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Sandia National Laboratories
Waste Isolation Pilot Plant

Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2009 PABC, Rev. 1. Supersedes ERMS 552500

Work Carried Out under Task 2 of the Analysis Plan for Calculation of Actinide Solubilities for the WIPP PABC, AP-143, Rev. 0
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1 INTRODUCTION

This revision (Rev. 1) of this analysis report documents several changes specified in the corrective action plan (CAP) for the corrective action request CAR IS-10-02-CAR-01. All of the additions to the text, figures, tables, and references in this revised report are identified with vertical bars in the left margins. All of the deletions are shown with red-line strikethrough. These changes include:

1. Addition of a reason for including the Nd(III) solubility data of Borkowski et al. (2009) in the uncertainty range and probability distribution for the WIPP Am(III) solubility model established for the CRA-2009 PABC by Xiong et al. (2009), despite the fact that they stated “Include only results from experimental studies published from January 1, 1990, through December 31, 2008” (Xiong et al., 2009, Section 2, criterion G1).

2. Submit all records related to this analysis to the WIPP Records Center for inclusion in the records package entitled “Calculation of Actinide Solubilities for the WIPP CRA-2009 PABC.”

3. Revise the uncertainty range and probability distribution for the WIPP Am(III) model by using the Nd(III) solubilities reported by Borkowski (2010) instead of those from Borkowski et al. (2009), which Xiong et al. (2009) included in their analysis. The results of Borkowski (2010), a more complete data set, superseded those of Borkowski et al. (2009).

Regarding item 1 above, inclusion of some of the results from Borkowski et al. (2009) (see Subsection 3.2 and Table 9 below) in the original version of this analysis was a deviation from the general criterion G1 of Xiong et al. (2009, Section 2), which stated, “Include only results from experimental studies published from January 1, 1990, through December 31, 2008.” Xiong et al. (2009) did not provide a reason for this deviation, an omission which was cited in CAR IS-10-02-CAR-01 and addressed in the CAP for this CAR (see item 1 in the CAP for CAR IS-10-02-CAR-01 in the SNL/WIPP Records Center). The reason that Xiong et al. (2009) included some of the results of Borkowski et al. (2009) that were unaffected by significant Nd(III)-borate complexation was because they were directed to do so in the management review of the original version of this analysis report (see comment 47 and the response to this comment on p. 22 of this review in the SNL/WIPP Records Center)..

Regarding item 2, we placed nine e-mail messages between Brush and Borkowski in the SNL/WIPP Records Center in the records package entitled, “Calculation of Actinide Solubilities for the WIPP CRA-2009 PABC (Work Associated with AP-143),” ERMS 548686. These e-mail messages requested and provided: (1) the numerical values of the results of the Nd(III) solubility experiments by Borkowski et al. (2009) that had values of pcH low enough to preclude significant complexation of Nd(III) by borate, thereby satisfying criterion G9 (see Section 2 of this revision); (2) information on the pcH range studied by Borkowski et al. (2009)

for inclusion in Table 9 of this revision; and (3) Borkowski's opinion on whether one or more $Am(OH)_x^{3-x}$ complexes with x > 4, which are not in the WIPP Am(III) model, could have been dominant in the experiments by Peretrukhin et al. (1996), thereby resulting in underpredictions of the results of these experiments (see Subsection 3.2 below).

Also regarding item 2, we placed four spreadsheets in the records package entitled, "Calculation of Actinide Solubilities for the WIPP CRA-2009 PABC (Work Associated with AP-143)," ERMS 548686. The file names of these spreadsheets are: (1) Xiong et al., 2009, Am(III) Uncertainty Analysis for the PABC, Rev 0, 091124.xls; (2) Xiong et al., 2009, Th(IV) Uncertainty Analysis for the PABC, Rev 0, 091124.xls; (3) Xiong et al., 2010b, Am(III) Uncertainty Analysis for the PABC, Rev 1, 100913.xls; and (4) Xiong et al., 2010b, Am(III) Uncertainty Analysis for the PABC, Rev 1, 110105.xls. The first two of these spreadsheets were used for the original version of this analysis; the other two were used for this revision.

Regarding item 3 above, we replaced the 82 Nd(III) solubilities from Borkowski et al. (2009) that Xiong et al. (2009) included in the original version of this analysis with 162 of the results from Borkowski (2010). Borkowski (2010) provided a more complete data set, which superseded that of Borkowski et al. (2009). Subsection 3.2 and Table 9 describe which results were included in the original version of this analysis and in this revision.

The changes resulting from item 3 (and another change described in Subsection 3.2 and Table 9) increased the total number of comparisons of measured and predicted Nd(III) and Am(III) solubilities by 95, from 346 in the original version of this analysis to 441 in the revised version. Subsection 3.2, pp. 47–56, describes the resulting changes in the Am(III) uncertainty range and probability distribution.

Finally, we also made several editorial changes in this revision. We marked these changes with vertical bars in the left margin and/or red-line strikethrough.

The text in the following paragraph, which does not include vertical bars in the left margin, is from the original version of this report (Xiong et al., 2009). The original version made statements that were correct at the time, but are no longer correct. For example, the statement that "This analysis report provides the results of our uncertainty analysis of Th(IV) and Am(III) solubilities for the Performance Assessment Baseline Calculation (PABC), a compliance-related calculation for the second Compliance Recertification Application (CRA-2009) for the U.S. Department of Energy's (DOE's) Waste Isolation Pilot Plant (WIPP) (U.S. DOE, 2009)," is no longer correct, because the CRA-2009 PABC has now been completed and will not be rerun using the results of this revision. However, we retained this statement from the original version of this report (and other similarly outdated statements as well) in this revised version to provide context for the rest of this report. In particular, please note that the results of this revised analysis were not used for the CRA-2009 PABC.

This analysis report provides the results of our uncertainty analysis of Th(IV) and Am(III) solubilities for the Performance Assessment Baseline Calculation (PABC), a compliance-related calculation for the second Compliance Recertification Application

(CRA-2009) for the U.S. Department of Energy's (DOE's) Waste Isolation Pilot Plant (WIPP) (U.S. DOE, 2009). The analysis described in this report was carried out under Task 2 of Brush and Xiong (2009a, Subsection 4.2).

The Th(IV) and Am(III) uncertainty ranges and probability distributions resulting from this analysis will replace those used for the performance-assessment (PA) calculations for the CRA-2009 (CRA-2009 PA), which were established by Xiong et al. (2005) for the PABC for the first WIPP CRA (CRA-2004 PABC). The ranges and distributions from this report will become part of the new WIPP PA baseline when approved by the U.S. Environmental Protection Agency (EPA).

Brush and Xiong (2009a, Subsection 4.2) stated that "Task 2 will consist of re-establishing uncertainty ranges and probability distributions for our calculated Th(IV), Np(V), and Am(III) solubilities. Because the EPA indicated that the uncertainty ranges and probability distributions for the solubilities of Th(IV), Np(V), and Am(III) established for the CRA-2004 PABC should be used again for the CRA-2009 PABC, the objective of this task is to develop new ranges and distributions for possible use in WIPP PA at some time in the future, not for the CRA-2009 PABC." Therefore, the use of the ranges and distributions obtained from this analysis for the CRA-2009 PABC is a deviation from Brush and Xiong (2009a).

Brush et al. (2009a, Subsection 4.2) also stated that this analysis would include re-establishing uncertainty ranges and probability distributions for Np(V). However, we did not include Np(V) in this analysis because PA does not sample the uncertainties associated with the solubilities of Np(V). Omission of Np(V) from this analysis is another deviation from Brush and Xiong (2009a). However, we will extend this analysis to Np(V) after we provide the uncertainty ranges and probability distributions for Th(IV) and Am(III) for the CRA-2009 PABC.

Furthermore, Brush and Xiong (2009a, Subsection 4.2) stated that Task 2 will be carried out "using EQ3NR to calculate solubilities under the conditions reported for the measured solubilities." The EPA, however, specified that the DOE continue to use FMT (Babb and Novak, 1997 and addenda; Wang, 1998) for the actinide-solubility calculations for the CRA-2009 PABC, instead of the EQ3/6 geochemical software package (Wolery and Jarek, 2003). Therefore, we used FMT for this analysis. This is our final deviation from Brush and Xiong (2009a).

Actinide solubilities (the sums of the concentrations of all of the dissolved actinide species in chemical equilibrium with actinide-bearing solid phases under the conditions expected in WIPP disposal rooms) and the concentrations of colloidal (suspended) actinides, calculated from the baseline solubilities, together constitute the actinide source term used in WIPP PA calculations. These solubilities are often referred to as the "baseline solubilities" because they comprise unique values calculated with FMT under the near-field chemical conditions predicted for the repository (Brush and Xiong, 2009a, Section 2).

PA codes use actinide solubilities that are the products of the baseline solubilities and sampled uncertainty factors that describe possible deviations of the Th(IV) and Am(III) thermodynamic speciation and solubility models from expected behavior. The reason for using these uncertainty factors is to adjust the baseline solubilities up if the model underpredicts the experimentally measured solubilities, or to adjust the baseline solubilities down if the model overpredicts the measured solubilities. For the CCA PA (U.S. DOE, 1996), the PAVT, and the CRA-2004 PA (U.S. DOE, 2004), these uncertainties were sampled from the combined range and probability distribution established for the Np(V) and Am(III) solubility models by Bynum (1996a, 1996b, 1996c), who did not include any results for Th(IV) in his analysis.

Xiong et al. (2005) established separate ranges and distributions for the Th(IV) and Am(III) solubility models for the CRA-2004 PABC. They also established a range and distribution for Np(V), but it was not used for the CRA-2004 PABC because PA does not sample the uncertainties in the solubility of Np in view of the fact that releases of this element do not affect the long-term performance of the WIPP (Brush and Garner, 2005). The Th(IV) and Am(III) ranges and distributions of Xiong et al. (2005) were reused for the CRA-2009 PA (U.S. DOE, 2009). Brush et al. (2005) provided additional information on the PA implementation of these uncertainties.

Finally, we gratefully acknowledge the contributions of E. J. (Jim) Nowak to this analysis and his many contributions to the WIPP Project over several decades. Jim passed away before he could sign this report as a coauthor or delegate signature authority.

Table 1 (see next page) defines the abbreviations, acronyms, initialisms, etc., used in this analysis report.

Table 1. Abbreviations, Acronyms, In4tialisms, etc.

Abbreviation, Acronym, or Initialism	Definition
Am, Am(III)	americium, americium in the +III oxidation state
am	amorphous
AP	analysis plan
aq	aqueous (dissolved in an aqueous solution)
atm	atmosphere(s)
Brine A	a synthetic WIPP brine representative of intergranular Salado-Fm. brines
C, c	carbon, crystalline
CAP	(SNL/WIPP QA) corrective action plan
CAR	(SNL/WIPP QA) corrective action request
CCA	(WIPP) Compliance Certification Application
CDF	cumulative distribution function
citrate	$(CH_2COO)_2C(OH)(COO)^{3-}$ or $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$
Cl, Cl^-	chloride, chloride ion
ClO_4, ClO^{4-}	perchlorate, perchlorate ion
Cm, Cm(III)	curium, curium in the +III oxidation state
CMS	(Sandia/WIPP software) Configuration Management System
CO_3, CO_3^{2-}	carbonate, carbonate ion
Col	colloidal (suspended in an aqueous or other solution)
cr	crystalline
CRA-2004	the first WIPP Compliance Recertification Application, submitted to the EPA in March 2004
CRA-2009	the second WIPP Compliance Recertification Application, submitted to the EPA in March 2009
D	the difference(s) between logs (base 10) of the measured and predicted actinide solubilities (S_m and S_p)
DOE	(U.S.) Department of Energy
EPA	(U.S.) Environmental Protection Agency
Eq.	equilibration
EQ3/6	a geochemical software package for speciation and solubility calculations (EQ3NR) and reaction-path calculations (EQ6)
ERDA-6	Energy Research and Development Administration (WIPP Well) 6, a synthetic brine representative of fluids in Castile brine reservoirs
fCO2	fugacity (similar to the partial pressure) of CO2
Fm.	Formation
FMT	Fracture-Matrix Transport, a geochemical speciation and solubility code

Table 1 continued on next page

Table 1. Abbreviations, Acronyms, Initialisms, etc. (continued)

Abbreviation, Acronym, or Initialism	Definition
G-Seep	a naturally-occurring brine formerly collected from G Drift in the WIPP underground workings and used for laboratory and modeling studies
GWB	Generic Weep Brine, a synthetic brine representative of intergranular Salado brines
H, H^+	hydrogen, hydrogen ion
HCO_3, HCO_3^-	bicarbonate, bicarbonate ion
H_2O	water
I	ionic strength, defined by $I = ½ \times \Sigma_i(M_i \times z_i^2)$, in which M_i and z_i are the molarity and charge of species *i*
I/O	(FMT) input and output files
K, K^+	potassium, potassium ion
LIB	Library
log	the common logarithm or logarithm (base 10)
M	molar
m	molal
mcr	microcrystalline
Mg, Mg^{2+}	magnesium, magnesium ion
mM	millimolar
N	bin number (see Subsection 5.2 for explanation)
Na, Na^+	sodium, sodium ion
NaTr	sodium trifluoromethanesulfonate (also abbreviated as sodium triflate)
Nd, Nd(III)	neodymium, neodymium in the +III oxidation state
NO_3, NO_3^-	nitrate, nitrate ion
NONLIN	a code used to fit parameters used in the FMT database to solubility, stability-constant, or other experimental data
Np, Np(IV), Np(V)	neptunium, neptunium in the +IV oxidation state , neptunium in the +V oxidation state
O	oxygen
OH, OH-	hydroxide, hydroxide ion
OPPIE	a scientific literature database search tool created by the Los Alamos National Laboratory Research Library
PA	performance assessment
PABC	(WIPP) Performance Assessment Baseline Calculations, carried out in 2005 and 2009
PAVT	(WIPP) Performance Assessment Verification Test, conducted in 1997

Table 1 continued on next page

Table 1. Abbreviations, Acronyms, Initialisms, etc. (continued)

Abbreviation, Acronym, or Initialism	Definition
phase 3	$Mg_2Cl(OH)_3 \cdot 4H_2O$
phase 5	Mg3(OH)5Cl·4H2O
pmH	the negative log (base 10) of the molal concentration of H+
ppm	parts per million
pcH	the negative log (base 10) of the molar concentration of H^+
p_{CO_2}	partial pressure (similar to the fugacity) of CO_2
pH	the negative log (base 10) of the activity of H^+
Pu, Pu(III), Pu(IV)	plutonium, plutonium in the +III oxidation state, plutonium in the +VI oxidation state
R	gas constant
Rev.	Revision
S_m	measured solubility
S_p	predicted solubility
SNL	Sandia National Laboratories
SO_4, SO_4^{2-}	sulfate, sulfate ion
SOTERM	(Actinide) Source Term, an appendix in the CCA and an attachment to Appendix PA in the CRA-2004
SPC	Salado Primary Constituents, a synthetic brine representative of intergranular Salado brines
T	temperature
Th, Th(IV)	thorium, thorium in the +IV oxidation state
TIC	total inorganic C (the sum of the dissolved species of inorganic C)
U, U(IV), U(VI)	uranium, uranium in the +IV oxidation state, uranium in the +VI oxidation state
WIPP	(U.S. DOE) Waste Isolation Pilot Plant
XRD	X-ray diffraction
μ^0, μ^0/RT	standard chemical potential, dimensionless standard chemical potential

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2 METHODS

The methods used for this analysis are similar to those used by Xiong et al. (2004, 2005). We compared experimentally measured solubilities of Th(IV), Nd(III), and Am(III) with the Th(IV) and Am(III) solubilities predicted using the thermodynamic models implemented in FMT (Babb and Novak, 1997 and addenda; Wang, 1998). We then constructed histograms and cumulative distribution functions (CDFs) of the differences between the logarithms (base 10) of the measured and predicted solubilities. We constructed separate histograms and CDFs for the Th(IV) and Am(III) models. These CDFs will be used for the CRA-2009 PABC.

This analysis does not include any comparisons for U(VI) because the DOE has not developed a thermodynamic speciation-and-solubility model for this element in this oxidation state. Instead, the EPA specified that an estimate of 1×10^{-3} M be used for the solubility of U(VI) in the WIPP brines Generic Weep Brine (GWB) and Energy Research and Development Administration (WIPP Well) 6 (ERDA-6), and the DOE has used this estimate beginning with the CRA-2004 PABC. Snider (2003) verified that GWB is the average composition of intergranular fluids collected from the Salado Formation (Fm.) at the original stratigraphic horizon of the repository and analyzed by Krumhansl et al. (1991). ERDA-6 is a synthetic brine representative of fluids in brine reservoirs in the Castile Fm. (Popielak et al., 1983). Furthermore, the EPA specified a fixed value for its estimate of the solubility of U(VI) in GWB and ERDA-6 (U.S. EPA, 2006).

We established ten general criteria for including results of experimentally measured solubilities in our comparisons of measured Th(IV), Nd(III), and Am(III) solubilities and predicted Th(IV) and Am(III) solubilities. We will also use these general criteria to extend this analysis to Np(V). They are:

> G1. Include only results from experimental studies published from January 1, 1990, through December 31, 2008.
>
> 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.).
>
> G3. Include only results from solubility studies. Exclude other studies that do not provide solubilities (e.g., studies of corrosion, leaching, sorption, or transport).
>
> 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).

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.

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 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 the value of the dimensionless standard chemical potential (μ^0/RT) is in the WIPP Th(IV) or Am(III) model (i.e., in the EPA-certified FMT database), and in which the quantity of solid initially present was sufficient to prevent complete dissolution of this solid during the experiments.

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).

G9. Include only results from studies with dissolved elements or species for which values of μ^0/RT and Pitzer ion-interaction parameters are in our models. Exclude studies with dissolved elements or species for which our models do not include values of μ^0/RT or Pitzer parameters.

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.

We also continued to use the specific criterion established by Xiong et al. (2005) for the experimentally measured solubilities of Th(IV):

S1. Include only results from experiments carried out with solutions with ionic strength $(I) \geq 3$ M or m.

Xiong et al. (2005, Subsection 5.2.3) described the reason for establishing S1.

Xiong et al. (2005) did not establish any specific criteria for experimentally measured solubilities of Nd(III), Am(III), or Cm(III). Furthermore, we did not establish any specific criteria for this comparison.

Nowak carried out multiple literature searches for published papers and unpublished reports on laboratory studies of actinide solubilities. For most of 2008, Nowak used Search Plus, Version 2.4, operated by Los Alamos National Laboratory (LANL). In late 2008, LANL switched from Search Plus to OPPIE. Nowak used OPPIE for the rest of 2008 and during 2009. Nowak also used Science Research Connection, operated by the DOE, during 2008 and 2009.

These literature searches identified thousands of published papers and unpublished reports on actinide chemistry (see Section 3 below). Therefore, Nowak conducted preliminary evaluations of these studies by applying the criteria described above to the information provided in the abstracts of these papers and reports. Because of the large number of papers and reports identified by the literature searches, it was not practical to document which criteria were used to include these studies in or exclude them from the final evaluations described below. Nowak excluded all papers and reports that, in his judgment, obviously failed to meet the criteria. In those cases in which it was not obvious that a paper or report should be excluded, Nowak retained them for the final evaluations. Furthermore, he requested that the final evaluations be performed by at least two of the authors of this report and that, if these two authors could not reach agreement, another author assist in the evaluations.

Therefore, Brush and Nowak carried out the final evaluations of laboratory studies of Th(IV) solubilities, and Ismail and Nowak conducted the final evaluations for Nd(III) and Am(III). The results of these evaluations are documented in Subsections 3.1 and 3.2 below.

Nowak used the commercially available software application Data Thief to obtain numerical values of experimental variables such as pcH or pmH and the resulting solubilities from scatter plots of the experimentally measured solubilities, if tabulations of these values were not provided by the investigators. Most of the published papers and unpublished reports did not include data tables.

Xiong then set up FMT input files to predict the solubilities of Th(IV), Nd(III), and Am(III) for the conditions reported for each of the measured solubilites in the laboratory studies selected by the final evaluations. However, if two or more identical results were reported (i.e., identical values of pcH or pH and solubility for two or more experiments), Xiong conducted only one FMT run for these experiments. Table 2 (see next page) provides information on FMT (Babb and Nowak, 1997 and addenda; Wang, 1998).

Xiong used the thermodynamic database FMT_050405.CHEMDAT (Nowak, 2005; Xiong, 2005) to predict Th(IV) and Nd(III) and Am(III) solubilities for the comparisons with the experimentally measured values. This is the same FMT database used by Xiong et al. (2005) for the uncertainty ranges and probability distributions for the CRA-2004 PABC and the CRA-2009 PA, and by Brush (2005) for the baseline solubilities for the CRA-2004 PABC and the CRA-2009 PA. Therefore, we did not recalculate any of the solubilities predicted by Xiong et al. (2005) for their comparisons if they were also included in our comparisons.

Table 2. Software Used for This Analysis.

Code	Version	Executable	Build Date	CMS Library	CMS Class
FMT	2.4	FMT_QB0204.EXE	09-03-98	LIBFMT	QB0204

J. J. Long carried out the FMT calculations under the PA run-control system used for WIPP compliance-related calculations. Table 3 provides run-control information for these calculations. The FMT code and databases are stored in the Sandia/WIPP Configuration Management System (CMS) libraries. Typing "libfmt" accesses the FMT library. The code and databases are stored in the directory PACMS: [CMS_WIPP_NONPA.FMT]. The calculations used for this analysis are in class PABC09-0 of the CMS library LIBPABC09_FMT.

Finally, Ismail generated frequency distributions of differences (D) between the logs of the measured and predicted actinide solubilities (S_m and S_p, respectively) and displayed them in tabular and histogram forms in Microsoft Excel spreadsheets using Excel's "histogram" data analysis tool in this commercial spreadsheet software. Negative values of D indicate that the Th(IV) or Am(III) model implemented in FMT predicted a solubility greater than the corresponding measured value (overprediction of solubility by the model); positive values of D indicate that the model predicted a solubility less than the measured value (underprediction). The Microsoft Excel files "PABC09 Th(IV) Uncertainty Analysis.xls" and "PABC09 Am(III) Solubility Uncertainty Analysis.xls" contain spreadsheets with S_m or S_p values (or logs thereof), frequency distributions, and histograms for this analysis. The bin numbers (N) in the histograms are defined as follows:

> Bin N contains values of D greater than $N - 0.15$ and less than or equal to N, where $D = \log_{10}(S_m) - \log_{10}(S_p)$.
>
> Examples of the definitions of bins follow:
>
> Bin -0.3 contains values of D greater than –0.45 and less than or equal to –0.3;
> Bin -0.15 contains values of D greater than –0.30 and less than or equal to –0.15;
> Bin 0 contains values of D greater than –0.15 and less than or equal to 0; and
> Bin 0.15 contains values of D greater than 0 and less than or equal to 0.15.

We will submit electronic copies of the files "PABC09 Th(IV) Uncertainty Analysis.xls" "PABC09 Am(III) Solubility Uncertainty Analysis.xls," and all of the other spreadsheets to the archived file PABC09_UNCERTAINTY.ZIP, which is stored in the CMS in class ANALYSIS of library LIBPABC09_FMT. We will also print out and submit paper copies of these spreadsheets to the SNL/WIPP Records Center for inclusion in the records package entitled "Calculation of Actinide Solubilities for the WIPP CRA-2009 PABC [work associated with AP-143]," ERMS 548686.

Table 3. Run-Control Information for the FMT Calculations Carried Out for This Analysis [A].

	File Names[1,2,3]	CMS Library	CMS Class
Script	EVAL_FMT_PABC09.COM	LIBPABC09_EVAL	PABC09-0
Script Input	EVAL_FMT_PABC09_*t*.INP	LIBPABC09_EVAL	PABC09-0
Script Log	EVAL_FMT_PABC09_*t*.LOG	LIBPABC09_FMT	PABC09-0
FMT:			
Input	FMT_050405.CHEMDAT	LIBPABC09_FMT	PABC09-0
Input	FMT_GENERIC.RHOMIN	LIBPABC09_FMT	PABC09-0
Input	FMT_PABC09_*w*_*n*.IN	LIBPABC09_FMT	PABC09-0
Input	FMT_PABC09_ *w*_*n*.INGUESS	LIBPABC09_FMT	PABC09-0
Output	FMT_PABC09_ *w*_*n*.OUT	LIBPABC09_FMT	PABC09-0
Output	FMT_PABC09_ *w*_*n*.FOR088	Not kept	Not kept

1. $$t \in \left\{\begin{array}{l}\text{ALTMAIER04, ALTMAIER05, ALTMAIER06, LANL\_08\_III,}\\ \text{MEINRATH91\_III, MEINRATH93\_III, PERETRUCHIN96\_III,}\\ \text{RAI97, RAO96\_III, RAO\_NOVAK96\_III, PERCHLOR}\end{array}\right\}$$
2. $$w \in \left\{\begin{array}{l}\text{ALTMAIER04IV, ALTMAIER05IV, ALTMAIER06IV, LANL\_08,}\\ \text{MEINRATH91\_III, MEINRATH93\_III, PERETRUCHIN96\_III,}\\ \text{RAI97IV, RAO96\_III, RAO\_NOVAK96\_III, PERCHLOR}\end{array}\right\}$$
3. $$n \in \left\{\begin{array}{l}\text{001 through 006 for ALTMAIER04IV}\\ \text{001 through 004 for ALTMAIER05IV}\\ \text{001 through 012 for ALTMAIER06IV}\\ \text{001 through 072 for LANL\_08}\\ \text{001 through 009 for MEINRATH91\_III}\\ \text{001 through 017 for MEINRATH93\_III}\\ \text{001 through 002 for PERETRUCHIN96\_III}\\ \text{001 through 080 for RAI97IV}\\ \text{001 through 032 for RAO96\_III}\\ \text{001 through 022 for RAO\_NOVAK96\_III}\\ \text{001 through 015 for PERCHLOR}\end{array}\right\}$$

[A] Run-control information for the new LANL runs is located in Xiong et al. (2010b).

3 RESULTS

Our literature searches yielded a grand total of 3,796 published papers and unpublished reports on possible laboratory studies of the solubilities of Th(IV), Nd(III), Am(III) and Cm(III). The final evaluations of these papers and reports for inclusion in this analysis are documented in Subsections 3.1 and 3.2 (see below). Subsections 3.1 and 3.2 also provide our results for the Th(IV) and the Am(III) models, respectively. These results are presented as histograms and as CDFs.

Table 4. Results of Literature Searches for Published Papers and Unpublished Reports on Th(IV), Nd(III), Am(III) and Cm(III) Solubility Studies.

Radioelement	Search Plus	Oppie	Science Research Connection	Total for Radio-element	Included in Final Evaluation (Table 5 or Table 9)	Included in Th(IV) or Nd(III) and Am(III) Comparison
Th(IV)	690	13	35	738	14	3
Nd(III)	1885	17	2	1904	16[A]	10[B]
Am(III)	595	5	36	636	3	1
Cm(III)	495	5	36	518	0	0

[A] We identified one paper (Lucchini et al., 2007) and two reports (Borkowski et al., 2009; Borkowski, 2010) because of our collaboration with Los Alamos National Laboratory — Carlsbad Operations, and another paper (Wood et al., 2002) by means other than a literature search.

[B] We included the results of Borkowski (2010) and Wood et al. (2002) in the uncertainty analysis for the Am(III) solubility model.

3.1 Th(IV) Solubility Model

This subsection and Table 5 document our final evaluations of published papers for the comparison of experimentally measured Th(IV) solubilities with those predicted using the WIPP Th(IV) speciation and solubility model in FMT.

None of the measured solubilities included in the comparisons for the WIPP Th(IV) model included any organic ligands. This is because none of the solubility studies that included organic ligands satisfied all of the criteria described in Section 2. Felmy et al. (2006) is included in Table 5 as an example of why a solubility study that included organic ligands failed to meet these criteria: they included 0.5–6 M $NaNO_3$ in all of their experiments, but NO_3^- is not included in the Th(IV) model.

Altmaier et al. (2004) measured the solubilities of $ThO_2(cr)$ and $ThO_n(OH)_{4-2n}\,xH_2O(am)$ in NaCl and $MgCl_2$ solutions with various ionic strengths (see Table 5 for additional information on these experiments). Xiong et al. (2004, 2005) did not consider the results in Altmaier et al. (2004) in their uncertainty analyses of Th(IV) solubilities for the CRA-2004 PABC because this paper came to their attention after they completed their analyses. For our analysis for the CRA-2009 PABC, we included all six of the uncentrifuged results from solutions with $I \geq 3$ M from Altmaier et al. (2004, Figure 2) according to criterion S1 (see Section 2 above): two from their 5 M NaCl solutions, two from their 2.5 M $MgCl_2$ solutions, and two from their 4.5 M $MgCl_2$ solutions (see Table 5 for additional information on these results and their FMT run numbers. However, we excluded the ultracentrifuged results of Altmaier et al. (2004) because this posttest phase-separation method was significantly different from those employed in the studies used to parameterize the WIPP Th(IV) solubility model (e.g., centrifugation or filtration) and appeared to support a significantly different solubility model than that established for the WIPP (i.e. ultracentrifugation showed that 99% or more of what had been interpreted as dissolved Th(IV) present as the $Th(OH)_4(aq)$ species appeared to be present as the eigencolloid $Th(OH)_4(col)$). The WIPP Th(IV) model was parameterized in the mid-1990s, before it was realized that the phase-separation methods used then might not have removed all of the $Th(OH)_4(col)$. Thus, we excluded the ultracentrifuged results of Altmaier et al. (2004) according to Criterion G5 (Section 2).

Although our model significantly overpredicts the solubility of Th(IV) from about pH = 6 to 13.5 in bicarbonate- (HCO_3^--) or carbonate-free (CO_3^{2-}-free) solutions, it is still adequate for WIPP compliance-related calculations because both the Th(IV) solubility and the total mobile concentration (dissolved plus colloidal) of Th(IV) predicted under these conditions are higher than they would be based on the ultracentrifuged results of Altmaier et al. (2004). This is because the concentration factors used to calculate the colloidal Th(IV) component of the WIPP mobile Th(IV) concentration are multiplied by a dissolved Th(IV) concentration (solubility) that is about 100 times higher than its actual value, based on the ultracentrifuged results of Altmaier et al. (2004).

Table 5. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Th(IV) Solubilities.

Reference	Solution(s) and Ionic Strength(s)	pH, pcH, or pmH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Altmaier et al. (2004)	(A) 0.5 M NaCl (B) 5 M NaCl (C) 0.25 M $MgCl_2$ (I = 0.75 M) (D) 2.5 M $MgCl_2$ (I = 7.5 M) (E) 4.5 M $MgCl_2$ (I = 13.5 M)	(A) pcH = 10.4 & 11-13.5 (B) pcH = 10.8 (C) pcH = 9.0 (D) pcH = 8.9 (E) pcH = 8.8	ThO_2(cr) & $ThO_n(OH)_{4-2n}$ xH_2O(am), which they referred to as "$Th(OH)_4$(am) or $ThO_2 \cdot xH_2O$(am)"	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Six uncentrifuged results (no duplicates) obtained at $I \geq 3$ M included in this analysis: FMT_PABC09_Altmaier04IV_001 through 006. Ultracentrifuged results excluded because the posttest phase-separation method was different than those employed in the studies used to parameterize the Th(IV) model and appeared to support a different model (see text).
Altmaier et al. (2005)	(A) Mostly $NaHCO_3$-Na_2CO_3-NaCl-NaOH with I = 0.5 M (B) Some with 0.25-2 M Na_2CO_3 & 0.1 M NaOH	(A) pcH = 4.5-7.5 & 8.5-13.5 (B) pcH = 13	$Th(OH)_4$(am) or $ThO_2 \cdot xH_2O$(am)	Not considered by Xiong et al. (2005) because this paper came to their attention after completion of their analysis. Most results excluded from this analysis because $I < 3$ M. All other results excluded because the $Th(OH)_y(CO_3)_z^{4-y-2z}$ complex(es) found to be important by Altmaier et al. (2005) are not in the WIPP Th(IV) model. Four results (no duplicates) obtained at $I \geq 3$ M modeled but excluded from this analysis: FMT_PABC09_Altmaier05IV_001 through 004.
Altmaier et al. (2006)	$NaHCO_3$-Na_2CO_3-NaCl with I = 0.1-4 M.	pcH = 8–11	$Th(OH)_4$(am) or $ThO_2 \cdot xH_2O$(am)	Most results excluded from this analysis because $I < 3$ M. All other results excluded because the $Th(OH)(CO_3)_4^{5-}$ complex found to be important by Altmaier et al. (2006) is not in the WIPP Th(IV) model. Twelve results (no duplicates) obtained at $I \geq 3$ M modeled but excluded from this analysis: FMT_PABC09_Altmaier06IV_001 through 012.

Table 5 continued on next page

Table 5. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Th(IV) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pH, pcH, or pmH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Altmaier et al. (2008)	(A) 0.2–5.26 m $CaCl_2$ (I = 1.2 to 15.78 m) (experiments with Th(IV)) (B) 2.40 m $Ca(ClO_4)_2$ (I = 7.20 m) (Th(IV))	pmH = 9.3-12.1 (all Th(IV))	Solutions with $CaCl_2$ < 1 M (entire pH range) or $CaCl_2$ > 1 M (pH < 11.5): $Th(OH)_4(am)$ or $ThO_2{\cdot}xH_2O(am)$. Solutions with $CaCl_2$ > 1 M (pH > 11.5): unidentified, possibly a Ca-Th solid(cr).	Most results excluded from this analysis because $I < 3$ M. Some results excluded because of ultracentrifugation. All other results excluded because the $Ca_4(Th(OH)_8)^{4+}$ complex found to be important by Altmaier et al. (2008) is not in the WIPP Th(IV) model.
Baston et al. (1996)	Nirex (0.02 M)	pH = 10-12	$ThO_2(am)$	Included in Xiong et al. (2004). Excluded by Xiong et al. (2005) and from this analysis because $I < 3$ M.
Felmy et al. (1991)	(A) 0.1 M $NaClO_4$ (B) 0.6 M NaCl (C) 1.2 M NaCl (D) 3.0 M NaCl (E) 0.6 M KCl	(A) pcH = 4.9-5.9 (B) pcH = 2.91–10.24 (C) pcH = 2.83–10.19 (D) pcH = 3.82–10.56 (E) pcH = 3.75–7.95	Th(IV) hydrous oxide (all)	All results included in Xiong et al. (2004). Forty-five results (no duplicates) obtained at $I = 3$ M included in Xiong et al. (2005) and this analysis: FMT_CRA1V_Felmy91_Rev1_055 through 099. $I = 3$ M results obtained at pcH ≤ 3.6 excluded because the solids dissolved before saturation was attained.
Felmy et al. (1997)	Information provided in previous publications	Information provided in previous publications	Information provided in previous publications	Excluded by Xiong et al. (2004, 2005) and from this analysis because this paper contains only previously published results (e.g., Felmy et al., 1991).

Table 5 continued on next page

Table 5. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Th(IV) Solubilities (continued.

Reference	Solution(s) and Ionic Strength(s)	pH, pcH, or pmH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Felmy et al. (2006)	(A) 0.5 M $NaNO_3$ & 0.01 M citrate (B) 3.0 M $NaNO_3$ & 0.01 M citrate (C) 6.0 M $NaNO_3$ & 0.01 M citrate (D) 0.5 M $NaNO_3$ & 10^{-4} to 10^{-2} M citrate (E) 0.5 M $NaNO_3$ & 10^{-4} to 10^{-2} M citrate	(A) pcH = 5.2–12.2 (B) pcH = 5.0–11.8 (C) pcH = 4.7–12.1 (D) pcH = 6-8 (E) pcH = 9.5-10.1	ThO_2(am) (all)	Excluded from this analysis because NO_3^- is not in the WIPP Th(IV) model.
Neck et al. (2002)	0.5 M NaCl	pcH = 1.11–13.7	$Th(OH)_4$(am) or $ThO_2 \cdot xH_2O$(am)	Included in Xiong et al. (2004). Excluded by Xiong et al. (2005) and from this analysis because I < 3 M.
Neck et al. (2003)	(A) 0.1 M NaCl (B) 0.5 M NaCl	(A) pcH = 1.00-1.75 (B) pcH = 1.03-1.28 & 11.03-13.43	ThO_2(cr) or $ThO_2 \cdot xH_2O$(mcr)	Not considered by Xiong et al. (2004) because this paper came to their attention after completion of their analysis. Excluded by Xiong et al. (2005) and from this analysis because I < 3 M.
Östhols et al. (1994)	0.5 $NaClO_4$ & 0, 0.1, & 0.97 atm CO_2	pH = 3.31–7.36 (continuous titrations) & 8.21-10.45 (batch experiments)	ThO_2(mcr)	Included in Xiong et al. (2004). Excluded by Xiong et al. (2005) and from this analysis because I < 3 M.

Table 5 continued on next page

Table 5. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Th(IV) Solubilities (continued.

Reference	Solution(s) and Ionic Strength(s)	pH, pcH, or pmH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Rai et al. (1995)	(A) 0.005-0.25 M $NaHCO_3$ (B) 0.1-2.0 M Na_2CO_3 (C) 0.1-2.0 M Na_2CO_3 & 0.1 M NaOH (D) 0.1-0.5 M NaOH & 1.0 M Na_2CO_3	Not provided	ThO_2(am)	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Excluded from this analysis because the $Th(OH)_y(CO_3)_z^{4-y-2z}$ complexes found to be important by Altmaier et al. (2005) under the conditions used by Rai et al. (1995) are not in the WIPP Th(IV) model.
Rai et al. (1997)	(A) 0.2 m NaCl (used only for U solubilities) (B) 1.0 m NaCl (used only for U solubilities) (C) 3.2 m NaCl (data from Felmy et al., 1991) (D) 4.0 m NaCl, (E) 6.0 m NaCl, (F) 1.0 m $MgCl_2$ (I = 3 m), (G) 1.82 m $MgCl_2$ (I = 5.46 m), & (H) 3.0 m $MgCl_2$ (I = 9 m)	(A) U not included in this analysis (B) U not included in this analysis (C) See entry for 3.0 M NaCl for Felmy et al. (1991) in this table (D) pcH = 3.02-5.16 (E) pcH = 3.32-5.28 (F) pcH = 3.84-4.94 (G) pcH = 3.17-5.46 (H) pcH = 3.52-5.65	ThO_2(am)	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Eighty-eight results (8 duplicates) obtained at $I \geq 3$ M included in this analysis: FMT_PABC09_Rai97IV_001 through 080. Results obtained from the most acidic solutions in each set of experiments (see Table 6) excluded because the solids dissolved before saturation was attained.

Table 5 continued on next page

Table 5. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Th(IV) Solubilities (continued.

Reference	Solution(s) and Ionic Strength(s)	pH, pcH, or pmH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Rai et al. (2000)	(A) 0.1 M NaCl (Set I of Rai et al., 2000) (B) 0.1 M NaCl (Set II) (C) 0.1 M NaCl (Set III) (D) 0.1 M NaCl (Set IV) (E) 0.1 M NaCl (Set V)	(A) pH = 2.0-4.7 & 1.5-2.2 (B) pH= 4.2-5.1 & 2.0-2.1 (C) pH = 1.9-4.2 & 1.9-3.0 (D) pH = 1.3-3.6 (E) pH = 1.4-3.5	(A) ThO_2(am) & ThO_2(am to cr) (B) ThO_2(am) & ThO_2(am to cr) (C) ThO_2(am) & ThO_2(am to cr) (D) ThO_2(cr) (E) ThO_2(cr)	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Most results excluded from this analysis because $I < 3$ M. All other results excluded because $T = 90$ °C.

Altmaier et al. (2005) measured the solubilities of $Th(OH)_4(am)$ and $ThO_2{\cdot}xH_2O(am)$, mostly with $NaHCO_3$-Na_2CO_3-$NaCl$ solutions with I = 0.5 M. They also carried out some experiments with Na_2CO_3 solutions with various ionic strengths (Table 5). Xiong et al. (2005) did not consider these results because this paper came to their attention after they completed their analysis. Inspection of the results in Altmaier et al. (2005, Figure 4b) led us to suspect that, in some of their experiments, the ionic strength might have equaled or exceeded 3 M. Therefore, we used Data Thief to extract the numerical values of the plotted CO_3^{2-} concentrations from their Figure 4b, and calculated the ionic strengths of the solutions. We found that four of these solutions had $I \geq 3$ M. According to criterion S1 (see Section 2), Xiong et al. (2005) would have included these results in their Th(IV) uncertainty range and probability distribution. We excluded them, however, because Altmaier et al. (2005) concluded that, at high CO_3^{2-} concentrations ($\log[CO_3^{2-}]$ greater than about -0.5) in their Figure 4b, the dominant aqueous species is (are) $ThOH(CO_3)_4^{5-}$ (or $ThOH(CO_3)_4^{5-}$ and $Th(OH)_2(CO_3)_4^{6-}$), neither of which is included in the WIPP Th(IV) model. Thus, we used criterion G9 to exclude these results.

The WIPP Th(IV) model includes the following $Th(OH)_y(CO_3)_z^{4-y-2z}$ complexes: $Th(CO_3)_5^{6-}$, $Th(OH)_3CO_3^-$, and $Th(OH)_4(aq)$. It does not include $ThOH(CO_3)_4^{5-}$ and $Th(OH)_2(CO_3)_2^{2-}$, both of which were identified by Altmaier et al. (2005, Figure 5) as important at high CO_3^{2-} concentrations. Furthermore, it does not include $Th(OH)_2CO_3(aq)$ and $Th(OH)_4CO_3^{2-}$, which – although not identified as important in their Figure 5 – were quantified by Altmaier et al. (2005): Nevertheless, the WIPP Th(IV) model is still adequate for WIPP compliance-related calculations. This is because none of the important $Th(OH)_y(CO_3)_z^{4-y-2z}$ complexes with $z > 0$ approaches the $Th(OH)_4(aq)$ concentrations predicted by Brush and Xiong (2009c) for the CRA-2009 PABC (4.52×10^{-8} M for GWB[1] and 4.76×10^{-8} M for ERDA-6[2]) until the log of the CO_3^{2-} concentration exceeds about −1 (see Altmaier et al., 2005, Figure 4b). By contrast, the total inorganic C (TIC) concentrations (essentially the sum of the concentrations of HCO_3^- and CO_3^{2-}) predicted by Brush and Xiong (2009c) were more than two orders of magnitude lower than that threshold (0.350 mM for GWB[3] and 0.448 mM for ERDA-6[4]). The reason why the TIC concentrations predicted for these WIPP brines are too low to form important $Th(OH)_y(CO_3)_z^{4-y-2z}$ complexes with $z > 0$ is because the brucite-hydromagnesite carbonation reaction will buffer the f_{CO_2} at 3.14×10^{-6} atm in both GWB[3] and ERDA-6[4]. The brucite-hydromagnesite carbonation reaction will also buffer the TIC at the values given above.

Altmaier et al. (2006) determined the solubilities of $Th(OH)_4(am)$ and $ThO_2{\cdot}xH_2O(am)$ in $NaHCO_3$-Na_2CO_3-$NaCl$ solutions with various ionic strengths (Table 5). We excluded most of

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[1] From the column labeled "GWB, Hydromagnesite, w Phase 3, w Organics (FMT Run 5)" in Table 13 of Brush et al. (2009c).

[2] From the column labeled "ERDA-6, Hydromagnesite, w Phase 3, w Organics (FMT Run 13)" in Table 14 of Brush et al. (2009c).

[3] From column labeled "GWB w Organics after Eq., w Phase 3, CRA-2009 PABC Run 5" in Table 8 of Brush et al. (2009c).

[4] From column labeled "ERDA-6 w Organics after Eq., w/o Phase 3, CRA-2009 PABC Run 13" in Table 9 of Brush et al. (2009c).

their results according to criterion S1 (Section 2) because they were obtained using $NaHCO_3$-Na_2CO_3-NaCl solutions with ionic strengths less than 3 M. However, we found 12 results from experiments with $I \geq 3$ M (see Altmaier et al., 2006, Figure 2). We used criterion G9 to exclude these data because the WIPP Th(IV) model does not include the $ThOH(CO_3)_4^{5-}$ complex, which Altmaier et al. (2006) found to be the dominant aqueous species. Nevertheless, the WIPP Th(IV) model is still adequate for WIPP compliance-related calculations for the reasons described above in our discussion of the data from Altmaier et al. (2005) (see above).

Altmaier et al. (2008) measured the solubilities of $Th(OH)_4$(am) and $ThO_2 \cdot xH_2O$(am), a (possible) Ca-Th solid, and Zr(IV) or Pu(IV) solids in $CaCl_2$ with various ionic strengths and in 2.40 m $Ca(ClO_4)_2$. We used criterion G6 (Section 2) to exclude most of their results because they were obtained from experiments with Zr(IV) or Pu(IV). We used criterion S1 to exclude the Th(IV) solubilities from 0.20 and 0.51 m $CaCl_2$ solutions. Finally, we used criterion G9 to exclude the Th(IV) solubilities from 1.02, 2.11, and 5.26 m $CaCl_2$ solutions (I = 3.06, 6.33, and 15.78 m, respectively) because Altmaier et al. (2008) concluded that, at high $CaCl_2$ concentrations (> 0.5 m for pcH = 11-12 according to their abstract, but > 0.2 m at pH = 12 from their Figure 5), the dominant aqueous species was $Ca_4(Th(OH)_8)^{4+}$, which is not included in the WIPP Th(IV) model.

Nonetheless, the Th(IV) model is still adequate for WIPP compliance-related calculations because the Ca concentration of WIPP brines is 0.00980 M for GWB[3] and 0.0112 M for ERDA-6.[4] (Note that the numerical values of these concentrations in molal units do not differ significantly from those in molar units: the output file for FMT Run 5 predicts a Ca concentration in GWB of 0.00980 M and 0.0113 m after equilibration with the important solids in WIPP disposal rooms.) Inspection of Figure 5 in Altmaier et al. (2008) demonstrates that both the total dissolved Ca concentration and the pcH must be much higher than the values expected in WIPP brines to increase the concentration of $Ca_4(Th(OH)_8)^{4+}$ to values greater than those expected when $Th(OH)_4$(aq) or $Th(OH)_4$(col) is the dominant species. For example, if the $CaCl_2$ concentration is 0.51 m, the pcH must be 12 or higher to increase the $Ca_4(Th(OH)_8)^{4+}$ concentration to values greater than those expected when $Th(OH)_4$(col) is the dominant mobile species. If the $CaCl_2$ concentration is 1.02 m, the pcH must be 11-11.5 or higher to increase the $Ca_4(Th(OH)_8)^{4+}$ concentrations greater than those expected when $Th(OH)_4$(col) is the dominant mobile species. Therefore, the absence of $Ca_4(Th(OH)_8)^{4+}$ from the Th(IV) model does not affect its validity under expected WIPP conditions.

Baston et al. (1996) measured the solubility of ThO_2(am) in a low-ionic-strength solution (Table 5). Xiong et al. (2004) included the results of Baston et al. (1996) in their analysis, but Xiong et al. (2005) excluded them because they were obtained from solutions with $I < 3$ M (see criterion S1 in Section 2). We also used criterion S1 to exclude these results.

Felmy et al. (1991) studied the solubility of Th(IV) hydrous oxide in 0.1 M $NaClO_4$, in NaCl solutions of various ionic strengths, and in 0.6 M KCl (Table 5). Xiong et al. (2004) included all of these results in their analysis. Xiong et al. (2005, Subsection 5.2.3), however, established criterion S1 based on their comparison of the solubilities measured by Felmy et al. (1991) and those predicted using the WIPP Th(IV) solubility model, and excluded most of them because they were obtained using solutions with $I < 3$ M. Furthermore, inspection of the remaining results showed that those obtained at the most acidic values of pH were essentially independent of pH. Xiong et al. (2005, p. 12) noted that:

> [T]his behavior can be explained by noting that in … the experiments at pH $\leq$ ~3.6 …, the Th(IV)-bearing solids were consumed before saturation was attained (see Felmy et al., 1991, p. 298). Therefore, the constant Th(IV) concentration of slightly less than 10^{-2} M in the experiments reflects the fact that the constant quantity of Th(IV) added at the start of these experiments was insufficient to saturate these solutions under these conditions… Thus, the concentrations in the experiments at pH $\leq$ ~3.6 … are not solubilities. Because the concentrations measured by Felmy et al. (1991) at pH $\leq$ ~3.6 are not solubilities, we excluded them from the revised An(IV) comparison.

Therefore, Xiong et al. (2005) excluded these acidic results, and we incorporated the reason for excluding these and similar results from other studies into criterion G7 (see Section 2; the descriptions of the results of Rai et al., 1997, in Subsection 3.1 and Tables 5 and 6; and the discussions of the results of Rao et al., 1996a, in Subsection 3.2 and Table 9). After applying criteria G7 and S1, Xiong et al. (2005) included 45 results from Felmy et al. (1991) in their analysis; we included the same 45 results in this analysis.

Felmy et al. (1997) reviewed the development of models for the solubility of Th(IV) solids in high-ionic-strength solutions. Xiong et al. (2004, 2005) excluded all of the results in Felmy et al. (1997) from their analyses, and we excluded it from this analysis, according to criterion G10 because this paper contains only previously published results (e.g., Felmy et al., 1991).

Felmy et al. (2006) measured the solubility of ThO_2(am) in $NaNO_3$ solutions with various ionic strengths and various concentrations of the organic ligand citrate (Table 5). We used criterion G9 (Section 2) to exclude their results because NO_3^- is not in the WIPP Th(IV) model.

Neck at al. (2002) measured the solubilities of $Th(OH)_4$(am) and $ThO_2 \cdot xH_2O$(am) in 0.5 M NaCl solutions (Table 5). Xiong et al. (2004) included these results in their analysis. Xiong et al. (2005) excluded them according to criterion S1 (Section 2) because they were obtained using solutions with I < 3 M. We also used criterion S1 to exclude them.

Neck et al. (2003) carried out solubility experiments with $Th(OH)_4$(am) and $ThO_2 \cdot xH_2O$(am) in 0,1 and 0.5 M NaCl solutions (Table 5). Xiong et al. (2004) did not consider the results in this paper because it came to their attention after they completed their analyses. Xiong et al. (2005) used criterion S1 (Section 2) to exclude them. We also used criterion S1 to exclude them.

Östhols et al. (1994) measured the solubility of ThO_2(mcr) in 0.5 M $NaClO_4$ under atmospheres with various concentrations of CO_2 (Table 5). Xiong et al. (2004) included these results in their analysis. Xiong et al. (2005) used criterion S1 (Section 2) to exclude them. We also excluded them.

Rai et al. (1995) measured the solubilities of ThO_2(am) and UO_2(am) in a variety of $NaHCO_3$, Na_2CO_3, and Na_2CO_3 and NaOH solutions with various ionic strengths (Table 5). Xiong et al. (2004, 2005) did not consider these results because this paper came to their attention after they completed their analyses. Based on their previous work and that of others, Rai et al. (1995, p. 1146) expected that "… it is probably that [sic] the dominant aqueous species of Th and U in these high-carbonate solutions are $Th(CO_3)_5^{6-}$ and $U(CO_3)_5^{6-}$, respectively." However, the response of the Th and U solubilities to variations in the concentration of OH^- in their experiments led them to speculate that the complexes $U(OH)_3CO_3^-$ or $U(OH)_4CO_3^{2-}$ or, from the oxidation-state analogy, $Th(OH)_3CO_3^-$ or $Th(OH)_4CO_3^{2-}$ could be dominant (Rai et al., 1995, p. 1148). Subsequently, Altmaier et al. (2005, 2006) demonstrated that, under the conditions of Rai et al. (1995), the important $Th(OH)_y(CO_3)_z^{4-y-2z}$ complexes are actually $Th(CO_3)_5^{6-}$, $Th(OH)(CO_3)_4^{-5}$, and $Th(OH)_2(CO_3)_2^{-2}$. Although the WIPP Th(IV) model includes $Th(CO_3)_5^{6-}$, it does not include $Th(OH)(CO_3)_4^{-5}$ and $Th(OH)_2(CO_3)_2^{-2}$. Therefore, Rai et al. (1995) used conditions under which there are two important $Th(OH)_y(CO_3)_z^{4-y-2z}$ species that are not in the WIPP Th(IV) model and we used criterion G9 (Section 2) to exclude them.

Rai et al. (1997) conducted solubility experiments with $Th(OH)_2$(am) in 4.0 and 6.0 M NaCl solutions and in $MgCl_2$ solutions with various ionic strengths (Table 5). Xiong et al. (2004, 2005) did not consider the results in this paper because it came to their attention after they completed their analyses. Initially, we decided to include all of their results obtained at $I \geq 3$ M according to criterion S1 (Section 2). However, many of the results of Rai et al. (1997) displayed the same feature observed by Xiong et al. (2005) in the results of Felmy et al. (1991) (see above): the results obtained at the most acidic pH values were independent of pH. Therefore, we used criterion G7 to exclude the most acidic results (see Table 6), which left 88 results for inclusion in this analysis.

Rai et al. (2000) performed solubility experiments with ThO_2(am) and ThO_2(cr) in 0.1 M NaCl solutions (Table 5). Xiong et al. (2004, 2005) did not consider this paper because it came to their attention after they completed their analyses. We used criteria S1 and G5 (Section 2) to exclude them. Criterion G5 also was applicable to some of these results because they were obtained at 90 °C, a temperature higher than that expected in the WIPP.

Figure 1 provides the histogram for our comparisons of experimentally measured and predicted Th(IV) solubilities for the CRA-2009 PABC and compares it to that obtained for the CRA-2004 PABC by Xiong et al. (2005). The current comparison includes a total of 140 measured and predicted solubilities, an increase of 95 from the 45 measured and predicted solubilities included in the previous comparison. The current distribution peaks at Bin −0.45 with a frequency of 15, with secondary and tertiary peaks at Bin 0.30 and Bin −0.60 (13 and 12 comparisons, respectively). Table 7 summarizes the statistical parameters of the current frequency distribution that are used by PA and compares them to those of the previous distribution.

Table 6. Results from Rai et al. (1997) Excluded from Th(IV) Comparisons Because of Complete Dissolution of Solids.

Run Time (days)	Solution	Maximum pcH	Number of Results Excluded	Figure in Rai et al. (1997) with Excluded Data
7	4.0 m NaCl	3.9	7	Figure 6
51	4.0 m NaCl	4.0	5	Figure 6
91	4.0 m NaCl	4.0	5	Figure 6
8	6.0 m NaCl	3.9	3	Figure 2
125	6.0 m NaCl	3.85	3	Figure 2
159	6.0 m NaCl	3.8	5	Figure 2
7	1.8 m $MgCl_2$	4.0	5	Figure 3
73	1.8 m $MgCl_2$	4.0	4	Figure 3
8	3.0 m $MgCl_2$	3.9	2	Figure 4

Inspection of Figure 1 reveals that the WIPP Th(IV) model; the thermodynamic database FMT_050405.CHEMDAT (Xiong, 2005), which includes phase 3 ($Mg_2Cl(OH)_3{\cdot}4H_2O$) but not phase 5 ($Mg_3(OH)_5Cl{\cdot}4H_2O$); and the speciation and solubility code FMT overpredicted the 140 measured solubilities included in the current analysis. This is because Figure 1 clearly contains more negative values of $D = \log_{10}(S_m) - \log_{10}(S_p)$ than positive values, which means that more of the predicted solubilities exceeded the measured solubilities than vice versa. The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Th(IV) solubilities are −0.346 and −0.520, respectively (Table 7), and the mean and median values of the sampled uncertainty factor are $10^{-0.346} = 0.451$ and $10^{-0.520} = 0.302$. (The WIPP PA codes use actinide solubilities that are the products of the baseline solubilities and the sampled uncertainty factors).

Xiong et al. (2005) used the same model, database, and code in their analysis, but slightly underpredicted the 45 measured solubilities in their analysis, all of which came from Felmy et al. (1991).

Table 8 provides values of the corresponding CDF for Th(IV) for the CRA-2009 PABC, and compares them to those obtained for the CRA-2004 PABC by Xiong et al. (2005). The current uncertainty analysis shows that the WIPP Th(IV) model, database, and code overpredicted the larger data set used for the CRA-2009 PABC to a greater extent than that used for the CRA-2004 PABC, although both extrema are farther from zero in the CRA-2009 PABC than in the CRA-2004 PABC. We will use the results in Table 8 to sample the uncertainties in the baseline solubilities of Th(IV), U(IV), and Pu(IV) for the CRA-2009 PABC. Figure 2 shows the CDFs plotted for both analyses.

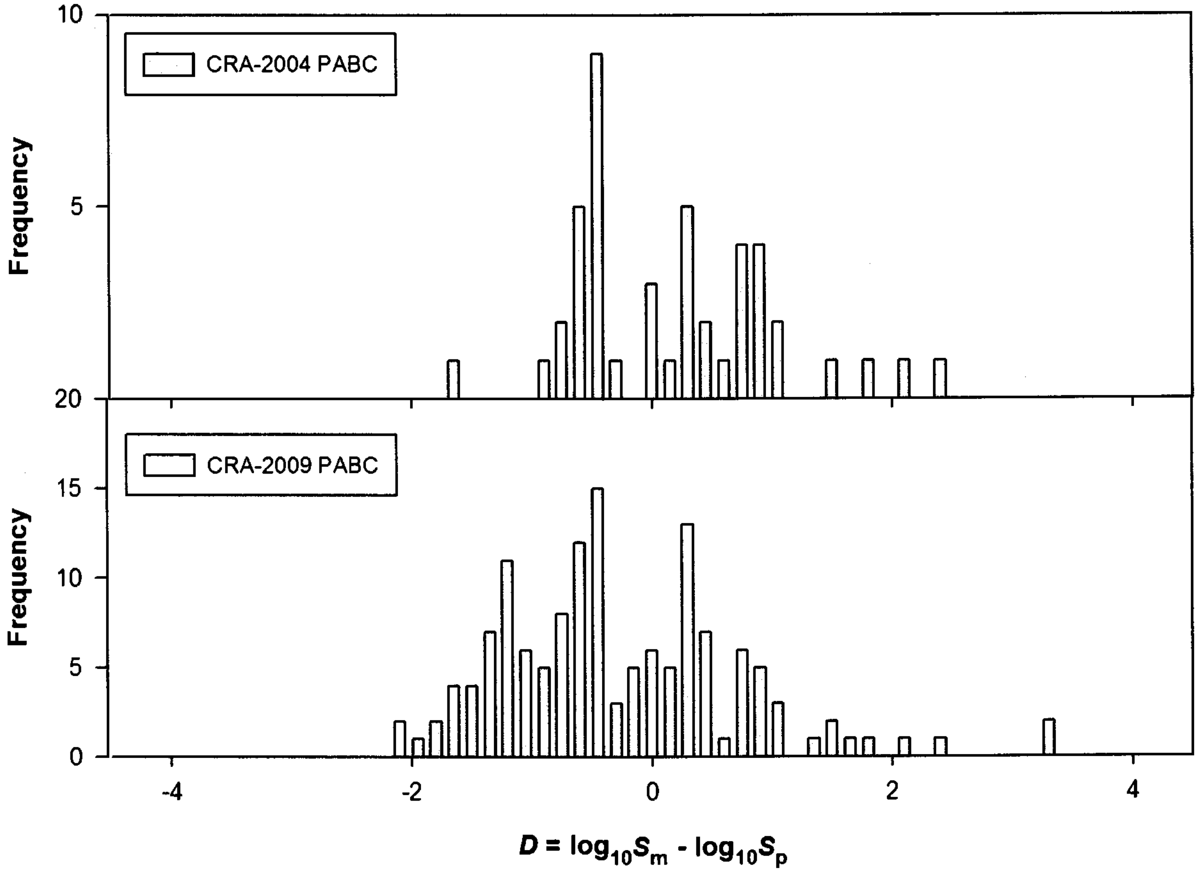

Figure 1. Comparison of the histograms of the difference $D = \log_{10} S_m - \log_{10} S_p$ for Th(IV) for the CRA-2004 PABC and CRA-2009 PABC.

Table 7. Comparisons of Selected Statistical Properties of the Distribution of $D = \log_{10}(S_m) - \log_{10}(S_p)$ for Th(IV) for the CRA-2004 PABC and CRA-2009 PABC.

Analysis	Mean	Median	Standard Deviation	Minimum	Maximum
CRA-2004 PABC	0.108	0.075	0.837	−1.80	2.40
CRA-2009 PABC [A]	−0.346	−0.520	0.995	−2.25	3.30

[A] This probability distribution was used to define the solubility multiplier SOLVAR for the oxidation-state IV model material SOLMOD4 in the WIPP PA Parameter Database for the CRA-2009 PABC.

Table 8. Comparisons of the CDFs of the Differences between Measured and Predicted Th(IV) Solubilities for the CRA-2004 PABC and CRA-2009 PABC.

X	$P(D < X)$ CRA-2004 PABC	$P(D < X)$ CRA-2009 PABC [A]
−2.25	0.0000	0.0000
−2.10	0.0000	0.0143
−1.95	0.0000	0.0214
−1.80	0.0000	0.0357
−1.65	0.0222	0.0643
−1.50	0.0222	0.0929
−1.35	0.0222	0.1429
−1.20	0.0222	0.2214
−1.05	0.0222	0.2643
−0.90	0.0444	0.3000
−0.75	0.0889	0.3571
−0.60	0.2000	0.4429
−0.45	0.4000	0.5500
−0.30	0.4222	0.5714
−0.15	0.4222	0.6071

Table 8 continued on next page

Table 8. Comparisons of the CDFs of the Differences between Measured and Predicted Th(IV) Solubilities for the CRA-2004 PABC and CRA-2009 PABC (continued).

X	$P(D < X)$ CRA-2004 PABC	$P(D < X)$ CRA-2009 PABC[A]
0.00	0.4889	0.6500
0.15	0.5111	0.6857
0.30	0.6222	0.7786
0.45	0.6667	0.8286
0.60	0.6889	0.8357
0.75	0.7778	0.8786
0.90	0.8667	0.9143
1.05	0.9111	0.9357
1.20	0.9111	0.9357
1.35	0.9111	0.9429
1.50	0.9333	0.9571
1.65	0.9333	0.9643
1.80	0.9556	0.9714
1.95	0.9556	0.9714
2.10	0.9778	0.9786
2.25	0.9778	0.9786
2.40	1.0000	0.9857
2.55	1.0000	0.9857
2.70	1.0000	0.9857
2.85	1.0000	0.9857
3.00	1.0000	0.9857
3.15	1.0000	0.9857
3.30	1.0000	1.0000

[A] This CDF was used to define the solubility multiplier SOLVAR for the oxidation-state IV model material SOLMOD4 in the WIPP PA Parameter Database for the CRA-2009 PABC.

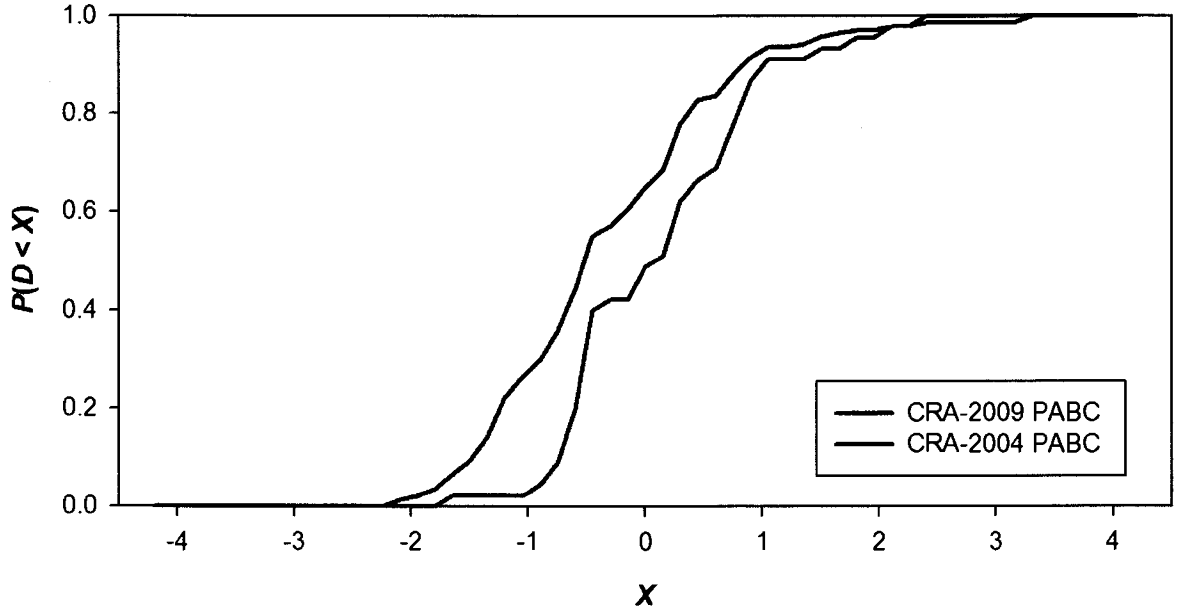

Figure 2. Comparison of plots of the CDFs for Th(IV) for the CRA-2004 PABC and CRA-2009 PABC.

3.2 Am(III) Solubility Model

This subsection and Table 9 document our final evaluations of published papers and unpublished reports for the comparison of experimentally measured Nd(III) and Am(III) solubilities with those predicted using the WIPP Am(III) speciation and solubility model in FMT.

No measured Cm(III) solubilities were included in this comparison because none of these studies met all of the criteria in Section 2.

Furthermore, no measured solubilities with organic ligands were included in this comparison because none of these studies met all of these criteria.

Borkowski et al. (2009) measured the solubilities of various Nd(III) solids in 5 m NaCl and the synthetic WIPP brines GWB and ERDA-6 (see Table 9 for additional information on these experiments). Nd(III), an oxidation-state analog of Am(III), was used along with Am(III) and Cm(III) to parameterize the WIPP Am(III) speciation and solubility model. Therefore, we considered all of the results of Borkowski et al. (2009) for inclusion in our uncertainty analysis of Nd(III) and Am(III) solubilities for the CRA-2009 PABC according to criterion G6 (see Section 2 above). However, Borkowski et al. (2009) concluded that, in many of their experiments in GWB or ERDA-6, complexation of Nd(III) by dissolved borate probably increased the solubility of Nd(III). Because there are no Nd(III)-borate species in the WIPP Am(III) solubility model, we asked Borkowski to select those experiments that had values of pcH low enough to preclude significant complexation of Nd(III) by borate, thereby satisfying criterion G9. Borkowski selected 18 runs with GWB (pcH $\leq$ 7.4) and 10 with ERDA-6 (pcH $\leq$ 8.1) and e-mailed us the numerical values of the results. We placed this e-mail in the SNL/WIPP Records Center in the records package entitled "Calculation of Actinide Solubilities for the WIPP CRA-2009 PABC [work associated with AP-143]," ERMS 548686. Borkowski also sent us the results of 54 runs with 5 m NaCl, because these solutions contained no borate. (We also placed this e-mail to the SNL/WIPP Records Center for inclusion in the same records package.) Therefore, we included a total of 82 results from Borkowski et al. (2009) in our Am(III) uncertainty analysis.

Inclusion of these results from Borkowski et al. (2009) in the original version of this analysis was a deviation from the general criterion G1 of Xiong et al. (2009, Section 2), which stated, "Include only results from experimental studies published from January 1, 1990, through December 31, 2008." Xiong et al. (2009) did not provide a reason for this deviation, an omission which was cited in CAR IS-10-02-CAR-01 and addressed in the CAP for this CAR (see item 1 in the CAP for CAR IS-10-02-CAR-01 in the SNL/WIPP Records Center). Therefore, we are providing a reason for this deviation here: Xiong et al. (2009) included the results of Borkowski et al. (2009) that were unaffected by significant Nd(III)-borate complexation because they were directed to do so in the management review of the original version of this analysis report (see comment 47 and the response to this comment on p. 22 of this review in the SNL/WIPP Records Center).

Subsequent to the completion of the original version of this report (Xiong et al. 2009), Borkowski (2010) issued a report containing tables of numerical values of the final values of pcH and Nd(III) solubilities presented graphically by Borkowski et al. (2009). However, comparisons of the numerical values in Borkowski (2010) and those e-mailed by Borkowski (see above) revealed that: (1) Borkowski (2010) contained more results than those e-mailed by Borkowski, and (2) the numerical values e-mailed by Borkowski could not be correlated with any of those in Borkowski (2010). Therefore, we used the FMT predictions by Xiong et al. (2010a, 2010b) with the numerical values from Borkowski (2010) to revise the comparisons of measured and predicted Nd(III) solubilities in this revision. To be consistent with the criteria used by Xiong et al. (2009) to select results that were unaffected by significant Nd(III)-borate complexation, we used the following 162 results reported by Borkowski (2010): all 120 results from the 5 M NaCl solutions, 28 results from GWB with pcH $\leq$ 7.4, and 14 from ERDA-6 with pcH $\leq$ 8.1.

Inclusion of these results from Borkowski (2010) in this revision is also a deviation from the general criterion G1 of Xiong et al. (2009, Section 2). The reason for this deviation is the same as that provided above.

Bunyakina & Storozhenko (2004) measured the solubility of $Nd_2(SO_4)_3 \cdot 8H_2O$ in solutions saturated with $MgSO_4$ and/or $Nd_2(SO_4)_3$ (see Table 9). Xiong et al. (2004, 2005) did not consider the results in Bunyakina & Storozhenko (2004) in their uncertainty analyses of Nd(III) and Am(III) solubilities for the CRA-2004 PABC because this paper came to their attention after they completed their analyses. We excluded these results from our analysis according to criterion G7 (see Section 2) because $Nd_2(SO_4)_3 \cdot 8H_2O$ is not in the WIPP Am(III) model.

Khalili et al. (1994) determined the solubilities of various Nd(III) solids in a synthetic brine similar to GWB (Table 9). According to criterion G7 (Section 2), Xiong et al. (2004, 2005) included 29 measured solubilities from solutions with pcH = 6.4 and 8.4 in their analyses because $Am(OH)_3$, the solubility-controlling solid in these experiments, is in the WIPP Am(III) model. However, they used the same criterion to exclude the results obtained from solutions with pcH = 10.4 and 12.4 because $Nd_2(CO_3)_3 \cdot 8H_2O$ and NdO(OH), the solubility-controlling solids in these runs, are not in the model, and because it is unclear whether all of the solids were identified at these values of pcH. After considering the results of Borkowski et al. (2009) (see text and Table 9 above), we used criterion G9 to exclude 24 of the 29 results included by Xiong et al. (2004, 2005) because the pcH of the solutions in these experiments exceeded 7.4, the pcH above which Borkowski concluded that complexation of Nd(III) by dissolved borate in GWB is significant. Therefore, we included 5 of the results of Khalili et al. (1994) in our analysis.

Lucchini et al. (2007) included preliminary results from Borkowski's study of the solubility of Nd(III) (see above and Table 9). Because Lucchini et al. (2007) was superseded by Borkowski et al. (2009), we excluded the former from our uncertainty analysis of Am(III) solubilities for the CRA-2009 PABC.

Makino et al. (1993) measured the solubilities of Nd(III) solids in 0.01 M $NaClO_4$ (Table 9). Xiong et al. (2004, 2005) did not consider these results because this paper came to their attention after they completed their analyses. Makino et al. (1993) stated that "the solid phase was identified as $Nd(OH)_3$(c) by X-ray diffraction [XRD] before and after the experiments." However, both of the posttest XRD patterns in their Figure 1 show that $Nd(OH)CO_3$(cr) was also present. Clearly, sufficient CO_3^{2-} was present in their solutions to convert at least some of the $Nd(OH)_3$(cr) to $Nd(OH)CO_3$(cr) during their undersaturation and/or oversaturation experiments, but it is unclear whether both of these solids were in equilibrium with the solutions or whether one solid was replacing another. It is also unclear what the TIC concentration of their solutions was, or even what the p_{CO_2} of the atmosphere in the headspace above their solutions was, because the p_{CO_2} of 0.1 ppm provided in the English summary of their paper was a detection limit (upper limit) for p_{CO_2}, not the actual concentration of CO_2 in the gaseous phase. Therefore, we excluded all 22 measured solubilities of Makino et al. (1993) according to criterion G8.

Meinrath and Kim (1991) measured the solubilities of $Nd_2(CO_3)_3$ and $Nd(OH)CO_3$ in 1 M $NaClO_4$ under atmospheres with various concentrations of CO_2 (Table 9). Xiong et al. (2004, 2005) did not consider the results in this paper because it came to their attention after they completed their analyses. According to criterion G7 (Section 2), we included all nine results obtained with 0.1 M $NaClO_4$ under a gaseous phase that contained 0.00031 atm CO_2 in our analysis because $Nd(OH)CO_3$, the solubility-controlling solid in these experiments (Table 9), is in the WIPP Am(III) model. However, we used the same criterion to exclude the results obtained from 0.1 M $NaClO_4$ under 0.01 and 1 atm CO_2 because $Nd_2(CO_3)_3$, the solubility-controlling solid in these runs, is not in the model.

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities.

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Borkowski et al. (2009)	(A) 5 m NaCl (B) GWB (C) ERDA-6	(A) pcH = 8.2–13.0 (B) pcH = 6.6–8.7 (C) pcH = 7.9–10.3	Presumably $Nd(OH)_3$, based on their thermodynamic predictions.	All 54 results from 5 m NaCl included in the original version of this analysis (Xiong et al., 2009). Eighteen results with pcH ≤ 7.4 from GWB included by Xiong et al. (2009) because Borkowski concluded that these results were not affected significantly by Nd(III)-borate complexation. Ten results with pcH ≤ 8.1 from ERDA-6 included by Xiong et al. (2009) be-cause Borkowski also concluded that these results were unaffected by borate. A total of 82 results (10 duplicates) included: FMT_PABC09_LANL_08_001 through 072. None of these results are included in this revision because all results in Borkowski et al. (2009) were superceded by those in Borkowski (2010) (see below). Inclusion of these results in the original version of this analysis was a deviation from criterion G1 of Xiong et al. (2009, Section 2); they included these results because they were directed to do so in the management review of the original version of this analysis (see text).

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Borkowski (2010)	(A) 5 m NaCl (B) GWB (C) ERDA-6	(A) pcH = 8.14–13.17 (B) pcH = 6.54–8.64 (C) pcH = 7.55–10.62	Presumably $Nd(OH)_3$, based on their thermodynamic predictions.	All 120 results from 5 M NaCl included in this revision. Twenty-eight results with pcH ≤ 7.4 from GWB are included in this revision because Borkowski concluded that they were not affected significantly by Nd(III)-borate complexation. Fourteen results with pcH ≤ 8.1 from ERDA-6 included in this revision because Borkowski concluded that these results were unaffected by borate. A total of 162 results (29 replicates) are included: FMT_LANL09_NACL_5M_PCH_001 through FMT_LANL09_NACL_5M_1E-2M_C_PCH_033; FMT_LANL09_GWB_PCH_001 through FMT_LANL09_GWB_1E-2M_C_PCH_004; and FMT_LANL09_ERDA-6_PCH_001 through FMT_LANL09_ERDA-6_001M_C_PCH_002. Inclusion of these results in this revision is a deviation from criterion G1 of Xiong et al. (2009, Section 2); the reason for this deviation is the same as that provided above for Borkowski et al. (2009).
Bunyakina & Storozhenko (2004)	Solutions saturated with $MgSO_4$ and/or $Nd_2(SO_4)_3$. Ionic strengths not provided.	Not provided	$Nd_2(SO_4)_3\cdot 8H_2O$	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Excluded from this analysis because $Nd_2(SO_4)3\cdot 8H_2O$ is not in the WIPP Am(III) model.

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Khalili et al. (1994)	Synthetic brine similar to GWB	pcH = 6.4, 8.4, 10.4, & 12.4	$Nd(OH)_3 \cdot nH_2O(am)$ at pcH = 6.4 & 8.4, $Nd_2(CO_3)_3 \cdot 8H_2O$ or "uncertain" at pcH = 10.4, NdO(OH) & $Nd(OH)_3$ or "uncertain" at pcH = 12.4	Twenty-nine results for pcH = 6.4 & 8.4 included by Xiong et al. (2004, 2005) because $Am(OH)_3$ is in the WIPP Am(III) model. Results for pcH = 10.4 & 12.4 excluded by Xiong et al. (2004, 2005) because $Nd_2(CO_3)_3 \cdot 8H_2O$ and NdO(OH) are not in the model, and because it is unclear that all of the solids were identified. Twenty-four of the 29 results included by Xiong et al. (2004, 2005) excluded from this analysis because the pcH in these runs exceeded 7.4, the pcH above which Borkowski concluded that complexation of Nd(III) by borate in GWB is significant (see text). Five results (5 duplicates) included: FMT_KHALILI_94_001.
Lucchini et al. (2007)	(A) GWB (B) ERDA-6	(A) pcH = 6.6–8.7 (B) pcH = 7.9–10.3	$Nd(OH)_3$ (both solutions), based on their thermodynamic predictions.	Not included in this analysis because a later report (Borkowski et al., 2009) superceded this paper.
Makino et al. (1993)	0.01 M $NaClO_4$ & 0.1 ppm CO_2	pcH = 7–13	$Nd(OH)_3(cr)$ with lesser amounts of $Nd(OH)CO_3(cr)$ (unclear whether both of these solids were in equilibrium one was replacing another).	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Excluded from this analysis because neither the TIC concentration of the aqueous phase nor the pCO_2 of the gaseous phase was provided, thus precluding predictions of Nd(III) solubilities for their experimental conditions.

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Meinrath & Kim (1991)	(A) 0.1 M $NaClO_4$ & 0.00031 atm CO_2	(A) pH = 4.1-4.3	(A) $Nd_2(CO_3)_3$ & $Nd(OH)CO_3$ initially, $Nd(OH)CO_3$ after 2 weeks	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. All nine results (no duplicates) from (A) included in this analysis because $Nd(OH)CO_3$ is in the WIPP Am(III) model: FMT_PABC09_Meinrath91_III_001 through 009. Results from (B) and (C) excluded because $Nd_2(CO_3)_3$ is not in the model.
	(B) 0.1 M $NaClO_4$ & 0.01 atm CO_2	(B) pH = 5.2-5.4	(B) $Nd_2(CO_3)_3$	
	(C) 0.1 M $NaClO_4$ & 1 atm CO_2	(C) pH = 5.7-6.2	(C) $Nd_2(CO_3)_3$	
Meinrath & Takeishi (1993)	(A) 0.1 M $NaClO_4$ & 0.0003 atm CO_2	(A) pH = 5.6-6.6	(A) $Nd_2(CO_3)_3$ & $Nd(OH)CO_3$ initially, $Nd(OH)CO_3$(mcr) after 5-7 days	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. All 17 results (no duplicates) from (A) and (B) included in this analysis because $Nd(OH)CO_3$, is in the WIPP Am(III) model: FMT_PABC09_Meinrath93_III_001 through 017. Results from (C), (D), and (E) excluded because $Nd_2(CO_3)_3$ is not in the model.
	(B) 0.1 M $NaClO_4$ & 0.003 atm CO_2	(B) pH = 5.4-6.3	(B) $Nd_2(CO_3)_3$ & $Nd(OH)CO_3$ initially, $Nd(OH)CO_3$(mcr) after 30-40 days	
	(C) 0.1 M $NaClO_4$ & 0.01 atm CO_2	(C) pH = 5.2-6.2	(C) $Nd_2(CO_3)_3\cdot(4.5\text{-}6\ H_2O)$	
	(D) 0.1 M $NaClO_4$ & 0.08 atm CO_2	(D) pH = 4.7-5.9	(D) $Nd_2(CO_3)_3\cdot(4.5\text{-}6\ H_2O)$	
	(E) 0.1 M $NaClO_4$ & 1 atm CO_2	(E) pH = 4.2-5.2	(E) $Nd_2(CO_3)_3\cdot(4.5\text{-}6\ H_2O)$	

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Peretrukhin et al. (1996)	1 & 5 M NaOH (experiments with Am(III))	Not provided	$Am(OH)_3$ aged by boiling for 3 hours (undersaturation runs) or $Am(OH)_3$, crystallinity unspecified (oversaturation runs)	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Four results (two duplicates) modeled but excluded from the Am(III) comparison because we predicted solubilities four to six orders of magnitude less than their measured values, possibly due to the presence of one or more $Am(OH)_x^{3-x}$ complexes with $x > 4$ in their experiments, but not in the WIPP Am(III) model: FMT PABC09 Peretruchin96_III_001 & 002.
Rao et al. (1996a)	0.1 M NaCl	pH = 4.8-9.0 (filtered samples in their Fig. 1) & 5.1-9.0 (41-day samples in their Fig. 2.	$Nd(OH)_3(cr)$	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Thirty-two of the 25 °C results (no duplicates) included in this analysis: FMT_PABC09_Rao96_III_001 through 032. Results obtained at $pH < 5.8$ excluded because the solids dissolved before saturation was attained.
Rao et al. (1996b)	(A) 0.1-1.0 M $NaHCO_3$ (B) 0.1-2.0 M Na_2CO_3	Not provided	$NaNd(CO_3)_2 \cdot 6H_2O(cr)$ (all)	Not considered by Xiong et al. (2004, 2005) because this paper came to their attention after completion of their analyses. Sixty results (38 duplicates) included in this analysis: FMT_PABC09_Rao-Novak96_III_001 through 022.

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Rao et al. (1999)	(A) 0.1-1.1 m $NaHCO_3$	(A) pH = 7.9-8.3	$NaNd(CO_3)_2{\cdot}6H_2O$ (all)	One-hundred-and-four results included in Xiong et al. (2004, 2005). Twenty-eight of the 104 results included by Xiong et al. (2004, 2005) excluded from this analysis because the pcH in these runs exceeded 7.4 or 8.1, the pcH above which Borkowski concluded that complexation of Nd(III) by borate in GWB or ERDA-6, respectively, is significant (see text). Seventy-six results (24 duplicates) included in this analysis: (FMT_CRA1V_RAO99_001 through 046, and 066 through 072.
	(B) 0.1-2 m Na_2CO_3	(B) pH = 10.4-10.8		
	(C) 2 M NaCl & 0.1-0.5 m $NaHCO_3$	(C) pH = 7.9-8.3		
	(D) 2 M NaCl & 0.1-2 m Na_2CO_3	(D) pH = 10.4-10.8		
	(E) 4 M NaCl & 0.1-2 m Na2CO3	(E) pcH = 10.4-10.8		
	(F) G Seep, a synthetic brine similar to GWB	(F) pcH = 5.6-7.8		
	(G) ERDA-6	(G) pcH = 6.2-10.6		
Runde et al. (1992)	0.1 M $NaClO_4$ & 0.0003, 0.01, & 1 atm CO_2	pH = 5.5 – 6.3	$Nd(OH)CO_3$ at 0.0003 atm CO_2, $Nd_2(CO_3)_3$ at 0.01 & 1 atm CO_2	Not considered by Xiong et al. (2004, 2005), because this paper came to their attention after completion of their analyses. Not included in this analysis because only K_{sp}'s reported, not actual solubility data.
Runde & Kim (1995)	(A) 5.0 M NaCl (B) 5.0 m NaCl & 0.01 atm CO2	(A) pcH = 6.7–13.8 (B) pcH = 6.6-9.3	(A) Am(OH)3(cr) (B) NaAm(CO3)3 ·xH2O(cr)	Seventy one results (18 duplicates) included in Xiong et al. (2004, 2005) and this analysis: FMT_CRA1V_Runde95-III_001 through 053.

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Silva (1982)	(A) 0.1 M $NaClO_4$ (B) 0.1 M $NaClO_4$	(A) pH = 5.7-9.5 (B) pH = 7.0-9.4	(A) $Nd(OH)_3(cr)$ (B) $Am(OH)_3(cr)$	Included in Xiong et al. (2004, 2005). Excluded from this analysis because this paper was published prior to 1990.
Wood et al. (2002)	(A) 0.03 m $NaTr^A$ (30 °C)	(A) pmH = 7.01-9.13	$Nd(OH)_3(cr)$	Not considered by Xiong et al. (2004, 2005, 2009) because this paper came to their attention after completion of their analyses. Most results excluded from this revision because T > 30 °C. Fifteen results (no duplicates) included in this revision: FMT_PABC09_PERCHLOR _001 through 015.
	(B) 0.03, 0.10, & 1.0 m $NaTr^A$ (50 °C)	(B) pmH = 6.494–9.548 (I = 0.03 m) pmH = 6.653-6.711 (I = 0.10 m) pmH = 6.681-6.809 (I = 1.0 m)		
	(C) 0.03, 0.10, & 1.0 m $NaTr^A$ (100 °C)	(C) pmH = 5.362–8.421 (I = 0.03 m) pmH = 5.739-5.744 (I = 0.10 m) pmH = 5.857-5.859 (I = 1.0 m)		
	(D) 0.03, 0.010, & 1.0 m $NaTr^A$ (150 °C)	(D) pmH = 4.791-5.890 (I = 0.03 m) pmH = 5.017-5.021 (I = 0.10 m) pmH = 5.139-5.141 (I = 1.0 m)		

[A] Sodium trifluoromethanesulfonate, abbreviated as "sodium triflate" or "NaTr," is a noncomplexing salt used to set the ionic strength. In FMT calculations, the noncomplexing medium, sodium perchlorate, is used as the supporting solution.

Table 9 continued on next page

Table 9. Final Evaluation of Published Papers for Comparisons of Measured and Predicted Am(III) Solubilities (continued).

Reference	Solution(s) and Ionic Strength(s)	pcH, pmH, or pH	Solubility-Controlling Solid	Evaluation and FMT Run Numbers for Results Included in This Analysis
Wood et al. (2002) (continued)	(E) 0.03, 0.10, & 1.0 m NaTr[A] (200 °C)	(E) pmH = 4.419-5.088 (I = 0.03 m) pmH = 4.472-4.473 (I = 0.10 m) pmH = 4.558-4.560 (I = 1.0 m)	See Wood et al. (2002) on previous page.	See Wood et al. (2002) on previous page.
	(F) 0.03, 0.10, & 1.0 m NaTr[A] (250 °C)	(F) pmH = 3.873-4.873 (I = 0.03 m) pmH = 4.050-4.068 (I = 0.10 m) pmH = 4.180-4.182 (I = 1.0 m)		
	(G) 0.03 & 0.10 m (290 °C)	(G) pmH = 3.493–6.898 (I = 0.03 m) pH = 3.406-5.221 (I = 0.10 m)		

[A] Sodium trifluoromethanesulfonate, abbreviated as "sodium triflate" or "NaTr," is a noncomplexing salt used to set the ionic strength.

Meinrath and Takeishi (1993) also measured the solubilities of $Nd_2(CO_3)_3$ and $Nd(OH)CO_3$ in 1 M $NaClO_4$ under atmospheres with various concentrations of CO_2 (Table 9). Xiong et al. (2004, 2005) did not consider these results because this paper came to their attention after they completed their analyses. According to criterion G7 (Section 2), we included all 17 results obtained with 0.1 M $NaClO_4$ under 0.0003 and 0.003 atm CO_2 because $Nd(OH)CO_3$, the solubility-controlling solid in these experiments (Table 9), is in the WIPP Am(III) model. However, we used the same criterion to exclude the results obtained from 0.1 M $NaClO_4$ under 0.01, 0.08, and 1 atm CO_2 because $Nd_2(CO_3)_3$, the solubility-controlling solid in these runs, is not in the model.

Peretrukhin et al. (1996) studied the solubilities of Tc(IV), Tc(V), Np(IV), Np(VI), Pu(III), Pu(IV), Am(III), and Am(VI) in strongly basic solutions. They carried out four experiments with Am(III), two in 1 M NaOH and two in 5 M NaOH (Table 9). Xiong et al. (2004, 2005) did not consider this paper because it came to their attention after they completed their analyses. We predicted Am(III) solubilities about four to six orders of magnitude less than their measured values (Table 10). Because we suspect that these differences were caused by one or more $Am(OH)_x^{3-x}$ complexes with $x > 4$ that were dominant in their experiments, but are not in the WIPP Am(III) model, we used criterion G9 (Section 2) to exclude these measured Am(III) solubilities.

Table 10. Comparison of Am(III) Solubilities Measured by Peretrukhin et al. (1996) with Those Predicted by FMT (This Analysis).

Run Type	Na(OH) Concentration (M)	Am(III) Solubility, Measured (M)	Am(III) Solubility, Predicted (M)
Undersaturation	1.0	5.9×10^{-7}	9.33×10^{-12}
Undersaturation	5.0	3.6×10^{-7}	5.04×10^{-12}
Oversaturation	1.0	6.9×10^{-6}	9.33×10^{-11}
Oversaturation	5.0	6.0×10^{-6}	5.04×10^{-11}

Rao et al. (1996a) measured the solubility of $Nd(OH)_3(cr)$ in 0.1 M NaCl at 25 and 90 °C. Xiong et al. (2004, 2005) did not consider these results because they came to their attention after they completed their analyses. Initially, we decided to include the 25 °C results of Rao et al. (1996a) and exclude their 90 °C results because the latter temperature is too high to be relevant to the WIPP. However, inspection of the 25 °C results showed that those with pH values < 5.8 were essentially independent of pH. This feature is similar to that observed by Xiong et al. 2005) in the results of Felmy et al. (1991) (see the discussion of these results in Subsection 3.1 above). Therefore, according to criterion G7 (Section 2), we included only the 32 solubilities measured by Rao et al. (1996a) at pH values > 5.8.

Rao et al. (1996b) measured the solubility of $NaNd(CO_3)_2 \cdot 6H_2O(cr)$ in $NaHCO_3$ and Na_2CO_3 solutions of various ionic strengths (Table 9). Xiong et al. (2004, 2005) did not consider this paper because it came to their attention after they completed their analyses. We included all 60 results in our analysis.

Rao et al. (1999) carried out solubility experiments with $NaNd(CO_3)_2 \cdot 6H_2O$ in $NaHCO_3$, Na_2CO_3, NaCl-$NaHCO_3$, and NaCl-Na_2CO_3 solutions of various ionic strengths; and in synthetic G Seep (a WIPP brine similar to GWB) and ERDA-6 (Table 9). Xiong et al. (2004, 2005) included all 104 results of this study in their analyses. For our analysis, however, we excluded 28 of the 104 results included by Xiong et al. (2004, 2005) according to criterion G9 because the pcH of the solutions in these experiments exceeded 7.4 or 8.1, the pcH above which Borkowski concluded that complexation of Nd(III) by dissolved borate in GWB or ERDA-6, respectively, is significant. Therefore, we included 76 of the results of Rao et al. (1999) in our analysis.

Runde et al. (1992) measured the solubilities of $Nd(OH)CO_3$ and $Nd_2(C0_3)_3$ under atmospheres with various concentrations of CO_2 (Table 9). Xiong et al. (2004, 2005) did not consider these results because they came to their attention after they completed their analyses. Runde et al. (1992) reported values of K_{sp}s instead of solubilities expressed as concentrations of dissolved Nd(III). Therefore, according to criterion G10 (Section 2), we excluded their results.

Runde and Kim (1995) measured the solubility of $Am(OH)_3(cr)$ in 5.0 M NaCl and that of $NaAm(CO_3)_3 \cdot xH_2O(cr)$ in 5.0 m NaCl under an atmosphere with 0.01 atm CO_2 (Table 9). Xiong et al. (2004, 2005) included all 71 results of this work in their analyses. We also included all 71 results in our analyses.

Silva (1982) conducted solubility experiments with $Nd(OH)_3$ and $Am(OH)_3$ in 0.1 M $NaClO_4$ (Table 9). Xiong et al. (2004, 2005) included all 37 results of this study in their analyses. For our analysis, however, we included only measured solubilities from papers published or unpublished reports issued from January 1, 1990, through December 31, 2008 (criterion G1 in Section 2). Therefore, we excluded the results of Silva (1982) from our analysis.

Wood et al. (2002) performed solubility experiments with $Nd(OH)_3(cr)$ in 0.03, 0.10, and 1.0 m sodium trifluoromethanesulfonate ($NaCF_3SO_3$) solutions at 30, 50, 100, 150, 200, 250, and 290 °C. (Sodium trifluoromethanesulfonate is often abbreviated as “sodium triflate” or “NaTr.”) Wood et al. (2002) used NaTr to set the ionic strength in their experiments because it dissolves to form species that do not complex Nd(III) in aqueous solutions. Xiong et al. (2004, 2005, 2009) did not consider these results because they came to their attention after they completed their analyses. We included the 15 results obtained at 30 °C in this revision, but excluded all results obtained at higher temperatures because they were above the acceptable temperature range of 20–30 °C specified in criterion G5 (Section 2).

Figure 3 provides the histogram for our revised comparison of experimentally measured and predicted Nd(III) and Am(III) solubilities and compares it to those obtained by Xiong et al. (2009) for the CRA-2009 PABC and Xiong et al. (2005) for the CRA-2004 PABC.

The current comparison includes a total of 441 measured and predicted solubilities, an increase of 95 from the 346 measured and predicted solubilities included in the original version of this analysis (Xiong et al., 2009). The revised distribution peaks at Bin 0.90 with a frequency of 32, with a secondary peak at Bin -0.30 (31 comparisons). Table 11 summarizes the statistical parameters of the current frequency distribution and compares them to those of the previous distributions.

Inspection of Table 11 reveals that the WIPP Am(III) model; the thermodynamic database FMT_050405.CHEMDAT (Xiong, 2005), which includes phase 3 but not phase 5; and the speciation and solubility code FMT overpredicted the 441 measured Nd(III) and Am(III) solubilities included in this revision. The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Am(III) solubilities are −0.0740 and −0.0925, respectively (Table 11), and the mean and median values of the sampled uncertainty factor are $10^{-0.0740} = 0.843$ and $10^{-0.0925} = 0.808$. (The WIPP PA codes use actinide solubilities that are the products of the baseline solubilities and the sampled uncertainty factors.)

Xiong et al. (2009) used the same model, database, and code, but obtained a negative skew in the original version of this analysis. (The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Am(III) solubilities were −0.142 and 0.072, respectively (Table 11), and the mean and median values of the sampled uncertainty factor were $10^{-0.142} = 0.721$ and $10^{0.072} = 1.18$. The negative mean implied that the overpredictions outweighed the underpredictions, while the positive median indicated that there were more underpredictions than overpredictions.) Xiong et al. (2005) also used the same model, database, and code, but obtained a positive skew: the positive mean implied that the underpredictions outweighed the overpredictions and the negative median indicated that there were more overpredictions than underpredictions for the 243 comparisons in their analysis.

Table 12 provides values of the corresponding CDF for Nd(III) and Am(III) for this revision and compares them to those obtained in the original version of this analysis for the CRA 2009 PABC by Xiong et al. (2009) and the CRA-2004 PABC by Xiong et al. (2005); Figure 4 shows these CDFs plotted for all three analyses. In this revision, the WIPP Am(III) model, database, and code slightly overpredicted the measured solubilities. In the original version of this analysis, they also slightly overpredicted the measured solubilities, whereas they slightly underpredicted the data used for the CRA-2004 PABC.

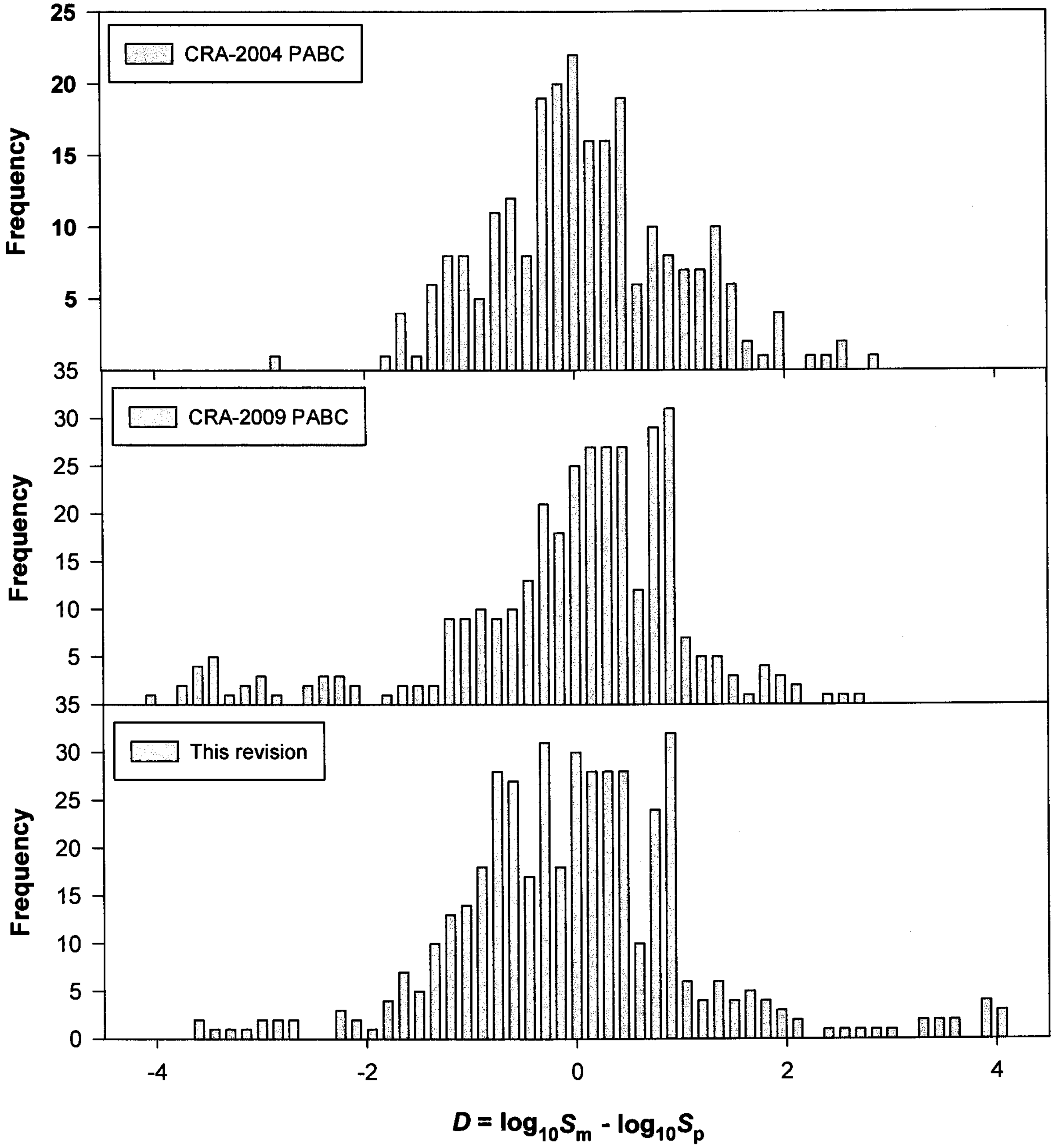

Figure 3. Comparison of the histograms of the difference $D = \log_{10} S_m - \log_{10} S_p$ for Nd(III) and Am(III) for the CRA 2004 PABC, the CRA-2009 PABC, and this revision.

Table 11. Comparisons of Selected Statistical Properties of the Distribution of $D = \log_{10}(S_m) - \log_{10}(S_p)$ for Nd(III) and Am(III) for the CRA-2004 PABC, the CRA-2009 PABC, and This Revision.

Analysis	Mean	Median	Standard Deviation	Minimum	Maximum
CRA-2004 PABC[A]	0.035	−0.031	0.900	−3.00	2.85
CRA-2009 PABC[B]	−0.142	0.072	1.17	−4.20	2.70
This revision[C]	−0.0740	−0.0925	1.19	−3.75	4.05

[A] This probability distribution was used to define the solubility multiplier SOLVAR for the oxidation-state III model material SOLMOD3 in the WIPP PA Parameter Database for the CRA-2004 PABC.

[B] This probability distribution was used to define the solubility multiplier SOLVAR for the oxidation-state III model material SOLMOD3 in the WIPP PA Parameter Database for the CRA-2009 PABC.

[C] This probability distribution was not used for the CRA-2009 PABC.

Table 12. Comparisons of the CDFs of the Differences between Measured and Predicted Nd(III) and Am(III) Solubilities for the CRA-2004 PABC, the CRA-2009 PABC, and This Revision.

X	$P(D < X)$, CRA-2004 PABC[A]	$P(D < X)$, CRA-2009 PABC[B]	$P(D < X)$, This Revision[C]
−4.20	0.0000	0.0000	0.0000
−4.05	0.0000	0.0029	0.0000
−3.90	0.0000	0.0029	0.0000
−3.75	0.0000	0.0087	0.0000
−3.60	0.0000	0.0202	0.0045
−3.45	0.0000	0.0347	0.0068
−3.30	0.0000	0.0376	0.0091
−3.15	0.0000	0.0434	0.0113
−3.00	0.0000	0.0520	0.0159
−2.85	0.0041	0.0549	0.0204
−2.70	0.0041	0.0549	0.0249
−2.55	0.0041	0.0607	0.0249
−2.40	0.0041	0.0694	0.0249
−2.25	0.0041	0.0780	0.0317
−2.10	0.0041	0.0838	0.0363
−1.95	0.0041	0.0838	0.0385
−1.80	0.0082	0.0867	0.0476
−1.65	0.0247	0.0925	0.0635
−1.50	0.0288	0.0983	0.0748
−1.35	0.0535	0.1040	0.0975
−1.20	0.0864	0.1301	0.1270
−1.05	0.1193	0.1561	0.1587
−0.90	0.1399	0.1850	0.1995
−0.75	0.1852	0.2110	0.2630
−0.60	0.2346	0.2399	0.3243
−0.45	0.2675	0.2775	0.3628
−0.30	0.3457	0.3382	0.4331
−0.15	0.4280	0.3902	0.4739
0.00	0.5185	0.4624	0.5420
0.15	0.5844	0.5405	0.6054
0.30	0.6502	0.6185	0.6689
0.45	0.7284	0.6965	0.7324
0.60	0.7531	0.7312	0.7551
0.75	0.7942	0.8150	0.8095

Table 12 continued on next page

Table 12. Comparisons of the CDFs of the Differences between Measured and Predicted Nd(III) and Am(III) Solubilities for the CRA-2004 PABC, the CRA-2009 PABC, and This Revision (continued).

X	$P(D < X)$, CRA-2004 PABC [A]	$P(D < X)$, CRA-2009 PABC [B]	$P(D < X)$, This Revision[C]
0.90	0.8272	0.9046	0.8821
1.05	0.8848	0.9249	0.8957
1.20	0.9259	0.9393	0.9048
1.35	0.9506	0.9538	0.9184
1.50	0.9588	0.9624	0.9274
1.65	0.9630	0.9653	0.9388
1.80	0.9794	0.9769	0.9478
1.95	0.9794	0.9855	0.9546
2.10	0.9835	0.9913	0.9592
2.25	0.9877	0.9913	0.9592
2.40	0.9959	0.9942	0.9615
2.55	0.9959	0.9971	0.9637
2.70	0.9959	1.0000	0.9660
2.85	1.0000	1.0000	0.9683
3.00	1.0000	1.0000	0.9705
3.15	1.0000	1.0000	0.9705
3.30	1.0000	1.0000	0.9751
3.45	1.0000	1.0000	0.9796
3.60	1.0000	1.0000	0.9841
3.75	1.0000	1.0000	0.9841
3.90	1.0000	1.0000	0.9932
4.05	1.0000	1.0000	1.0000
4.20	1.0000	1.0000	1.0000

[A] This CDF was used to define the solubility multiplier SOLVAR for the oxidation-state III model material SOLMOD3 in the WIPP PA Parameter Database for the CRA-2004 PABC.

[B] This CDF was used to define the solubility multiplier SOLVAR for the oxidation-state III model material SOLMOD3 in the WIPP PA Parameter Database for the CRA-2009 PABC.

[C] This CDF was not used for the CRA-2009 PABC.

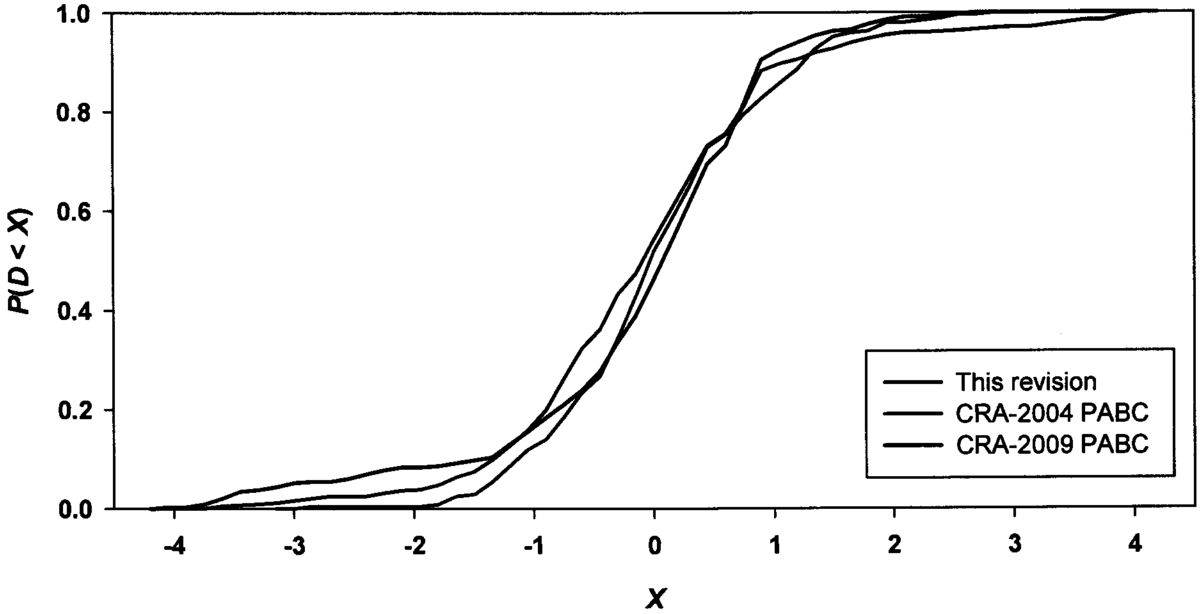

Figure 4. Comparison of plots of the CDFs for Nd(III) and Am(III) for the CRA-2009 PABC, the CRA-2004 PABC, and this revision.

4 CONCLUSIONS

This revision (Rev. 1) of this analysis report documents several changes specified in the CAP for CAR IS-10-02-CAR-01. Section 1 of this revision describes these changes in detail.

This analysis report provides the results of our uncertainty analysis of Th(IV) and Am(III) solubilities for the CRA-2009 PABC. The analysis described in this report was carried out under Task 2 of Brush and Xiong (2009a, Subsection 4.2).

The Th(IV) and Am(III) uncertainty ranges and probability distributions resulting from this analysis will replace those used for the CRA-2009 PA, which were established by Xiong et al. (2005) for the CRA-2004 PABC. The ranges and distributions from this report will become part of the new WIPP PA baseline when approved by the EPA.

The Th(IV) comparison included a total of 140 measured and predicted solubilities, an increase of 95 from the 45 comparisons of Xiong et al. (2005) for the CRA-2004 PABC. The WIPP Th(IV) model overpredicted the measured solubilities in the current analysis. The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Th(IV) solubilities are −0.346 and −0.520, respectively (see Table 7), and the mean and median values of the sampled uncertainty factor are $10^{-0.346} = 0.450$ and $10^{-0.520} = 0.302$. (PA codes use actinide solubilities that are the products of the baseline solubilities and the sampled uncertainty factors). Xiong et al. (2005) used the same model, database, and code; but slightly underpredicted the measured solubilities in their analysis.

The revised Nd(III) and Am(III) comparison included a total of 441 measured and predicted solubilities, an increase of 95 from the 346 comparisons of Xiong et al. (2009) for the CRA-2009 PABC. The revised comparison overpredicted the measured solubilities. The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Am(III) solubilities are −0.0740 and −0.0925, respectively (Table 11), and the mean and median values of the sampled uncertainty factor are $10^{-0.0740} = 0.843$ and $10^{-0.0925} = 0.808$ (Table 11). Xiong et al. (2009) used the same model, database, and code; but the results were negatively skewed in the original version of this analysis. (The mean and median values of the log of the sampled uncertainty factor used to adjust the baseline Am(III) solubilities were −0.142 and 0.072, respectively).

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Xiong, Yongliang Yongliang Xiong

From: Domski, Paul S
Sent: Monday, January 24, 2011 9:16 AM
To: Xiong, Yongliang
Subject: RE: Signature Authority for Uncertainty Analysis, Rev. 1

Dear Yongliang,

I hereby authorize you to sign for me as a review requester on any of the Document Review and Comment Forms, NP 6-1-1, if necessary; and as a coauthor on my approval line on page 1 of our analysis report entitled "Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2009 PABC, Rev. 1. Supersedes ERMS 552500" while I am out of my Carlsbad office in January 2011.

Thanks.

Paul Domski
S.M. Stoller Corp
(505) 604-6736

From: Xiong, Yongliang
Sent: Friday, January 21, 2011 4:19 PM
To: Domski, Paul S
Subject: FW: Signature Authority for Uncertainty Analysis, Rev. 1

Paul,

Please also send your signature authority.

Yongliang

From: Brush, Laurence H
Sent: Friday, January 21, 2011 12:12 PM
To: Xiong, Yongliang
Cc: Leigh, Christi D
Subject: Signature Authority for Uncertainty Analysis, Rev. 1

Yongliang,

I hereby authorize you to sign for me as a review requester on any of the Document Review and Comment Forms, NP 6-1-1, if necessary; and as a coauthor on my approval line on page 1 of our analysis report entitled "Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2009 PABC, Rev. 1. Supersedes ERMS 552500" while I am out of my Carlsbad office in January 2011.

I will send you the final version of this analysis report after Christi has approved it. Please print out or have Shannon print out this version for submittal to the Sandia/WIPP Records Center. It will be correctly paginated, and the table of contents and lists of figures and tables will be updated.

I have attached a copy of the final, revised spreadsheet to this e-mail message for Shannon to print out and put in Records

Thank you very much in advance!

Larry Brush

Chavez, Mario Joseph Mario Chavez

From: Long, Jennifer J
Sent: Monday, January 24, 2011 11:43 AM
To: Chavez, Mario Joseph
Subject: Signature Authority

Mario,

I give you signature authority for the Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2009 PABC, Rev. 1 analysis.

Thanks!
Jennifer Long

Chavez, Mario Joseph Mario Chavez

From: Clayton, Daniel James
Sent: Friday, January 07, 2011 7:52 AM
To: Brush, Laurence H; Chavez, Mario Joseph
Subject: RE: Our Report and Your DRC

Looks good, here is the updated DRC

2011 01 06_Xio et
al Uncer Ana...

Mario,

I give you signature authority for the Uncertainty Analysis of Actinide Solubilities for the WIPP CRA-2009 PABC, Rev.1 analysis and related DRCs

Dan Clayton

From: Brush, Laurence H
Sent: Thursday, January 06, 2011 2:07 PM
To: Clayton, Daniel James
Subject: Our Report and Your DRC

Daniel,

I think we have fixed everything that you identified in your recent review. Thank you very much!

Larry

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Casey, Shannon Leigh Shannon Casey

From: Leigh, Christi D
Sent: Monday, January 24, 2011 2:12 PM
To: Casey, Shannon Leigh
Subject: RE: Uncertainty Analysis, Rev. 1

I give Shannon Casey signature authority for the document on my behalf.

Christi Leigh

From: Casey, Shannon Leigh
Sent: Monday, January 24, 2011 11:46 AM
To: Leigh, Christi D
Subject: RE: Uncertainty Analysis, Rev. 1

Christi,

You also need to give someone authority to sign the document on your behalf.

Thanks!
Shannon

From: Leigh, Christi D
Sent: Monday, January 24, 2011 10:31 AM
To: Casey, Shannon Leigh
Subject: FW: Uncertainty Analysis, Rev. 1

To Whom It may Concern:

I accept the changes that have been made to this document and I give Shannon Casey signature authority on this DRC

Christi Leigh

From: Brush, Laurence H
Sent: Friday, January 21, 2011 12:11 PM
To: Leigh, Christi D
Subject: Uncertainty Analysis, Rev. 1

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