ± 0.07	0.264 ± 0.02	0.258 ± 0.04	0.265 ± 0.03
ERDA-6	1.200 ± 0.25	0.924 ± 0.18	0.734 ± 0.08	0.952 ± 0.28
ERDA-6 Org	0.650 ± 0.07	0.543 ± 0.09	0.742 ± 0.05	0.788 ± 0.17
Humid	0.008 ± 0.01	0.006 ± 0.01	0.018 ± 0.01	0.004 ± 0.01

Source: Averages calculated from data in Roselle 2013, Appendix A. Note that negative corrosion rates in Appendix A-1 are not considered in the calculation over averages.

Table 2. Average Corrosion Rates (µm/Yr) For Steel Samples Averaged Over All Time Segments (Roselle 2013)

Brine	CO_2 Concentration (ppm)			
	0	350	1500	3500
GWB	0.141 ± 0.07	0.190 ± 0.05	0.195 ± 0.05	0.318 ± 0.07
GWB Org	0.147 ± 0.06	0.175 ± 0.05	0.213 ± 0.06	0.303 ± 0.08
ERDA-6	0.248 ± 0.16	0.342 ± 0.40	0.511 ± 0.11	0.952 ± 0.26
ERDA-6 Org	0.228 ± 0.16	0.194 ± 0.18	0.267 ± 0.08	0.645 ± 0.11
Humid	0.010 ± 0.01	0.016 ± 0.03	0.005 ± 0.01	0.010 ± 0.01

Source: Averages calculated from data in Roselle 2013, Appendix A. Note that negative corrosion rates in Appendix A-1 are not considered in the calculation over averages.

1.1.2 WIPP 2014 Recertification and Corrosion Performance Assessment Parameters

In a letter from J. Edwards, USEPA to J. Franco, DOE, (Transmitting Fourth Set of Completeness Comments Related to the 2014 WIPP Compliance Recertification Application, Response 4-C-2, 4-C-3 and 4-C-6, EPA Docket EPA-HQ-OAR-2014-0609-0024, ERMS 564885) three questions were posed by EPA to DOE regarding corrosion parameters that incorporated Roselle's data. These variables correspond to the PA parameters CORRMCO2, HUMCORR, and STOIFX, respectively (Table 3). The questions can be summarized as:

1. **EPA Comment 4-C-2**: "*Please provide a justification for why the experimental corrosion data gathered from [Roselle's] experiments above 0 ppm CO_2 concentrations were not included in the development of the parameter CORRMCO2. Please update the range, median and distribution for the CORRMCO2 parameter that reflects this experimental data.*"

2. **EPA Comment 4-C-3**: *"Please justify why the DOE does not use the available and WIPP-relevant data in the derivation of corrosion rates that indicate corrosion will occur under humid conditions.[HUMCORR]"*

3. **EPA Comment 4-C-6**: *"The stoichiometric coefficient used in PA for gas generation due to steel corrosion (STOIFX) has been maintained at its historical value of 1. This parameter of "1" assumes no green rust will form on steel. The assumption is contradicted in Appendix SOTERM Section 2.3.4 of the CRA-2014 which includes the following statement:*

   Roselle (Roselle 2013) states that green rust is the most likely corrosion product in experiments with low atmospheric CO2 concentration s (<350 ppm).

   Given the contradictions, the DOE should discuss why a value of "1" should be used for the parameter STOIFX."

Responses were provided for each comment and recapped below.

1. **DOE Response 4-C-2**: The DOE accepts the EPA position and proposes to modify the STEEL:CORRMCO2 parameter to reflect a cumulative distribution that considers the 0 and 350 ppm CO_2 experimental results, which DOE believes to bracket the conditions expected in the WIPP (Zeitler and Hansen 2015a, 2015b). This will also incorporate an updated equilibration gas phase concentration with DATA0.FM2 of 0.58 ppm CO_2 (Domski and Xiong 2015). The new statistics for the cumulative distribution function of STEEL:CORRMCO2 are presented in Table 3.

2. **DOE Response 4-C-3**: Based on the EPA comment, DOE will reanalyze the applicability of data from iron corrosion experiments at 0 and 350 ppm CO_2 (Roselle 2013). It was determined that the selection of corrosion rates based solely on 0 ppm CO_2 experiments may not completely reflect iron corrosion under WIPP conditions because there is a predicted value of 0.58 ppm CO_2 in the gas phase when in equilibrium with WIPP brines. Therefore, it is appropriate to also consider data from corrosion experiments performed under conditions with nonzero CO_2 concentrations. Therefore, the 350 ppm data will be used with the 0 ppm data to construct a distribution for the STEEL:HUMCORR parameter via linear interpolation between the two data sets (Zeitler and Hansen 2015c, 2015d). The results will be a cumulative distribution function that can be used as a cumulative distribution to describe the STEEL:HUMCORR parameter (Table 3).

3. **DOE Response 4-C-6**: The corrosion products in Roselle's experiments have not been quantitatively identified, and he found no indication that the most likely corrosion product observed by Telander and Westerman (1993), being $Fe(OH)_2$, will differ significantly from his results or that green rust, a transient product, would be the major product. Section 2.3.4 of Appendix SOTERM -2014 incorrectly refers to Roselle's work and has been revised. The major product is $Fe(OH)_2$ or possibly its successor, $Fe(II)_2(OH)_3Cl(cr)$, as time evolves. DOE maintains that the mole ratio of hydrogen gas to iron should be 1 in the anoxic corrosion of iron in the absence of CO_2. It is therefore recommended that the parameter STOIFX not change from its current value of 1 (Table 3).

Table 3. Steel Corrosion Pa Parameters

			CRA 2009	CRA 2014	EPA Comments (2016)	
Parameter	Definition	Attribute	"Value"	"Value"	"Value"	Unit
STEEL:CORRMCO2	Generic steel in waste, Inundated corrosion rate for steel without CO_2 present	Distribution	Uniform	Student	Cumulative	--
		Maximum	3.17E-14	1.84E-14	3.96E-14	m/s
		Mean	1.59E-14	6.06E-15	6.76E-15	m/s
		Median	1.59E-14	6.06E-15	5.58E-15	m/s
		Minimum	0.00E+00	3.29E-16	0.00E+00	m/s
		St. Dev.	9.15E15	4.05E-15	5.84E-15	m/s
		Degrees of Freedom	N/A	6.03E+01	1.25E+02	None
HUMCORR	Rate of anoxic steel corrosion under humid conditions	Mean	Constant = 0	Constant = 0	2.68E-16	m/s
		Median			1.90E-16	m/s
		St. Dev.			3.27E-16	m/s
		Min.			0.00E+00	m/s
		Max			1.02E-15	m/s
STOIFX	Stoichiometric coefficient for gas generation	Constant	1	1	1[a]	None

[a] Roselle report will not be revised. Reports which supersedes Roselle (2013) will be issued. Perceived contradictory statements will be addressed as part of EPA comment review process.

Upon responding to 4-C-6, it was determined by Sandia National Laboratories that the characterization of Roselle's corrosion coupons and the validation of hydrogen gas parameters should be completed as set out in the original TP 06-02. The quantitative characterization of corrosion products will be carried out in TP 06-02, Rev. 3, and determination of the mol H_2 gas generated and the corresponding mol H_2 to Fe ratio will be determined, per this Analysis Plan. Then the STOIFX parameter value will be re-evaluated. The STEEL:CORRMCO2 and STEEL:HUMMCORR parameters were adjusted according to the justifications specified in the 4-C-2 and 4-C-3 DOE 2014 CRA Response Letters (Sisk-Scott and Zeitler, 2015a and 2015b).

1.1.3 Hydrogen Gas Generation Rate for Steel

In the Average-Stoichiometry Model, which is currently implemented in BRAGFLO, hydrogen gas generation is assumed to result from the microbial degradation of CPR materials and the anoxic corrosion of steel. As the corrosion reactions (1-8) in Table 4 illustrate, a lack of corrosion product identification or incorrect assumptions regarding the stable corrosion products will lead to incorrect estimates of the amount of H_2 gas produced. In the case of Reaction (2) versus Reaction (6), if iron hydroxide reacts to form magnetite the ratio of moles H_2 gas produced to moles Fe reacted is 4:3 and a 24% overestimate is possible. This will change the current STOIFX parameter value (2014 CRA) from 1 to 1.3. Whereas, if iron hydroxide reacts to form hibbingite, as per Reaction (8), then the ratio is 1:1, which will leave the STOIFX parameter unchanged. This can have a substantial effect on the gas generation rate, since uncertainties in the STOIFX parameter are larger than all the other cumulative errors in the experiments.

Table 4. Corrosion Reactions And Their Corresponding H_2/Fe Mol Ratios

Corrosion Reaction	mol H_2	mol Fe	mol H_2/mol Fe
1.) $Fe + 2H_2O \rightarrow Fe(OH)_2 + H_2$	1	1	1.0
2.) $3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$	4	3	1.3
3.) $Fe + \left(\frac{4+2x}{3}\right) H_2O = \left(\frac{4-x}{3}\right) H_2 + xFe(OH)_2 + \left(\frac{1-x}{3}\right) Fe_3O_4$	1	1	1.0
4.) $3Fe(OH)_2 \rightarrow Fe_3O_4 + H_2 + H_2O$	1	N/A	N/A
5.) $2Fe(OH)_2 + Cl^- + H^+ \rightarrow Fe(II)_2(OH)_3Cl(cr) + H_2O$	N/A	N/A	N/A
6.) $Fe + H_2O + CO_2 \rightarrow FeCO_3 + H_2$	1	1	1.0
7.) $6\ Fe + CO_2 + 15\ H_2O \rightarrow Fe(III)_2Fe(II)_4(OH)_{12}CO_3 \cdot 2H_2O + 7\ H_2$	7	6	1.2
8.) $2Fe(cr) + 3H_2O(l) + Cl^- + H^+ = Fe(II)_2(OH)_3Cl(cr) + 2H_2(g)$	2	2	1.0

The current STOIFX parameter value is inferred from the predominant mechanism (Reaction 1) for steel corrosion based on experiments performed by Telander and Westerman (1993 and 1997) and Roselle (2009, 2010, 2011a, 2011b, and 2013) mentioned earlier. The parameter STOIFX represents the stoichiometric coefficient for hydrogen gas generation due to the anoxic corrosion of steel. However, note that the value of the STOIFX term depends on the phase formed as seen in Table 4. Therefore, in order to model the long-term H_2 gas generation rate in an anoxic disposal environment it is critical to measure both the H_2 gas production and document the phase formations over time.

Roselle's steel corrosion data provided in Tables 1 and 2 were used to determine the rate of gas generation due to anoxic corrosion of steel (q_{rgc}) by equation PA.67 in Appendix PA of the 2014 CRA (DOE, 2014).

$$q_{rgc} = \left(R_{ci}S_{b,eff} + R_{ch}S_g^*\right)D_s\rho_{Fe}X_c(H_2|Fe)M_{H_2} \tag{10}$$

where

D_s = surface area concentration of steel in the repository (m^2 surface area steel/ m^3 disposal volume)

M_{H_2} = molecular weight of H_2 (kg H_2/mol H_2)

R_{ci} = corrosion rate under inundated conditions (m/s) [CORRMCO2]

R_{ch} = corrosion rate under humid conditions (m/s) [HUMCORR]

$S_{b,eff}$ = effective brine saturation due to capillary action in the waste materials

$$S_g^* = \begin{cases} 1 - S_{b,eff}, & if\ S_{b,eff} > 0 \\ 0, & if\ S_{b,eff} = 0 \end{cases}$$

ρ_{Fe} = molar density of steel (mol/m^3)

$X_c(H_2|Fe)$ = stoichiometric coefficient for gas generation due to corrosion of steel (mol H_2/mol Fe) [STOIFX]

Three of the variables in equation (10) are directly associated with the steel corrosion data represented in Roselle's studies. These variables are R_{ci}, the steel corrosion rate under inundated conditions; R_{ch}, the corrosion rate under humid conditions and $X_c(H_2|Fe)$, the stoichiometric coefficient for gas generation.

In Roselle's experiments, the calculation of mass loss data and the resulting corrosion rates for each of the relevant experiment coupons was determined (R_{ci} *and* R_{ch}). The determination of the corrosion products was not completed but will be carried out according to TP 06-02 Rev. 3. Upon identification of the corrosion products, the reaction pathways will be determined and their consequent mol ratios for H_2 and Fe established in this Analysis Plan. The hydrogen gas generation rate calculation will not be within the scope of this Analysis Plan, since the gas generation rates are calculated directly within the PA model code BRAGFLO.

1.2 Objectives

The analysis described in this plan is a compliance decision analysis with the objective of recalculating the stoichiometric coefficient (STOIFX) for gas generation due to corrosion of steel for compliance calculations. The objectives are laid out in the original version of TP 06-02, "Iron and Lead Corrosion in WIPP-Relevant conditions." It should be pointed out that in the first writing of TP 06-02, very little was known about green rust. Since the findings from Roselle, the importance of green rust is now understood, and in this analysis plan, the role played by this phase in corrosion of steel will be examined. The corrosion reactions will be established and compared to previous reaction pathways. The resultant Fe corrosion reactions established will then enable the mol H_2 gas production and the hydrogen gas generation rate (BRAGFLO) to be determined.

2 Approach

The objective of Roselle's experiments was to determine steel corrosion rates under WIPP-relevant conditions. Specifically, his experiments aimed to determine the corrosion rates of iron-based metal and the nature of the corrosion products formed. A detailed discussion of the methods used and experimental setup of the corrosion studies can be found in Roselle (2009). The original test plan (TP-06-02) has been modified recently (TP-06-02 Rev 3) to include experimental work to identify the corrosion products present in Roselle's experiments. If the corrosion products observed as a result of the work conducted under TP 06-02, Rev. 3 are different from those previously reported; the STOIFX parameter derived for CRA-2014 PA will be re-examined.

First the appropriate reaction or sets of reactions [Reaction (1-8)] will be identified. Based on those reactions, the hydrogen gas generated can be determined. This mol H_2 gas generated can then be used to calculate the mol H_2/mol Fe ratio. This will impart a STOIFX parameter value, which PA can apply in the calculations of the gas generation rates within the PA model code BRAGFLO.

3 Software List

Commercial off-the-shelf spreadsheet programs, such as Excel, will be used for data manipulation and plotting.

4 Tasks

4.1 Task 1 – Determination of STOIFX parameter value for Gas Generation Rate Calculations

Once the corrosion products have been determined according to TP 06-02 Rev. 3, the methods outlined in the Approach Section will be used to calculate a mol H_2/mol Fe ratio (STOIFX parameter).

4.2 Task 2 – Application of Results

Once the data analysis is completed a report will be generated and submitted to provide insight into the extent to which metals within the WIPP (specifically iron) might augment previous expected corrosion behavior. These results will also be used to formulate new gas generation parameters, if needed, for use in the WIPP PA.

At Sandia National Laboratories-Carlsbad, the Technical and Research Staff will be performing Tasks 1-2. All tasks will be completed by September 30th, 2016.

5 Special Considerations

No special considerations have been identified.

6 Applicable Procedures

All applicable WIPP quality assurance procedures will be followed when conducting these analyses. Training of personnel will be done in accordance with the requirements of NP 2-1, *Qualification and Training*. Specifically, the following Nuclear Waste Management Procedures (NPs) and Activity/Project Specific Procedures (SPs) are applicable:

- NP 6-1 – *Document Review Process*
- NP 9-1 – *Analyses*
- NP 17-1 – *Records*
- NP 19-1 – *Software Requirements*
- NP 20-2 – *Scientific Notebooks*
- SP 13-1 – *Chain of Custody*
- SOP CPG-CHEM-TWD-2011-001 – *ES&H Standard Operating Procedure (ES&H SOP) for Activities in the Sandia National Laboratories/Carlsbad Program Group Laboratory, Building NPHB (U)*
- Standard Operating Procedure (SOP) for Oxygen Deficiency Hazard Alarm Response for Carlsbad (Building NPHB)

7 References

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