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date: *June 27, 2022*

to: Sandia National Laboratory WIPP Records Center

from: Paul S. Domski and Martin B. Nemer, SNL WIPP Geochemistry *signature on file*

subject: Revised Literature Screening Criteria for the WIPP Actinide Solubility Uncertainty Analysis for CRA-2024

Introduction

On June 30, 2021, Sandia National Laboratory (SNL) presented to Carlsbad Field Office of the Department of Energy (CBFO) proposed revisions to the general literature screening criteria used for selecting experimental studies to be included in the actinide uncertainty analysis. The motivation to revise the existing screening criteria was to simplify the language for clarity and refine the experimental data selection strategies. At the June 30th meeting, a working group was formed to revise the criteria. The group was comprised of Anderson Ward of CBFO, Don Reed and Jeremy Beam of Los Alamos National Laboratory, and Martin Nemer and Paul Domski of SNL. The intent of this working group was to meet regularly and come to a consensus on the revisions to the general literature screening criteria, and to present the revised criteria to CBFO and to the EPA at a technical exchange.

The WIPP literature screening criteria are used to determine which experimental studies, or specific data, or subsets of data, from an experimental study, are included in the actinide uncertainty analysis. Each of the screening criteria must be met for a study to be included in the uncertainty analysis. However, exceptions may be considered on a case-by-case basis, provided the justification for any exception is well documented. These screening criteria are intended for use in the WIPP actinide uncertainty analysis, they are NOT intended to be used to select parameters to be included in the WIPP actinide solubility model, i.e., the thermodynamic database.

The revised screening criteria are listed below, Table 2 provides a side-by-side comparison of the old criteria with the new criteria with notes, and finally, a discussion of how the parameter ranges for criterion G11 were determined is provided.

Literature Screening Criteria for the CRA-2024 Actinide Uncertainty Analysis

Applicability:
These screening criteria are applicable to the selection of experimental data from the scientific literature for the purpose of validating the WIPP actinide solubility model under conditions

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WIPP:4.0.1:PA:QA-L:577493

modeled in PA. In this context, it is necessary to differentiate the two types of data typically considered in modeling, training data and test data. Training Data are those data used to fit free parameters to a given model, e.g., laboratory measurements of solubility which are used to fit the log K of a specific mineral phase. These screening criteria are ***not*** *intended for use in selecting Training Data, or to fit free parameters to the WIPP actinide solubility model for inclusion in the thermodynamic database. These criteria are applicable only to the selection of Test Data. Test Data are those data used to validate the WIPP actinide solubility model. For example, solubility measurements taken from the literature are compared to those predicted by the model parameterized with the log K fitted with the Training Data. The Test Data (S_m) and the model predictions (S_s) are used to calculate the difference, or D values as $D = \log_{10}(S_m) - \log_{10}(S_s)$. The D values are then used to create an empirical distribution of model-prediction errors, which are sampled in PA and added to the baseline solubility values.* The new screening criteria, G-1 through G-10, are listed below.

G1 – Time Frame: *Preference given to data from studies after January 1990 with the emphasis on the period between the closure date of the most recent recertification cycle and the current recertification cycle. The closure date for the literature search is set to one year before the required parameter feed to performance assessment for the current recertification cycle. Studies prior to 1990 may be acceptable, provided the experimental and analytical methods are provided and defensible, and satisfies the remainder of the criteria listed herein.*

G2 – Sources: *Include data from studies in peer-reviewed journals, unpublished undergraduate/graduate theses or dissertations, national and international laboratories and organizations (e.g., officially released reports from government and educational national and international laboratories.), as well as studies originating from industry.*

G3 – Type of Data: *Include only those studies that provide solubility data. Exclude studies that do not provide solubility data (e.g., studies of corrosion, leaching, sorption, or transport).*

G4 – Solvent and Composition: *Include only data from studies in which water was the solvent and the solution composition characterized; exclude studies in which no aqueous phase was present (e.g., solids, molten metal or salts, or pure organic liquids).*

G5 – Temperature and Pressure: *Include only data obtained from studies that were performed at pressures and/or temperatures at, or close to, those currently included in the WIPP model.*

G6 – Use of Oxidation-State Analogs*: Include data from studies that contain actinides currently in the WIPP model, or their appropriate oxidation-state analogs.*

G7 – Phase Characterization and Thermodynamic Equilibrium: *Include data from studies with a well-characterized solubility-controlling solid (both the starting and final solid phases) for which solubility parameters are in the WIPP model. Characterization of the final phase(s) may be complicated due to the presence of low-crystallinity hydrated phases, which are not easily identified. These amorphous phases should be characterized by a combination of methods, including a detailed description of how they were synthesized and elemental identification (e.g., component analysis by SEM and/or dissolution followed by ICP/MS) as XRD analysis may not*

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be definitive. Other methods of solid characterization may include, but are not limited to surface techniques, X-ray diffraction, and elemental composition. The experimental procedure should discuss solid-phase synthesis procedures, including descriptions of precursors (solids and solutions); and whether equilibrium (including meta-stability) was obtained. Determination of equilibrium typically includes demonstration of stable concentrations and/or chemical conditions as a function of time.

***G8 – Applicability**: Include data from studies in which the participating chemical components (i.e., aqueous species and solid phases that may affect actinide solubility) are included the WIPP model. Exceptions include the use of non-participating cations and/or anions, or additional known and characterized dissolved elements that have been demonstrated to not strongly complex or effect the solubility of the actinide(s) of interest.*

***G9 – Repeatability and Reproducibility:** Include only data from studies in which: 1) The investigators provided a sufficient description of their experiments to allow the work to be repeated by a qualified investigator; 2) sufficient experimental data are provided to allow thermodynamic calculations; and 3) the solution separation technique is understood and justifiable.*

***G10 – WIPP-Relevant Conditions:** Include data from experimental studies carried out under conditions [e.g., pcH, ionic strength, and total inorganic carbon (TIC)] similar to those expected for WIPP, as designated by the Chemical Conditions Conceptual Model.*

Experimental studies/data included in the WIPP actinide uncertainty analysis must meet the following conditions:

Table 1. Parameter ranges for literature screening criteria for CRA-2024.

Ionic Strength (m)	$5.0 \leq I \leq 9.5$ m[A]
	$Mg \leq 1.6$ M
	$Ca \leq 0.5$ M
pcH	$8.5 \leq pcH \leq 10.7$
Total Inorganic Carbon	$TIC = 0.0 - 2.0 \times 10^{-2}$ M

Table 2 provides a comparison of the previous version of each screening criteria with revised criteria with notes that summarize the changes.

[A] The WIPP brines are predominantly sodium – chloride type brines but include an array of other dissolved ionic species (e.g., K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-}, HCO_3^-, $B(OH)_4^-$, and Br^-), and as such the G10 ionic strength range mainly reflects the Na - Cl predominance. However, in the scientific literature actinide/lanthanide solubility studies are typically performed in single electrolyte solutions, mainly NaCl, $MgCl_2$, and $CaCl_2$, therefore, it is necessary to set WIPP appropriate upper bounds on dissolved Mg and Ca in this criterion. Note that the Mg and Ca limits are applicable to both single and multi-electrolyte solutions.

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Table 2. Comparison of the Old Criteria with the New

Former Criteria	Updated Criteria	Notes
G1. Include only results from experimental studies published from January 1, 1990, through *End Date*.	**G1 – Time Frame**: Preference given to data from studies after January 1990 with the emphasis on the period between the closure date of the most recent recertification cycle and the current recertification cycle. The closure date for the literature search is set to one year before the required parameter feed to performance assessment for the current recertification cycle. Studies prior to 1990 may be acceptable, provided the experimental and analytical methods meet modern standards are defensible, and the remainder of these criteria.	In previous uncertainty analysis studies published before 1990 were not considered, the update allows for older relevant data. The updated criterion also provides a more general time frame based on project milestones.
G2. Include results from both papers published in peer-reviewed journals and unpublished reports (e.g., officially released reports from government laboratories such as Los Alamos National Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, etc.).	**G2 – Sources**: Include data from studies in peer-reviewed journals, unpublished undergraduate/graduate theses or dissertations, national and international laboratories and organizations (e.g., officially released reports from government and educational national and international laboratories.), as well as studies originating from industry.	The updated criterion more explicitly lists acceptable sources of experimental studies.
G3. Include only results from solubility studies. Exclude other studies that do not provide solubilities (e.g., studies of corrosion, leaching, sorption, or transport).	**G3 – Type of Data**: Include only those studies that provide solubility data. Exclude studies that do not provide solubility data (e.g., studies of corrosion, leaching, sorption, or transport).	Slight rewording, no significant changes were made to the original.
G4. Include only results from studies in which water was the solvent. Exclude studies in which other solvents were used (e.g., solids, molten metal or salts, or organic liquids).	**G4 – Solvent and Composition**: Include only data from studies in which water was the solvent and the solution composition characterized; exclude studies in which no aqueous phase was present (e.g., solids, molten metal or salts, or pure organic liquids).	The update clarifies that the aqueous solution composition must be well defined/characterized and eliminates the ambiguity from the old G8 criterion.
G5. Include only results obtained from studies at pressures at or close to atmospheric, at temperatures at or close to those expected in the WIPP (i.e., 20 30 °C), and with posttest phase-separation methods similar to those used for the WIPP, because these were the conditions and methods used to parameterize the Th(IV) and Am(III) speciation and solubility models for WIPP compliance-related PA calculations.	**G5 – Temperature and Pressure**: Include only data obtained from studies that were performed at pressures and/or temperatures at, or close to, those included in the WIPP model.	The old criterion combined two different criterion: 1) the T&P conditions; and 2) the post-test phase separation method. The update simplifies this to only the T&P conditions, and moves the post-test separation methods to G10.
G6. Include only results from studies of Th(IV); and Nd(III), Am(III), and Cm(III); because these are the elements used to parameterize the WIPP Th(IV) and Am(III) solubility models. Exclude studies of U(IV), Np(IV), and Pu(IV); and Pu(III) because there could be	**G6 – Use of Oxidation-State Analogs**: Include data from studies that contain actinides, or their appropriate oxidation-state analogs, currently in the WIPP model.	The update is more general and will allow a greater number of studies to be considered for inclusion in the uncertainty analysis.

Former Criteria	Updated Criteria	Notes
systematic differences between the solubilities of these elements and those of their oxidation-state analogs used to parameterize the models; and because the difficulties inherent in maintaining these elements in these oxidation states could introduce experimental artifacts in the results obtained with these elements.		
G7. Include only results from studies with a characterized solubility-controlling solid for which solubility data are in the WIPP Th(IV) or Am(III) model (i.e., in the EPA-certified thermodynamic database), and in which the quantity of solid initially present was sufficient to prevent complete dissolution of this solid during the experiments (EPA, 2016).	**G7 – Phase Characterization and Thermodynamic Equilibrium:** Include data from studies with a well-characterized solubility-controlling solid (both the starting and final solid phases) for which solubility parameters are in the WIPP model. Characterization of the final phase(s) may be complicated due to the presence of low-crystallinity hydrated phases, which are not easily identified. These amorphous phases should be characterized by a combination of methods, including a detailed description of how they were synthesized and elemental identification (e.g., component analysis by SEM and/or dissolution followed by ICP/MS) as XRD analysis may not be definitive. Other methods of solid characterization may include, but are not limited to surface techniques, X-ray diffraction, and elemental composition. The experimental procedure should discuss solid-phase synthesis procedures, including descriptions of precursors (solids and solutions); and whether equilibrium (including meta-stability) was obtained. Determination of equilibrium typically includes demonstration of stable concentrations and/or chemical conditions as a function of time.	The updated criterion specifies the condition of equilibrium and the direction from which it is achieved, as well phase characterization.
G8. Include only results from studies with aqueous solutions of known composition. Exclude studies performed with groundwaters, sedimentary pore waters, and soil solutions that may contain unknown quantities of species that can be complexants or adsorbents (e.g., humic acids or other dissolved organic compounds, microbial colloids, or pseudocolloids).	**G8 – Applicability**: Include data from studies in which the participating chemical components (i.e., aqueous species and solid phases that may affect actinide solubility) are included the WIPP model. Exceptions include the use of non-participating cations and/or anions, or additional known and characterized dissolved elements that have been demonstrated to not strongly complex or effect the solubility of the actinide(s) of interest.	The update reiterates G4 in that the aqueous solution must be well characterized, while also allows for non-solubility affecting entities NOT included in the WIPP model to be present in the experimental data.
G9. Include results from studies with dissolved elements or species that are present in WIPP brines. Exclude studies with dissolved elements or species that are absent in WIPP repository brines and for which our models do not include		The old G9 is now included in the new G8, and the new G9 replaces the old G10.

Former Criteria	Updated Criteria	Notes
association/dissociation constants or Pitzer parameters (EPA, 2016).		
G10. Include only results from studies for which the investigators provided a complete description of their experiments and the original solubilities. Exclude literature reviews and summaries, and studies in which the authors only provided average dissolved concentrations or solubility products, thus necessitating back-calculation of the solubilities.	**G9 – Repeatability and Reproducibility**: Include only data from studies in which: 1) The investigators provided a sufficient description of their experiments to allow the work to be repeated by a qualified investigator; 2) sufficient experimental data are provided to allow thermodynamic calculations; and 3) the solution separation technique is understood and justifiable.	The updated criterion explicitly defines the required conditions of the experiment as described in the literature being evaluated. Also, the update includes the old G5 post-test separation techniques.
G11. Include only results from experimental studies carried out under conditions at or close to those predicted for WIPP disposal rooms. Specifically, include only results from experiments in which: 1. $I \geq 3$ m or M, 2. pcH = 8.0–11.2, and 3. Total inorganic C (TIC) = 0-2.0E-02 M (EPA, 2016)	**G10 – WIPP-Relevant Conditions** Include data from experimental studies carried out under conditions [e.g., pcH, ionic strength, and total inorganic carbon (TIC)] similar to those expected for WIPP, as designated by the Chemical Conditions Conceptual Model. Experimental studies/data included in the WIPP actinide uncertainty analysis must meet the following conditions: 1) $5.0 \leq I \leq 9.5$ m - Mg $\leq$ 1.6 M - Ca $\leq$ 0.5 M 2) $8.5 \leq$ pcH ≤ 10.7 3) TIC = 0.0 - 2.0 □ 10-2 M	The ranges specified in the updated criterion were decided upon with consideration of the chemistry of unreacted Salado brines compositions and the reacted brine compositions from previous actinide baseline solubility calculations, and with the recognition that the ranges must reflect, with reasonable uncertainty, those of the WIPP Chemical Conditions Conceptual Model.

Development of the WIPP Specific Criterion for the Actinide Uncertainty Analysis

CRA-2014 Performance Assessment

Criterion G11, or the WIPP specific criterion, was established for CRA-2014 (Brush and Domski, 2013) to narrow the range of chemical conditions considered in the technical literature to be more consistent with those expected for WIPP, and to better represent the conditions at which the WIPP An(III) and An(IV) models were parameterized.

The parameter ranges established by Brush and Domski (2013) and the rationale for these ranges are listed in Table 3.

Table 3. Parameter ranges for literature screening criteria for CRA-2014.

$I \geq 3$ m or M
pcH = 8.0–11.2
TIC = 0-1.4 × 10^{-2} M

Paraphrased from Bush and Domski (2013):

1) *Ionic Strength*: We established the specification that I be ≥ 3 m or M so as to apply the same criterion to the solubility experiments carried out with Nd(III), Am(III) or Cm(III) as that previously applied to experiments with Th(IV) (criterion S1). We did not specify an upper limit of I because all of the results included after applying criterion G11 had values of I within a factor of two greater than those predicted for the WIPP brines GWB and ERDA-6.
2) *pcH*: We established a pcH range of 8.0–11.2 by rounding the pcH of 9.54 predicted for GWB to 9.5 and setting the lower limit of the range 1.5 units of pcH below this value. Similarly, we rounded the pcH of 9.69 predicted for ERDA-6 to 9.7 and set the upper limit 1.5 units above it.
3) *Total Inorganic Carbon (TIC)*: Criterion G11 specifies that the lower limit of the TIC range be 0 to ensure that this revised analysis includes CO_2-free Th(IV) solubility measurements, and CO_2-free Nd(III), Am(III), and Cm(III) solubilities. Inclusion of CO_2-free conditions is appropriate because the speciation and solubilities predicted by the Th(IV) and Am(III) models for the invariant points for GWB and ERDA-6 described above are more like those in CO_2-free systems than high-f_{CO_2} or high-HCO_3^- and/or high-CO_3^{2-} systems. The upper limit of the TIC range was set by multiplying the TIC content of ERDA-6, the higher of the two brines, by $10^{1.5}$ or 31.6. This is consistent with the lower and upper limits of the pcH range, which are 1.5 pcH units below and above the values in GWB and ERDA-6, respectively, rounded to two significant figures.

While the parameter ranges, and the reasoning for choosing those ranges, was well thought out by Brush and Domski (2013), the ranges tended to be either too broad, in the case of ionic strength and pcH, or too restrictive for TIC. The narrow TIC range excluded too many studies, while the

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broad ranges of I and pcH allowed experimental data that were outside of the expected conditions at the WIPP. The original G11 criterion was only used for the CRA-2014 PA (Brush and Domski, 2013).

The CRA-2014 SEN4 Performance Assessment

Following the CRA-2014 the EPA issued Technical Support Document (TSD) 194.24 which evaluated the selection criteria used for the actinide uncertainty analysis, and specifically the G11 criterion which was new for CRA-2014. The EPA states:

> *"The Criterion G11 pcH and ionic strength limitations appear reasonable and do not systematically exclude specific categories of data. However, because TIC was limited to 0 – 0.014 M, no Th(IV) solubilities measured with any carbonate in solution were included in the calculation of the CRA-2014 PA Th(IV) solubility uncertainty distribution (Brush and Domski 2013c). In addition, only a single solubility measurement in a solution containing carbonate from Rao et al. (1999) was included in the Am(III) solubility uncertainty distribution calculation because of the limits on pcH for solubility measurements in WIPP brines."*
>
> *"Consequently, the upper limit on TIC in Criterion G11 for both the +III and +IV actinide solubility uncertainty determination should be revised upward to 0.02 M."*

Thus, the revised "SEN4" G11 criterion was created (Table 4):

Table 4. Parameter ranges for literature screening criteria for SEN4.

$I \geq 3$ m or M
pcH = 8.0–11.2
TIC = 0-2.0 × 10^{-2} M

In addition, for CRA-2014 SEN4 the EPA provided explicit direction to include selected data from the studies of Neck et al. (2009) and Altmaier et al. (2008). From page 90 of EPA's draft TSD the EPA designates these exceptions as follows:

> *"A2: Include only +III actinide solubility results from concentrated $CaCl_2$ brine experiments with pcH < 10. This pcH limit is included because Neck et al. (2009) found that Cm(III) forms significant $Cax[Cm(OH)_y]^{2x+3-y}$ aqueous species at pcH > 10. Significant concentrations of these species are unlikely to form in WIPP repository brines because of the low calcium concentrations maintained by anhydrite precipitation.*
>
> *A3: Include only Th(IV) actinide solubility results from concentrated $CaCl_2$ brine experiments with pcH < 10. This limit is included because Brendebach et al. (2007) and Altmaier et al. (2008) found that significant concentrations of the $Ca_4[Th(OH)_8]^{4+}$ aqueous species form in concentrated $CaCl_2$ solutions at pcH > 10. Significant*

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concentrations of this species are unlikely to form in WIPP repository brines because of the low calcium concentrations maintained by anhydrite precipitation."

This SEN4 G11 criterion and the A2 and A3 directives were used for the CRA-2014 SEN4, CRA-2019 DPA, EPA completeness comment CC1-GEOCHEM-1, and for the Replacement Panels Performance Assessment (RPPA).

Revision of the General Criterion G11 (G10) for CRA-2024

Revision of the general screening criteria resulted in two of the criteria being combined (see Table 2) with G11 becoming G10 in the revised criteria. The new G10 ranges for ionic strength and pcH (total inorganic carbon did not change) were informed with consideration of WIPP brine compositions; the equilibrated compositions from past actinide baseline solubility calculations, and unreacted brines collected from the Salado formation in the WIPP underground. In the memorandum by Domski (2018) 31 WIPP brine compositions (19 unreacted native Salado brines and 12 reacted/equilibrated brines) were evaluated and ranges of ionic strength (I) and pcH were assigned, the SEN4 TIC range was retained. For the current revision the data considered by Domski (2018) has been reevaluated and new ranges have been specified for ionic strength and pcH, while the TIC range is same as that specified for SEN4.

For each of the brine properties (I, pcH, and TIC) Domski (2018) created PDF, CDF, probability – probability plots (P – P plot), and quantile – quantile plots (Q – Q plots) to determine if the data were normally distributed, and ± 2σ to the mean applied for the 95% confidence interval. Domski (2018) showed that none of the three properties displayed normal distributions, thus, the ± 2σ rule did not apply. Although the data did not obey normality the ± 3σ rule of thumb was applied to each property an expert judgement confidence interval that we believe bounds conditions expected in the WIPP repository under the current WIPP Conceptual Model. Table 5 shows the ± 3σ minimum and maximum values resulted in a wide pcH range (4.6 – 11.8), an ionic strength range (5.7 – 9.1) that is too focused, and a narrow TIC range (0 – 8.7E-04).

Table 5. Statistics for WIPP brine properties.

	pcH	I (m)	TIC (M)
Minimum	6.9	5.9	6.4E-06
Maximum	9.9	8.2	7.8E-04
Mean	8.2	7.4	2.4E-04
Median	7.3	7.6	1.4E-04
σ	1.2	0.6	2.1E-04
3σ	3.6	1.7	6.3E-04
-3σ	4.6	5.7	-4.0E-04
+3σ	11.8	9.1	8.7E-04

Table 6 shows the parameter ranges specified by Domski (2018):

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Table 6. Parameter ranges specified by Domski (2018).

$5.5 \leq I \leq 9$ m
$6.0 \leq pcH \leq 11$
TIC = 0.0 - 2.0 × 10^{-2} M

The pcH range, $6.0 \leq pcH \leq 11$, specified by Domski (2018) is too broad, and the low-end value, 6.0, is too far outside of the expected WIPP repository conditions to define the lower pcH limit. To better understand the range of pcH for the equilibrated (reacted) brines, Table 7 provides the statistics for the 19 GWB and ERDA-6 brines which have been equilibrated with repository materials (halite, anhydrite, brucite, and hydromagnesite, or magnesite), the 19 unreacted Salado formation brines are not included in Table 7.

Table 7. Statistics for Equilibrated WIPP brine pcH.

	pcH
Minimum	9.39
Maximum	9.94
Mean	9.60
Median	9.59
σ	0.20
3σ	0.59
-3σ	9.0
+3σ	10.2

The last two rows in Table 7 show the 3σ sigma minimum and maximum, which for the purpose of the screening criteria provide a pcH range, $9.0 \leq pcH \leq 10.2$, that is too exclusive. However, using this range as guidance and extending the pcH range by ±0.5 pcH units to $8.5 \leq pcH \leq 10.7$ we have an acceptable range that is based on the expected WIPP conditions.

The ionic strength range (5.7 – 9.1 m) based on the 3σ rule (Table 5) is too narrow for the purposes of literature screening as it would screen out many studies. Increasing the total range to 5.0 – 9.5 molal would be much more inclusive for the purpose of the uncertainty analysis.

The WIPP brines, are predominantly sodium – chloride type brines but include an array of other dissolved ionic species (e.g., K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-}, HCO_3^-, $B(OH)_4^-$, and Br^-), and as such the G10 ionic strength range mainly reflects the Na - Cl predominance. However, in the scientific literature actinide/lanthanide solubility studies are typically performed in single electrolyte solutions, mainly NaCl, $MgCl_2$, and $CaCl_2$, therefore, it is necessary to set WIPP appropriate upper bounds on dissolved Mg and Ca in this criterion.

Table 8 provides the magnesium and calcium data for the WIPP brines, these data include both unreacted Salado formation brines and brines in equilibrium with halite, anhydrite, brucite, and hydromagnesite.

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Table 8. Statistics for Mg and Ca for WIPP brines.

	Mg (M)	Ca (M)
Minimum	1.9E-02	5.5E-03
Maximum	1.0E+00	3.2E-02
Mean	6.2E-01	9.4E-03
Median	6.3E-01	8.5E-03
σ	3.4E-01	5.0E-03
3σ	1.0E+00	1.5E-02
-3σ	-4.1E-01	-5.6E-03
+3σ	1.6E+00	2.4E-02

The ± 3σ was applied to the mean of the Mg and Ca data (Table 8), and while the range for Mg is appropriate (Mg ≤ 1.6 M, where a 1.6 M solution of $MgCl_2$ has an ionic strength of 4.8), the upper limit of the Ca range 2.4E-02 M is too low for practical purposes. Therefore, it is suggested that the Ca range be set to Ca ≤ 0.5 M, where a 0.5 M $CaCl_2$ solution has an ionic strength of 1.5. This is a very generous upper limit for the Ca concentration for the purposes of WIPP. Note that the Mg and Ca limits are applicable to both single and multi-electrolyte solutions.

The suggested parameter ranges for the G10 criterion for use in CRA-2024 are listed in Table 9.

Table 9. Parameter ranges for literature screening criteria for CRA-2024.

Ionic Strength (m)	$5.0 \leq I \leq 9.5$ *m*[B]
	$Mg \leq 1.6$ *M*
	$Ca \leq 0.5$ *M*
pcH	$8.5 \leq pcH \leq 10.7$
Total Inorganic Carbon	$TIC = 0.0 - 2.0 \times 10^{-2}$ *M*

Conclusions

The updated literature/data screening criteria for the actinide uncertainty analysis for CRA-2024 have been completed. These criteria improve upon the criteria as documented in Brush and Domski (2013) by simplifying and clarifying the language, combining aspects of like criteria, and reevaluating the parameter ranges for the WIPP specific criteria. These criteria will be used for CRA-2024, and perhaps for future uncertainty analysis, however, if changes are made to the WIPP actinide solubility models, or there are changes to reactants in the model (e.g., the inclusion of cementitious materials, or other reactants not currently considered), then these criteria may be revised for those purposes.

[B] The WIPP brines are predominantly sodium – chloride type brines but include an array of other dissolved ionic species (e.g., K^+, Mg^{2+}, Ca^{2+}, SO_4^{2-}, HCO_3^-, $B(OH)_4^-$, and Br^-), and as such the G10 ionic strength range mainly reflects the Na - Cl predominance. However, in the scientific literature actinide/lanthanide solubility studies are typically performed in single electrolyte solutions, mainly NaCl, $MgCl_2$, and $CaCl_2$, therefore, it is necessary to set WIPP appropriate upper bounds on dissolved Mg and Ca in this criterion. Note that the Mg and Ca limits are applicable to both single and multi-electrolyte solutions.

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