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To: Records Center

From: Todd R. Zeitler

Subject: A summary of EPA/DOE defined parameters to be implemented in the CRA-2019 PA

Introduction

Some parameter values to be utilized in the CRA-2019 PA have been defined by the U.S. Environmental Protection Agency (EPA) and agreed to by the U.S. Department of Energy (DOE) (Peake 2018 and Veal 2017). The specified parameter values represent changes to CRA-2014 PA inputs, including three sampled parameters (GLOBAL:PBRINE, BOREHOLE:TAUFAIL, and WAS_AREA:HYMAGCON) and six constant parameters (REFCON:STCO_31, REFCON:STCO_32, REFCON:STCO_35, REFCON:STCO_36, REFCON:STCO_43, and REFCON:STCO_46) and are summarized in Table 1 and Table 2, respectively.

This memo provides a concise listing of the revised CRA19 analysis parameter names and values to allow for data entry into the Performance Assessment Parameter Database (PAPDB) from a single source document.

GLOBAL:PBRINE Parameter

As agreed to by the EPA and DOE (Peake 2018 and Veal 2017), a cumulative distribution (derived by the EPA) is to be used for the GLOBAL:PBRINE parameter (Table 1). The distribution referred to by Peake (2018) is that enumerated in Table B-1 of the technical support document (TSD) related to the PBRINE parameter (U.S. EPA 2017a) that supported the EPA's 2017 recertification decision (U.S. EPA 2017b). The EPA previously directed this distribution for use by the DOE as part of the CRA14_SEN4 sensitivity study (Zeitler and Day 2016) and the distribution thus already exists in the PAPDB as version 4 of the PBRINE parameter. Since these parameters were directed by EPA to be used in a sensitivity study, they were not previously justified for use in compliance calculations per NP-9-1. EPA has since directed their use in a compliance calculation for the CRA-2019. For completeness, the values that comprise the EPA-directed distribution are listed in Table 3. The new distribution is fundamentally different in terms of values and basis from that proposed by the DOE as part of the CRA-2014 PA. The

impact of the EPA's recommended change to the distribution is to, on average, increase the probability of intersecting brine for an inadvertent drilling intrusion.

BOREHOLE:TAUFAIL Parameter

As agreed to by the EPA and DOE (Peake 2018 and Veal 2017), the minimum value in the uniform distribution for the BOREHOLE:TAUFAIL parameter should be changed from the value used in the CRA-2014 PA (2.22 Pa) to 1.60 Pa (see Table 1). The change to the distribution referred to by Peake (2018) is described on p.iii in the TSD on the TAUFAIL parameter (U.S. EPA 2017c) that supported the EPA's 2017 recertification decision (U.S. EPA 2017b). The EPA previously directed this distribution for use by the DOE as part of the CRA14_SEN4 sensitivity study (Zeitler and Day 2016) and the distribution thus already exists in the PAPDB as version 7 of the TAUFAIL parameter.

WAS AREA:HYMAGCON Parameter

As agreed to by the EPA and DOE (Peake 2018), the distribution for the WAS_AREA:HYMAGCON parameter should be changed from that used in the CRA-2014 PA to one derived by the EPA (see Table 1). The new distribution referred to by Peake (2018) is described in Table 12-1 of the TSD on chemistry-related issues (U.S. EPA 2017d) that supported the EPA's 2017 recertification decision (U.S. EPA 2017b). The general impact of the change to the distribution on PA calculations is an, on average, lower amount of brine produced from the modeled hydromagnesite to magnesite conversion reaction.

REFCON:STCO 31, REFCON:STCO 32, REFCON: STCO 35, REFCON:STCO 36, REFCON:STCO 43, and REFCON:STCO 46 Parameters

As agreed to by the EPA and DOE (Peake 2018), the stoichiometric coefficients defining the sulfidation reactions with iron and iron hydroxide are to be set to zero (0). The parameters listed in Table 2, when set to zero, turn off the FeOH₂ and metallic Fe sulfidation reactions. The setting of these parameters to a value of zero referred to by Peake (2018) is described on p.12 of the TSD on chemistry-related issues (U.S. EPA 2017d) that supported the EPA's 2017 recertification decision (U.S. EPA 2017b). The EPA previously directed the zeroing out of these stoichiometric coefficients for use by the DOE as part of the CRA14_SEN4 sensitivity study (Zeitler and Day 2016) and thus these values already exist in the PAPDB as version 2 of the respective parameters. The general impact of the change to these stoichiometric coefficients on PA calculations is that less hydrogen sulfide gas will be consumed and less water will be produced in the waste areas.

Table 1: EPA-Defined Sampled Parameters for the CRA-2019 PA that Differ from Those of the CRA-2014 PA

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value¹	Source
GLOBAL:PBRINE	none	Prob. that Drilling Intrusion In Excavated Area Encounters Pressurized Brine	Cumulative	(See Table 3 for distribution data)	0.26345	Peake 2018, Veal 2017, U.S. EPA 2017a
BOREHOLE:TAUFAIL	Pa	Effective shear strength for erosion	Uniform	Min = 1.60 Max = 77 Mean = 39.3	39.3	Peake 2018, Veal 2017, U.S. EPA 2017c
WAS_AREA:HYMAGCON	mol kg ⁻¹ sec ⁻¹	Rate of conversion of hydromagnesite to magnesite	Uniform	Min = 0 Max = 3.4 x 10 ⁻¹⁰ Mean = 1.7 x 10 ⁻¹⁰	1.7 x 10 ⁻¹⁰	Peake 2018, U.S. EPA 2017d

¹ For material properties defined by cumulative distributions, default values are calculated as weighted (i.e., not arithmetic) means.

Table 2: EPA-Defined Constant Parameters for the CRA-2019 PA that Differ from Those of the CRA-2014 PA

Parameter	Units	Description	Value	Source
REFCON:STCO_31	none	FeOH2 Sulfidation: H2 Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_32	none	FeOH2 Sulfidation: H2O Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_35	none	FeOH2 Sulfidation: FeOH2 Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_36	none	FeOH2 Sulfidation: FeS Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_43	none	Metallic Fe Sulfidation: Fe Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d
REFCON:STCO_46	none	Metallic Fe Sulfidation: FeS Stoichiometric Coefficient	0	Peake 2018, U.S. EPA 2017d

Table 3: Distribution Data for GLOBAL:PBRINE for the CRA-2019 PA

Rank	GLOBAL:PBRINE	Probability of Sampling GLOBAL:PBRINE	Cumulative Distribution Function (CDF)
1	0.04	0.002	0.002
2	0.05	0.002	0.004
3	0.06	0.002	0.006
4	0.07	0.008	0.014
5	0.08	0.009	0.023
6	0.09	0.02	0.043
7	0.1	0.037	0.08
8	0.11	0.029	0.109
9	0.12	0.031	0.139
10	0.13	0.046	0.185
11	0.14	0.038	0.223
12	0.15	0.042	0.264
13	0.16	0.03	0.294
14	0.17	0.035	0.33
15	0.18	0.033	0.363
16	0.19	0.023	0.385
17	0.2	0.028	0.414
18	0.21	0.016	0.429
19	0.22	0.025	0.455
20	0.23	0.023	0.478
21	0.24	0.009	0.487
22	0.25	0.024	0.512
23	0.26	0.021	0.533
24	0.27	0.013	0.546
25	0.28	0.017	0.563
26	0.29	0.014	0.577
27	0.3	0.016	0.593
28	0.31	0.016	0.609
29	0.32	0.024	0.633
30	0.33	0.02	0.653
31	0.34	0.02	0.673
32	0.35	0.016	0.689
33	0.36	0.023	0.713
34	0.37	0.023	0.735
35	0.38	0.024	0.759

Rank	GLOBAL:PBRINE	Probability of Sampling GLOBAL:PBRINE	Cumulative Distribution Function (CDF)
36	0.39	0.015	0.774
37	0.4	0.022	0.796
38	0.41	0.029	0.825
39	0.42	0.027	0.851
40	0.43	0.023	0.875
41	0.44	0.015	0.89
42	0.45	0.018	0.908
43	0.46	0.019	0.927
44	0.47	0.012	0.939
45	0.48	0.013	0.953
46	0.49	0.012	0.964
47	0.5	0.012	0.976
48	0.51	0.006	0.982
49	0.52	0.004	0.986
50	0.53	0.006	0.993
51	0.54	0.004	0.997
52	0.55	0.001	0.998
53	0.56	0.001	0.999
54	0.57	0.001	1

References

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