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Defense Waste Management Programs
4100 National Parks Highway
Carlsbad, NM 88220

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to: Russell Chris Camphouse, (08881) rccamph@sandia.gov

from: Ramesh Sarathi, (08881) rsarath@sandia.gov

subject: ***Explanation of CAPMIC definition and usage in PA calculations***

This memo is intended to address recent questions regarding how the parameter CAPMIC (which is used in calculating mobile actinide concentration limits) is defined and employed in Performance Assessment (PA) calculations. It clarifies the original intent of CAPMIC, explains how it is used, gives examples of where it is inconsistently defined, and recommends a path forward to resolve issues.

Historical Definition and Usage of CAPMIC

Conflicting and misleading definitions of CAPMIC date back to the 1996 CCA Appendix SOTERM (SOTERM-1996) and the original Parameter Record Package for Colloidal Actinide Source Term Parameters (Papenguth 1996). The intended definition of CAPMIC is given in SOTERM-1996 (page 68, lines 24-37) and the Parameter Record Package (pdf-page 11) as part of the discussion of how the experimental data is used to determine values for the parameters PROPMIC and CAPMIC:

> *The CAPMIC value is defined as the actinide concentration in molarity at which no growth* [of microbes] *was observed. For cases where growth clearly diminished as actinide concentration increased, but the actinide concentration was not great enough to stop growth, CAPMIC values were determined by linear extrapolation of population numbers, and then adding an order-of-magnitude to account for uncertainty. ...it appears that the toxicity effects are due to chemical toxicity rather than radiotoxicity.*

The discussion in SOTERM-1996 continues (page 68, lines 33-37) and explains how CAPMIC is intended to be used in PA calculations:

> *CAPMIC values are used similarly to the CAPHUM values ..., except that the upper limit for microbe concentration is due to toxicity rather than geometric limitations imposed by the colloid itself. Consequently, for microbes, the total concentration of mobile actinides in a performance assessment realization is used in the comparison, rather than the amount of actinides associated with the microbes.*

This statement clearly establishes that CAPMIC is defined with respect to the total amount of dissolved/dispersed actinide in the system. This is reflected in the footnotes of Table SOTERM-14 (page 69, SOTERM-1996) and in the notes for the table on pdf-page 22 of the Parameter Record Package:

> *[CAPMIC is defined in] units of moles total mobile actinide per liter,*

and,

> *CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e. the sum of dissolved plus colloidal actinide).*

Table 2 "Microbe toxicity results" on pdf-page 15 of the Parameter Record Package gives further details on how the CAPMIC parameters are derived from the toxicity experiment data.

The equations used in PA to calculate the microbial colloid solubility limit enhancement term were correspondingly formulated on the basis that CAPMIC is defined as a total mobile actinide concentration. The equations used in the CCA are outlined in SOTERM-1996 (excerpt from page 77, lines 13-15):

9 *Dissolved* = **Model Solubility** * 10 ***Sampled from Solubility Distribution***

10 ***Humic = Dissolved * Proportionality Constant***
11 if ***Dissolved * Prop. Const.*** < **Humic Cap**, otherwise
12 **Humic = Humic Cap**

13 ***Microbe*** = ***Dissolved*** * **Proportionality Constant**
14 if the ***Total Mobile*** < **Microbe Cap**, otherwise
15 **Microbe = Microbe Cap**

16 **Mineral = Database Concentration**

17 **Intrinsic = Database Concentration**

18 ***Total Mobile = Dissolved + Humic + Microbe*** + Mineral + Intrinsic

Figure 1 –Equations to calculate the total mobile actinide concentration limit as specified in the CCA

The actual code (an ALEGEBRA input file) used to calculate the Total Mobile (variable TOTSOL) and the Microbe (variable MIC) terms outlined above is given in Appendix-PANEL of the 1996 CCA (PANEL-1996) (excerpt from page 35):

```
!AM=32,SOLMOD3=45,SOLAM3=53,PHUMOX3=49
LIMIT BLOCKS 32
DIS=MAKEPROP(10**SOLSIM[B:53]*SOLSIM[B:45])
HUM=MAKEPROP(MIN(CAPHUM,10**SOLSIM[B:53]*SOLSIM[B:45]*PHUMSIM[B:49]))
MIC1=MAKEPROP(10**SOLSIM[B:53]*SOLSIM[B:45]*PROPMIC)
TOT=MAKEPROP(DIS+HUM+MIC1+CONCINT+CONCMIN)
TOTNM=MAKEPROP(DIS+HUM+CONCINT+CONCMIN)
TOTSOL = MAKEPROP(IFLT0(CAPMIC-TOT,MIN(TOTNM+CAPMIC,TOT),TOT))
MIC= MAKEPROP(IFLT0(CAPMIC-TOT,TOTSOL-TOTNM,MIC1))
LOGSOLM=MAKEPROP(LOG10(TOTSOL))
```

Figure 2 – ALGEBRA code listing for the total mobile actinide concentration limits as specified in the CCA

Unfortunately, there are multiple issues with the formulations in both listings. Line 14 in Figure 1 is consistent with the concept that CAPMIC is a total mobile actinide concentration. Line 15, however, employs CAPMIC as if it were a microbe-associated actinide concentration rather than a total mobile actinide concentration. Thus the formulation in SOTERM-1996 simultaneously and erroneously uses two different definitions for CAPMIC in the same equation. The equations in the CCA ALGEBRA file listing (Figure 2) contain flawed logic and simplify to *Microbe = minimum(Dissolved * Proportionality Constant, Microbe Cap)*, regardless of how *Total Mobile* compares to *Microbe Cap.*

These flaws appear to have been recognized and partially addressed in 1998. A Corrective Action Request (CAR) (W-98-003, ERMS 249852) was filed that identified that "there is a logic error in putting the cap on microbial colloid concentrations" and that "it should be compared to total radionuclide concentrations, not just microbial concentrations." Following the CAR, the code PANEL was modified (in version 4.00) so that it performed the total mobile concentration limit calculations internally (previously the calculations were performed as a pre-processing step using ALGEBRA) and to address the inconsistent logic. The contemporaneous PANEL Design Document (PANEL-4.00-DD) lists the equations as (page 33):

Dissolved Solubility = **Model Solubility** * 10 ^*Sampled from Solubility Distribution*

Humic Colloid Concentration = *Dissolved Solubility* * ***Proportionality Constant***
if *Dissolved* * ***Prop. Const.*** < **Humic Cap.** otherwise
Humic Colloid Concentration = **Humic Cap**

Microbe Colloid Concentration = *Dissolved Solubility* * **Proportionality Constant**
if the *Total Mobile* < **Microbe Cap.** otherwise
Microbe Colloid Concentration = **Max (0, microbe cap - Dissolved - Himic - Mineral)**

Mineral Colloid Concentration = **Database Concentration**

Intrinsic Colloid Concentration = **Database Concentration**

Total Mobile = *Dissolved* + *Humic* + *Microbe* + Mineral + Intrinsic

LOGSOLM = log_{10}(*Total Mobile*)

Figure 3 – Equations to calculate the total mobile actinide concentration limit as specified in the PANEL DD.

Note that the comparison of *Total Mobile* to *Microbe Cap* remains, but the equation for the *Microbe Colloid Concentration* has changed (although the printed equation erroneously omits the intrinsic colloid contribution). No discussion of the change or the equations is given in the Design Document, but the equations are discussed in later Analysis Package reports. Garner (2003) (page 7) states:

> *The mobilized concentration for microbial colloids is zero if there is no microbial activity. If microbial activity is present, the* [microbial-bound actinide] *concentration is obtained by multiplying the dissolved component by the value of PROPMIC. However, the microbial colloidal* [actinide] *concentration cannot make the total mobilized concentration exceed the value of CAPMIC.*

This explains the *max(0, microbe cap - Dissolved - Humic - Intrinsic - Mineral)* term. Additional discussion of the microbial colloid actinide concentration enhancement equation and CAPMIC is given in Garner and Leigh (2005) (page 23).

Before discussing the details of the equations further, it is important to clarify their context in PA calculations. These equations <u>are not</u> used to calculate time-varying concentrations over the course of a simulation. Rather, these equations are used to calculate a fixed concentration limit (i.e. a pseudo-solubility limit that includes both the "dissolved" solubility and the mobile concentration enhancements due to dispersed colloids). This value is constant over the course of a single simulation but variable <u>between</u> model realizations because the dissolved solubility limit is multiplied by an uncertainty modifier (SOLVAR), a parameter that is sampled probabilistically.

Returning to the equations, the microbial colloid contribution term can be divided into three regions:

1. if (Dissolved+Humic+Mineral+Intrinsic+Dissolved*PROPMIC) < CAPMIC, then Microbial = Dissolved*PROPMIC
2. if (Dissolved+Humic+Mineral+Intrinsic) < CAPMIC but (Dissolved+Humic+Mineral+Intrinsic+Dissolved*PROPMIC) > CAPMIC, then Microbial = CAPMIC - (Dissolved+Humic+Mineral+Intrinsic)
3. if (Dissolved+Humic+Mineral+Intrinsic) > CAPMIC, then Microbial = 0

The terms *Dissolved*, *Humic*, *Microbial*, *Mineral*, and *Intrinsic* each refer to the respective and additive contributions to the total mobile concentration limit for a particular model realization. These equations, and the code contained in PANEL, simplify to:

$$Microbial = min[(Dissolved * PROPMIC), max(0, CAPMIC - (Dissolved + Humic + Mineral + Intrinsic))].$$

The entire term $max(0, CAPMIC - (Dissolved + Humic + Mineral + Intrinsic))$ is the "cap" on the microbe-bound portion of the total mobile concentration limit, and the value varies between realizations because the *Dissolved* (and *Humic*) terms vary between realizations.

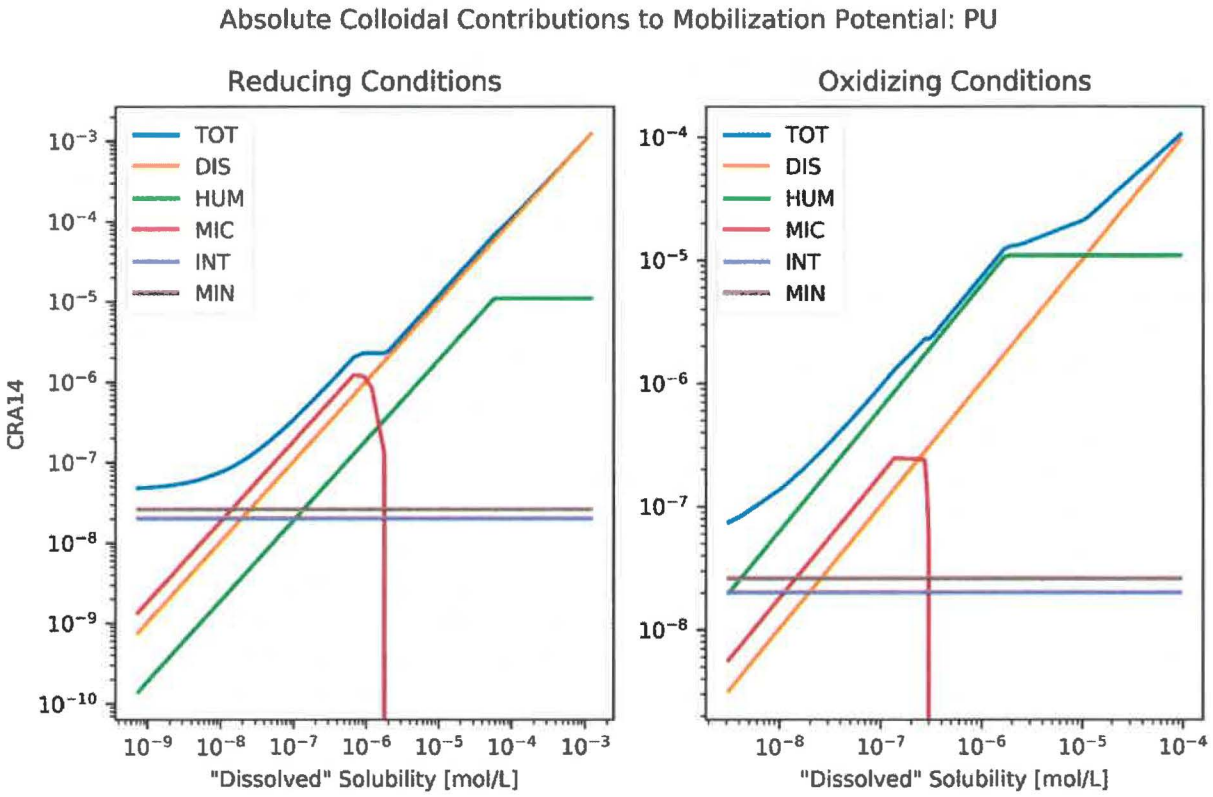

Figure 4 – Contributions to the total mobile concentration limit as a function of sampled dissolved solubility limit, CRA14 data

The red lines in Figure 4 show the mobile concentration enhancement due to microbial colloids for Pu(III) (left) and Pu(IV) (right) as a function of the Pu dissolved solubility limit values used across the CRA-2014 model realizations. The three conditionals produce a "/_" shape (the kinks near the top of the caret are artifacts of the limited number of sampled points (i.e. the limited number of CRA-2014 model realizations) used to produce the graph). The microbial contribution increases linearly, reaching a maximum when the dissolved contribution is such that $(Dissolved + Humic + Mineral + Intrinsic + Dissolved * PROPMIC) = CAPMIC$. After this point, the microbial contribution decreases sharply to zero. In those model realizations where *Dissolved+Humic+Mineral+Intrinsic* exceeds CAPMIC, there is no microbial colloid enhancement to the total mobile concentration.

Considering that CAPMIC is defined akin to a toxicity limit, and that these equations are used to calculate fixed total mobile concentration limits and not time-varying concentrations, the behavior where the microbial contribution decreases to zero is reasonable. PROPMIC, the proportionality constant between microbe-bound actinides and dissolved actinides, is defined assuming a constant bounding concentration of microbes in the brine in the waste panels. In those realizations where the dissolved solubility limit causes the total mobile concentration limit to be greater than the toxicity limit, one would expect the concentration of microbes in the brine in the waste panels to be smaller (i.e. microbe growth is limited), thus PROPMIC to be smaller, and the microbial contribution to be smaller. The $max(0, CAPMIC - (Dissolved + Humic + Mineral + Intrinsic))$ term achieves this same effect without directly altering PROPMIC.

Inconsistencies in CAPMIC Definition and Usage

While inconsistencies in the definition of CAPMIC and in the microbial colloid enhancement equations were rectified from 1998 forward in the PANEL source code, PANEL documentation (PANEL-4.00-DD), and PANEL Analysis Package reports (Garner 2003, Garner and Leigh 2005, Kim 2013), various inconsistencies remained in other documents. For example, the Parameter Record Package (pdf-page 2 of Papenguth 1996) defines CAPMIC as the "maximum concentration of each actinide associated with mobile microbes" with units "moles microbe-bound actinide per liter of dispersion," Table SOTERM-8 (page 46 of SOTERM-1996) refers to CAPMIC as the "maximum (cap) concentration of actinide associated with mobile microbes," and Table SOTERM-14 (page 69) refers to CAPMIC as the "maximum sorbed on microbes." These are also the definitions found in the PA Parameter Database and in subsequent versions of SOTERM (pages 30 and 51 of SOTERM-2004, pages 82 and 83 of SOTERM-2009, and pages 99 and 100 of SOTERM-2014). Those descriptions and definitions are in direct conflict with the definition of CAPMIC as "the actinide concentration in molarity at which no growth [of microbes] was observed" as set forth in alternate sections of the 1996 CCA SOTERM (SOTERM-1996, page 68) and the Parameter Record Package (Papenguth 1996, pdf-page 11). The conflicting definitions have different unit bases in addition to different meanings.

Similarly, the equations involving CAPMIC were not updated and corrected for SOTERM-2004 (page 56) or SOTERM-2009 (page 90) (and remained identical with what was published in SOTERM-1996), but were updated in SOTERM-2014 to be consistent with those used in PANEL (excerpt from page 108):

4 Dissolved = Baseline Solubility × 10 Sampled from Solubility Uncertainty Distribution (SOTERM.74)

5 IF (Dissolved × Proportionality Constant of Humic Colloids < Humic Cap),
6 THEN Humic = Dissolved × Proportionality Constant of Humic Colloid, (SOTERM.75)

7 ELSE Humic = Humic Cap

8 Mineral = Database Concentration (a constant value) (SOTERM.76)

9 Intrinsic = Database Concentration (a constant value) (SOTERM.77)

10 Microbial_temp = Dissolved × Proportionality Constant of Microbial Colloids,
11 Total Mobile_temp = Dissolved + Humic + Microbial_temp + Mineral + Intrinsic

12 IF (Total Mobile_temp < Microbial Cap),
13 THEN Microbial = Microbial_temp. (SOTERM.78)

14 ELSE IF((Dissolved + Humic + Mineral + Intrinsic) > Microbial Cap),
15 THEN Microbial = 0
16 ELSE Microbial = Microbial Cap – (Dissolved + Humic + Mineral + Intrinsic)

17 Total Mobile = Dissolved + Humic + Microbial + Mineral + Intrinsic (SOTERM.79)

Figure 5 – Excerpt from SOTERM-2014, page 108, describing the concentration limit equations

While the divergence between the PANEL documentation and reports and Appendix SOTERM has generated much confusion, the usage of the CAPMIC parameter in PANEL was consistent with its definition and units from 1998 through 2014 as a toxicity limit.

Redefinition of CAPMIC in SOTERM-2014

However, SOTERM-2014 included a redefinition of the basis of CAPMIC (page 84) (also see Reed et al 2013, pages 74-75):

- *Fourth, CAPMIC values were changed for all elements to a concentration based on microbial biomass and sorption capacity. This adds more realism to the model and accounts for variability in the toxicity data – which was used in prior CRAs to determine this value.*
- *Fifth, a biomass-based number was used for CAPMIC. The new biomass-based CAPMICs are less than the total mobile values in the case of the +3 oxidation state.*

This redefinition of CAPMIC, from a toxicity limit to a sorption capacity, while physically and experimentally reasonable, causes multiple issues in the context of PA.

The first issue is that this redefinition of the CAPMIC basis is inconsistent with the equations in PANEL that utilize CAPMIC. Not only was CAPMIC derived from toxicity experiments; the concentration limit equations were developed to employ CAPMIC as if it were akin to a toxicity limit, not a sorption limit. Furthermore, because the unit basis changed from a *total mobile actinide concentration* to a *microbe-associated actinide concentration,* the unit basis is not consistent with the equations.

The redefinition, however, is consistent with the mistaken definition of CAPMIC as the *maximum concentration of actinide associated with mobile microbes* as is implied in SOTERM-2009 (and prior SOTERM documents). Thus, this change in units makes the new CAPMIC units consistent with the description in the parameter database (prior to the 2014 change, the units described in the database were inconsistent with the actual units for CAPMIC).

The second issue is that, because of the redefinition of the CAPMIC basis and the ensuing inconsistency with the PANEL equations, the calculated microbial colloid solubility enhancement terms were underpredicted for CRA-2014.

Impact Assessment

For illustration purposes, let us define two different CAPMIC variables: CAPMIC_TOT will correspond to the original CAPMIC that is defined with respect to the total mobile actinide concentration limit, and CAPMIC_ADS will correspond to the modified CAPMIC that is defined with respect to the microbial colloid associated actinide concentration limit. We can then construct a relationship between the two values and calculate CAPMIC_TOT values from the CAPMIC_ADS values supplied in CRA-2014. To do so, we first use CAPMIC_ADS and PROPMIC to solve for the *dissolved* solubility limit at which CAPMIC_ADS becomes limiting: $DIS = CAPMIC\_ADS/PROPMIC$. We then calculate the total mobile actinide concentration limit corresponding to this dissolved solubility, which is CAPMIC_TOT.

I.e., the equation

$$TOTAL\ MOBILE = DISSOLVED + HUMIC + MICROBIAL + MINERAL + INTRINSIC$$

becomes:

$$CAPMIC\_TOT = (CAPMIC\_ADS/PROPMIC) + min(CAPMIC\_ADS/PROPMIC * PHUM, CAPHUM) + CAPMIC\_ADS + CONCMIN + CONCINT.$$

Table 1 – Comparison of CAPMIC_ADS and CAPMIC_TOT values using CRA-2014 and Salado brine parameters

Element/ Valency	SOLSOH	CONCMIN	CONCINT	PHUM	CAPHUM	PROPMIC	CAPMIC _ADS	Calculated CAPMIC _TOT
	mol-dissolved-actinide/L	mol-mineral-associated-actinide/L	mol-colloidal-actinide/L	mol-humic-associated-actinide/mol-dissolved-actinide	mol-humic-associated-actinide/L	mol-microbe-associated-actinide/mol-dissolved-actinide	mol-microbe-associated-actinide/L	mol-total-mobile-actinide/L
	(Salado brine only)			(Salado brine only)				(Salado brine only)
Th(IV)	6.05E-08	2.60E-08	2.00E-08	6.30E+00	1.10E-05	1.76E+00	2.30E-06	1.19E-05
U(IV)	6.05E-08	2.60E-08	3.00E-08	6.30E+00	1.10E-05	1.76E+00	2.30E-06	1.19E-05
U(VI)	1.00E-03	2.60E-08	3.00E-08	1.20E-01	1.10E-05	1.76E+00	2.30E-06	3.82E-06
Np(IV)	6.05E-08	2.60E-08	2.00E-08	6.30E+00	1.10E-05	1.76E+00	2.30E-06	1.19E-05
Np(V)	2.77E-07	2.60E-08	2.00E-08	9.10E-04	1.10E-05	1.76E+00	2.30E-06	3.65E-06
Pu(III)	2.59E-06	2.60E-08	2.00E-08	1.90E-01	1.10E-05	1.76E+00	2.30E-06	3.90E-06
Pu(IV)	6.05E-08	2.60E-08	2.00E-08	6.30E+00	1.10E-05	1.76E+00	2.30E-06	1.19E-05
Am(III)	2.59E-06	2.60E-08	4.00E-09	1.90E-01	1.10E-05	3.20E-01	3.10E-08	1.76E-07

Note, the source of this data is the WIPP PA Parameter Database. There are slight discrepancies compared to Table SOTERM-21 (SOTERM-2014, page 100). That table erroneously lists the CONCINT value for U(IV) as 2e-8 (it should be 3e-8, the same as for U(VI)). It also lists the CONCINT value for Np(V) as ND (not derived). The Np(IV) value is used for Np(V).

Table 1 lists the CAPMIC_TOT values corresponding to the CAPMIC_ADS values that were defined for CRA-2014. Note that these example calculations were done for Salado brine only (the brine-specific parameters are noted) and using CRA-2014 parameter values. The baseline solubilities (SOLOH) are also included in the table for reference, but are not used in calculating CAPMIC_TOT. As expected, the calculated CAPMIC_TOT values are larger than the CRA-2014 CAPMIC_ADS values. This indicates that the microbial colloid actinide concentration limits were underpredicted because they were capped using values with inconsistent units.

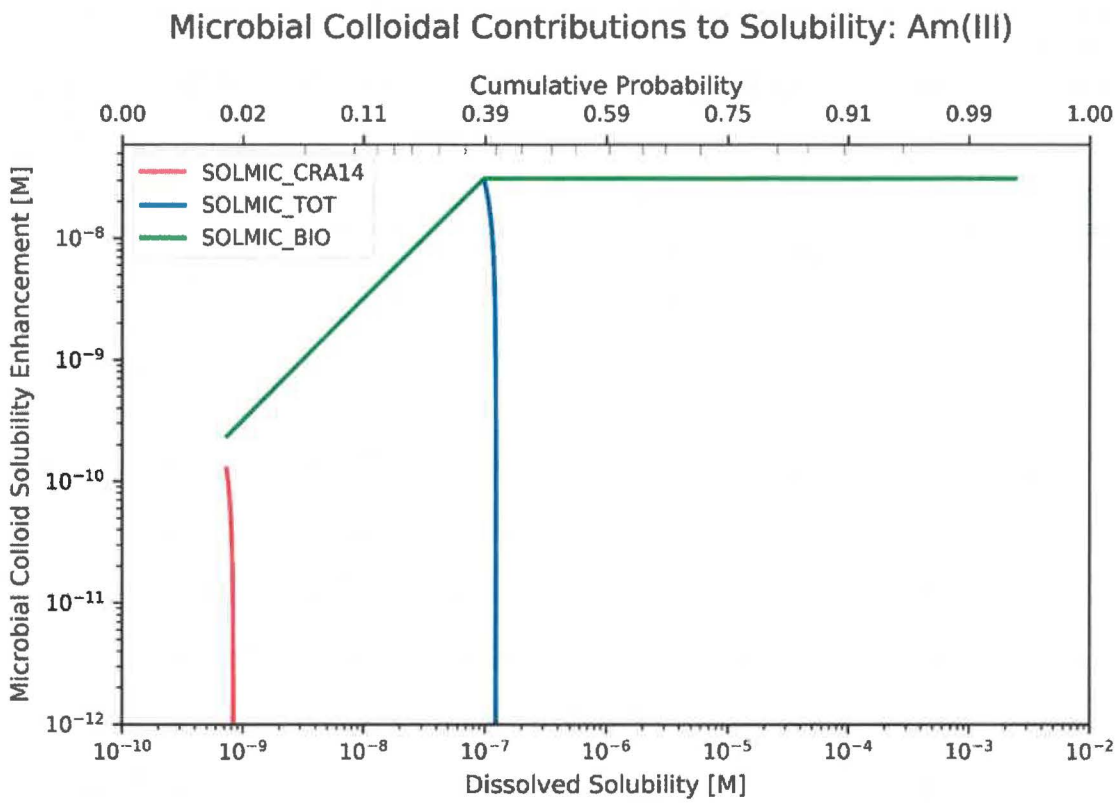

Figure 6 – Microbial colloid enhancement term for Am(III) calculated using CAPMIC_ADS, CAPMIC_TOT

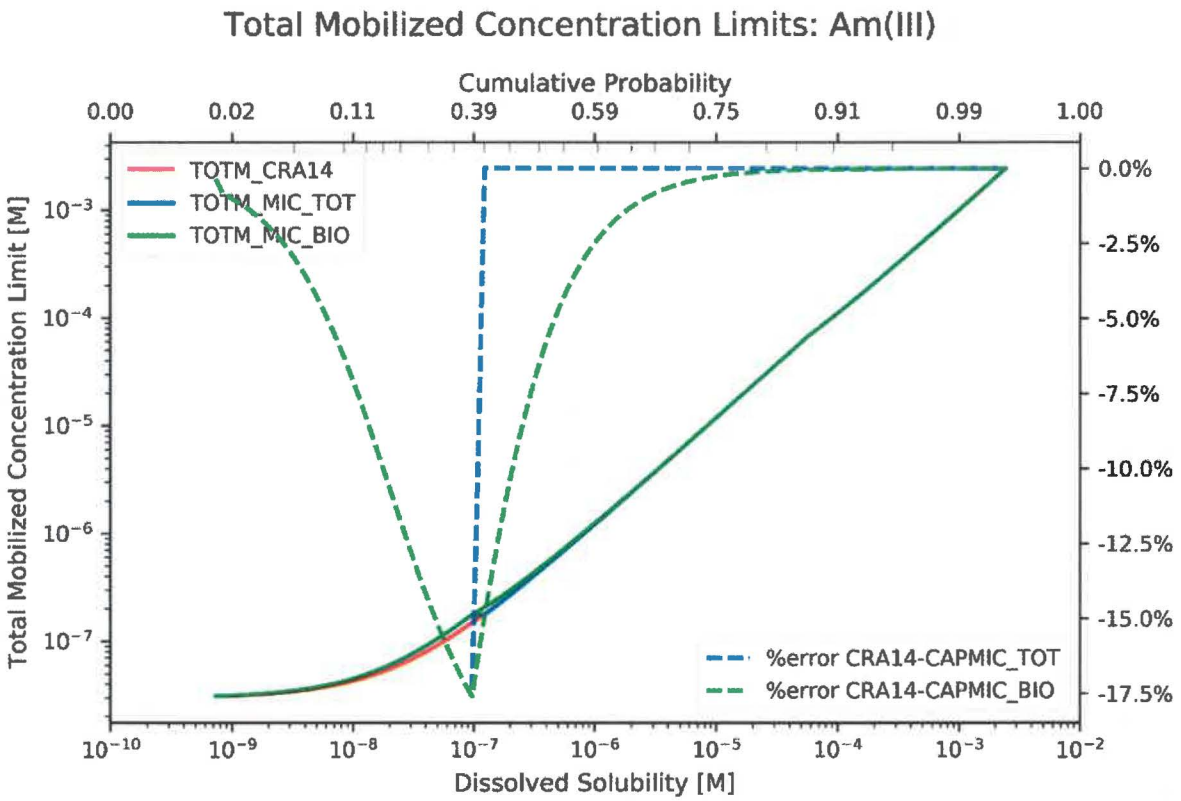

Figure 7 – Total mobile concentration limit for Am(III) calculated using CAPMIC_ADS,. CAPMIC_TOT

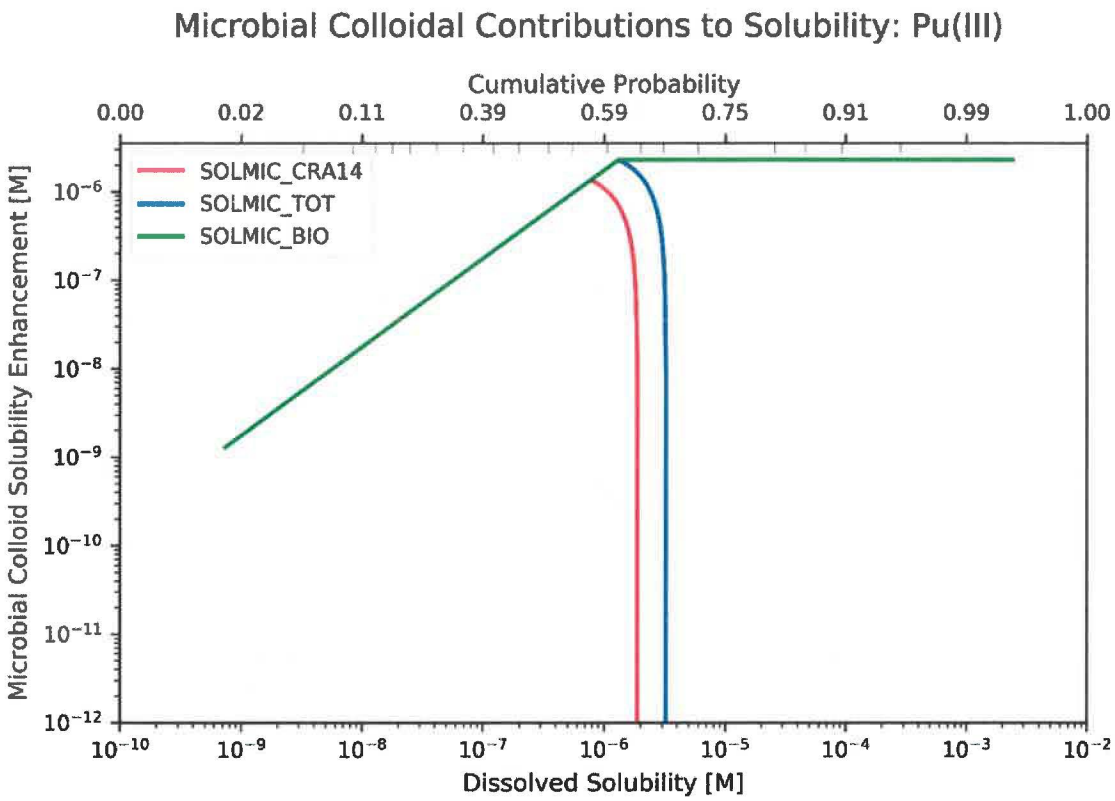

Figure 8 – Microbial colloid enhancement term for Pu(III) calculated using CAPMIC_ADS, CAPMIC_TOT

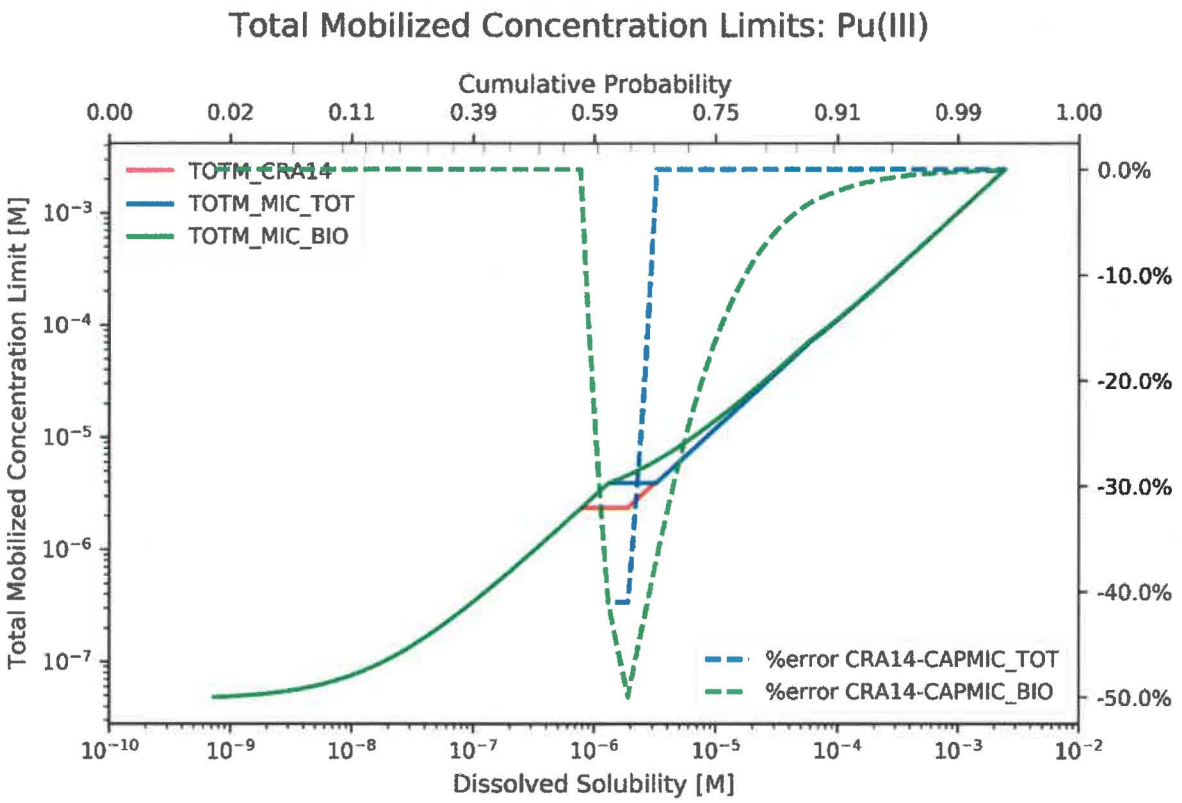

Figure 9 – Total mobile concentration limit for Pu(III) calculated using CAPMIC_ADS, CAPMIC_TOT

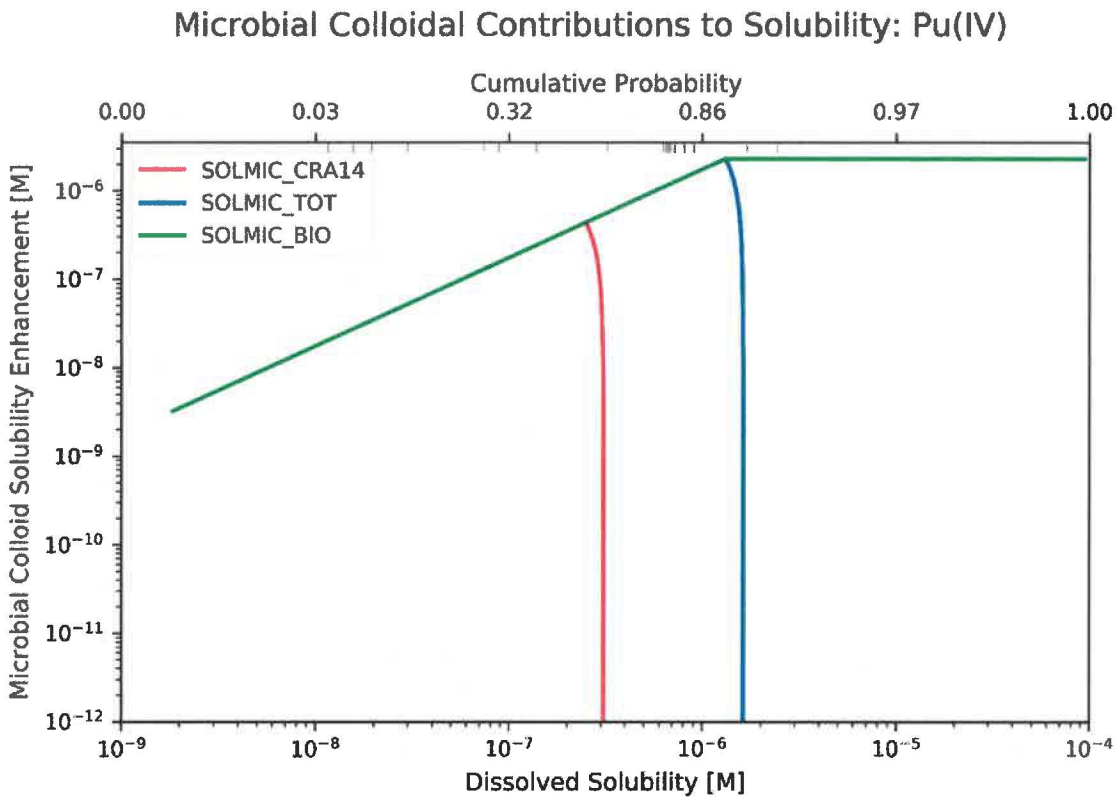

Figure 10 – Microbial colloid enhancement term for Pu(IV) calculated using CAPMIC_ADS, CAPMIC_TOT

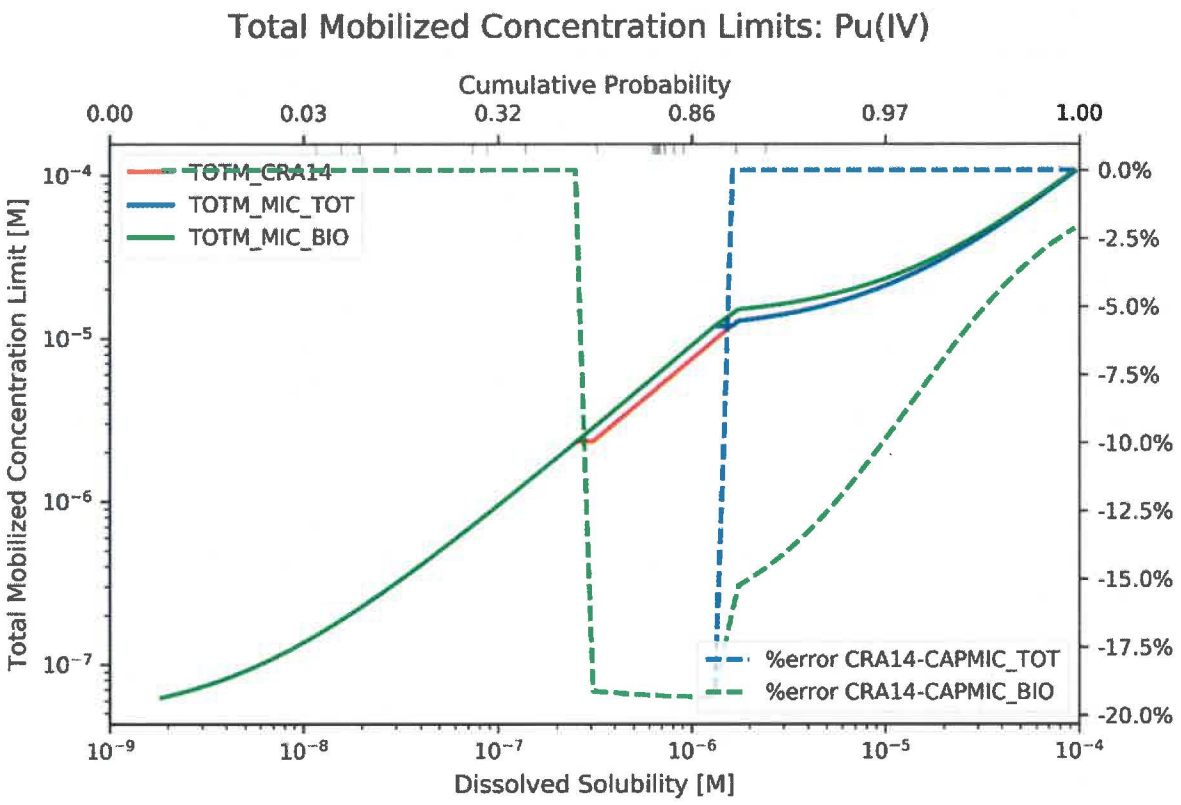

Figure 11 – Total mobile concentration limit for Pu(IV) calculated using CAPMIC_ADS, CAPMIC_TOT

Figure 6, Figure 8, and Figure 10 show the microbial colloid enhancement term as a function of the stochastic dissolved solubility limit, for Am(III), Pu(III), and Pu(IV). The red curves illustrate the microbial colloid enhancement terms as calculated in CRA-2014 (i.e. using the biomass-based CAPMIC values (CAPMIC_ADS in Table 1) with units microbe associated actinide per liter along with the equation in PANEL that requires CAPMIC to have units of total mobile actinide per liter). The blue and green curves illustrate two possible alternatives for making the units consistent between the parameter CAPMIC and the equation that employs it. The blue curves were generated using the CAPMIC_TOT values (i.e. CAPMIC_ADS values with units adjusted to total mobile actinide per liter) along with the currently implemented microbial colloid enhancement equation. The green curves were generated using the CAPMIC_ADS values directly, but the equation was changed to apply the cap directly on the quantity *Dissolved*PROPMIC* (as was intended when the biomass-based values were derived). Both methods result in the cap being enforced at the same dissolved solubility limit value. However, the currently implemented equation causes the microbial enhancement to drop to zero after the cap is reached while the altered equation causes the value to plateau at the capped value.

For Am(III), the CAPMIC_ADS value is so low that, with the CRA-2014 method (red curve), there is no microbial colloid contribution to the total mobile actinide concentration over the vast majority of the range of sampled/calculated dissolved solubility limit values. This is not the case when applying CAPMIC_TOT values or when using the modified equation. For Pu(III) and Pu(IV), both CAPMIC_ADS and CAPMIC_TOT are large enough that microbial colloids contribute to mobility enhancement.

The impact of the difference between the methods is better captured in Figure 7, Figure 9, and Figure 11. Those figures show the resulting total mobile concentration limits as a function of the stochastic dissolved solubility limit (solid curves) and the percent error in the CRA-2014 total mobile concentration limits (dashed curves) for Am(III), Pu(III), and Pu(IV). The x-axis at the top of the figure shows the cumulative probability corresponding to dissolved solubility (bottom x-axis). For Am(III), errors (of underprediction) greater than 10% but less than a maximum of 18% occur at low dissolved solubilities and over a small portion of the distribution. Because the errors occur over a small percentage of realizations, and because the errors both are small and occur over small solubility limit values (i.e. low consequence values), the impact on Am(III) releases will be minimal. For Pu(III), errors greater than 10% but less than a maximum of 50% occur at higher dissolved solubilities, and, for the alternative equation (green curves), over a large portion of the distribution. For Pu(IV), errors greater than 10% and less than a maximum of 20% occur over a wide portion of the distribution.

Regarding other radionuclides, the results for Th(IV), U(IV), and Np(IV) will be similar or identical to the Pu(IV) (the only difference is that U(IV) has a slightly higher CONCINT value; the parameters are otherwise identical). Both U(VI) and Np(V) have constant dissolved solubility limits in PA (there is no solubility uncertainty modifier for the V or VI valencies). For U(VI), the dissolved solubility limit is large enough (1e-3 mol/L, as mandated by the EPA) that CAPMIC is enforced, but the resulting microbial enhancement term is negligible in comparison. For Np(V), the *Dissolved *PROPMIC* term is small enough that neither CAPMIC_ADS nor CAPMIC_TOT is evoked. Thus the inconsistent CAPMIC definition has no impact on either U(VI) or Np(V) total mobilized concentration limit values for CRA-2014.

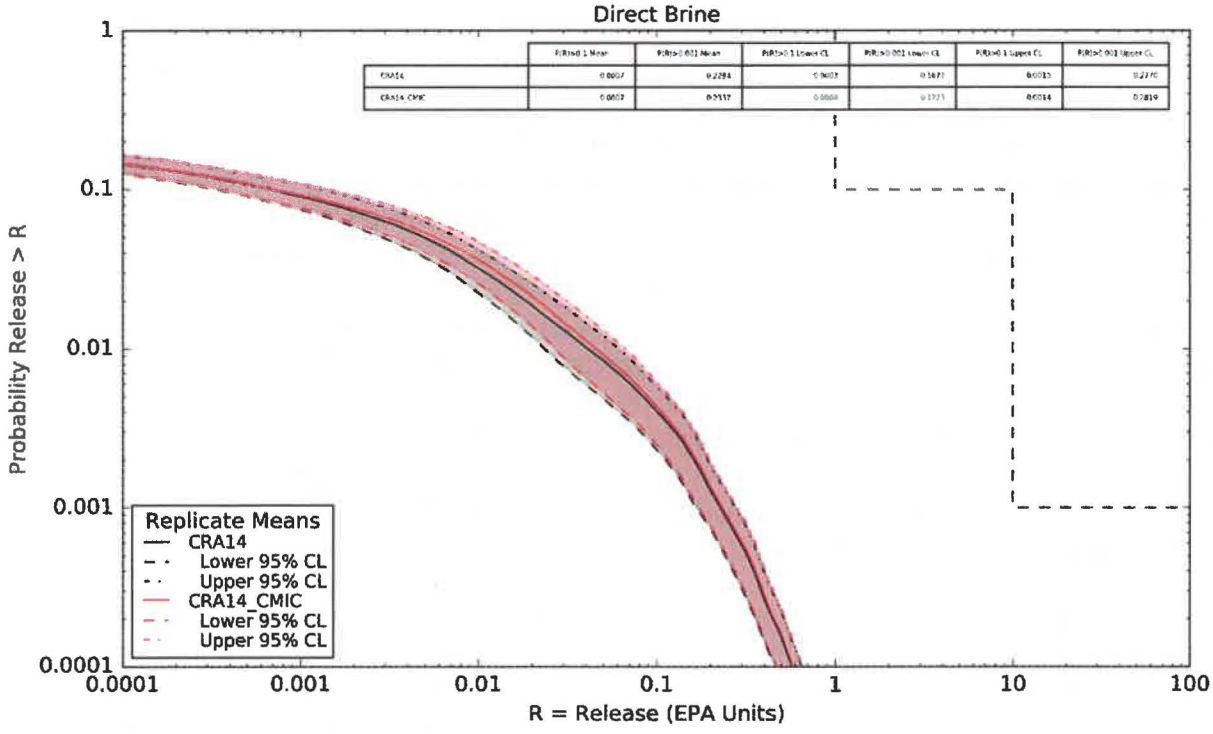

Figure 12 – Impact on CRA-2014 DBR releases

A partial PA calculation was run to assess the impact of the error on the CRA-2014 releases. Figure 12 shows the impact on DBR releases (microbial colloids do not impact *from Culebra* releases because the microbial, mineral, and intrinsic colloids are assumed to filter out and thus not transport through the Culebra). For these results, the code PANEL was altered to produce results consistent with the green curves in the previous figures. The CAPMIC_ADS values were used directly, but the cap was enforced on the value *Dissolved*PROPMIC*. Thus the microbial colloid -associated actinide concentration limit term was calculated as:

$$Microbial = \min\begin{cases} Dissolved * PROPMIC, \\ \underbrace{CAPMIC}_{microbe-adsorption\ limit} \end{cases}$$

There is no change in mean DBR releases at P(R)>0.1; but there is a 2% increase in mean DBR releases at P(R)>0.001. This change is not significant to alter any previous conclusions.

Summary and Recommendations

In summary, the parameter CAPMIC was both defined and implemented inconsistently beginning with the 1996 CCA and the original Parameter Record Package. Both documents simultaneously and conflictingly define CAPMIC as "the actinide concentration in molarity at which no growth [of microbes] was observed" (i.e. a total mobile actinide concentration), the likely intended definition, and "maximum concentration of each actinide associated with mobile microbes" (i.e. microbe-bound actinide concentration). The CCA calculations contained flawed logic and attempted to simultaneously use both definitions (even though each has a different unit basis), but the logic flaw caused only the second definition to be invoked. The inconsistency in the implementation was addressed in 1998 in the PANEL Design Document (and the source code) and in subsequent PANEL Analysis Package reports (and PA calculations), but inconsistencies in the definition remained in subsequent Appendix SOTERM documents and in the Parameter Database. In CRA-2014 the unit basis of CAPMIC was changed, resulting in a new inconsistency between the parameter and the equations in which it is used.

Results were shown that illustrate the magnitude of the discrepancy. The discrepancy is negligible for Am(III), but non-conservative for Pu(III) and Pu(IV). The impact is that the low-probability/high-consequence (P(R)>0.001) CRA-2014 mean DBR releases were underpredicted by 2%, while the P(R)>0.1 mean DBR releases were unchanged. These changes do not alter prior conclusions.

As the biomass-based CAPMIC values were adopted in 2014 and will continue to be used, the equation used to calculate the microbial colloid-associated actinide concentration limit in PANEL will be changed to

$$Microbial = \min\begin{cases} Dissolved * PROPMIC, \\ \underbrace{CAPMIC}_{microbe-adsorption\ limit} \end{cases}$$

to be consistent with the new CAPMIC unit basis of microbe-associated actinide concentration. This equation causes the Microbial contribution to plateau at large dissolved solubility limit values (rather than decrease to zero), which will result in slightly larger total actinide concentration limits. The current description of CAPMIC in the parameter database, *maximum concentration of actinide on microbe colloids* (e.g. the maximum microbe-associated actinide concentration limit at which PROPMIC applies), is consistent with the updated CAPMIC basis.

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