MODEL ERROR RESOLUTION DOCUMENT

Complete only applicable items.

INITIATION

1. Originator:	2. Date:	3. ERD No.
Al A Eddebbarh/ Shaoping Chu	5/22/2008	MDL-NBS-HS-000020 ERD 02

4. Document Identifier:	5. Document Title:
MDL-NBS-HS-000020 REV02 AD 02	Particle Tracking Model and Abstraction of Transport Processes

6. Description of and Justification for Change (Identify applicable CRs and TBVs):
This ERD addresses CR-12112 associated with *Particle Tracking Model and Abstraction of Transport Processes*, MDL-NBS-HS-000020 REV02 AD 02.

CR-12112:

During the process of examining mass balance calculations from FEHM Version 2.24-01, it was noticed that the filtration logic for colloids passing between units in the rock matrix was not filtering out any of the particles based on particle size versus pore size. An examination of the FEHM source code showed that in the subroutine inmptr.f, there is a line that sets the random seed (rseed), which was previously read from the multi-species particle tracking file, to zero. This logic is only implemented for the coupled GoldSim/FEHM model, and was done so because the TSPA-LA GoldSim model passes the random seed to FEHM. The problem with this logic is that the random seed is later used inside the subroutine inmptr.f (and before the random seed passed from GoldSim is assigned in FEHM). A random seed of zero will force the random seed function used by FEHM to pass back a random number of zero. When this random number of zero is used in conjunction with the logic in inmptr.f, to sample colloid sizes and assign one to each potential particle, each particle is given a particle size of zero which will make it smaller than any sampled pore size and negate its chances of getting permanently filtered. This problem is also found in FEHM Version 2.25.

In addition in FEHM Version 2.24-01 and older versions, the backspace statement in the following logic does not use the correct file unit number, therefore only every other line of the distribution will be read. This problem occurs when the "mptr" macro is provided in a separate file than the main "dat" file, which is the case for the TSPA model files and many other runs of the model. When the mptr macro is contained in the "dat" file, the problem will not occur.

(see attached)

CONCURRENCE

	Printed Name	Signature	Date
7. Checker	Kenneth Rehfeldt	Kenneth Rehfeldt	5/23/2008
8. QCS/QA Reviewer	Peter Persoff	Peter Persoff	05/23/2008

APPROVAL

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(continued from Block 6)

I Background Information

This ERD presents additional simulations that explicitly exclude colloid filtration and negate the colloid filtration process and provides results that are consistent with the implementation in TSPA. Although the process of colloid filtration is correctly implemented in the simulations in MDL-NBS-HS-000020 REV 02 AD 02, the coding logic identified in CR-12112 negates the colloid filtration process in the TSPA simulations. Thus, from the perspective of TSPA, colloid filtration is treated conservatively as physical straining at fracture-matrix interfaces resulting in size exclusion and preferential transport of colloids within the fracture domain.

The analyses presented in this ERD supplement the work already presented in MDL-NBS-HS-000020 REV 02 AD 02. The work in this ERD does not specifically address the second part of the CR. Rather, the second issue was addressed in the Impact Analysis attached to Software Problem Report SPR 20080505001. In that analysis it was shown that the error in sampling made no significant difference to the Normalized Cumulative Breakthrough for radionuclides irreversibly attached to colloids.

Changes required to address the CR are presented in Section III of this ERD. Product output DTNs: MO0705TRANSTAT.000 REV 01 and LA0506BR831371.002 REV 00 of the parent document are revised to reflect the addition of input and output files for transport simulations without colloid filtration. The changes to MDL-NBS-HS-000020 REV 02 AD 02 in this ERD as a result of errors identified in CR-12112 do not have any impact on the conclusions of the parent document, or to the conclusions of any existing downstream technical products such as the TSPA-LA or the SAR.

II Inputs and Software

Direct inputs to this error resolution analysis include the following DTNs: MO0705TRANSTAT.000 REV 01 and LA0506BR831371.002 REV 00. The two DTNs are product output from the parent report and are qualified as shown in the TDMS. Other direct inputs to this analysis are the same as presented in MDL-NBS-HS-000020 REV 02 AD 02 and are not repeated here.

The software codes controlled under IM-PRO-003, *Software Management*, used in this analysis are: FEHM V2.24-01 (STN: 10086-2.24-01), FEHM V2.23 (STN: 10086-2.23-01), and PARTICLE_STAT V1.0 (STN: 11241-1.0-00).

III Analysis and Results

To address CR-12112, simulations were performed without colloid filtration (i.e., the process of colloid filtration negated). These new simulations are constructed to be consistent with the simulations in the TSPA. In the work presented below, the sections impacted are presented with both the original simulations results and then the new results for the case labeled “without colloid filtration.” The case without filtration is the version of the UZ abstraction model that was implemented in TSPA.

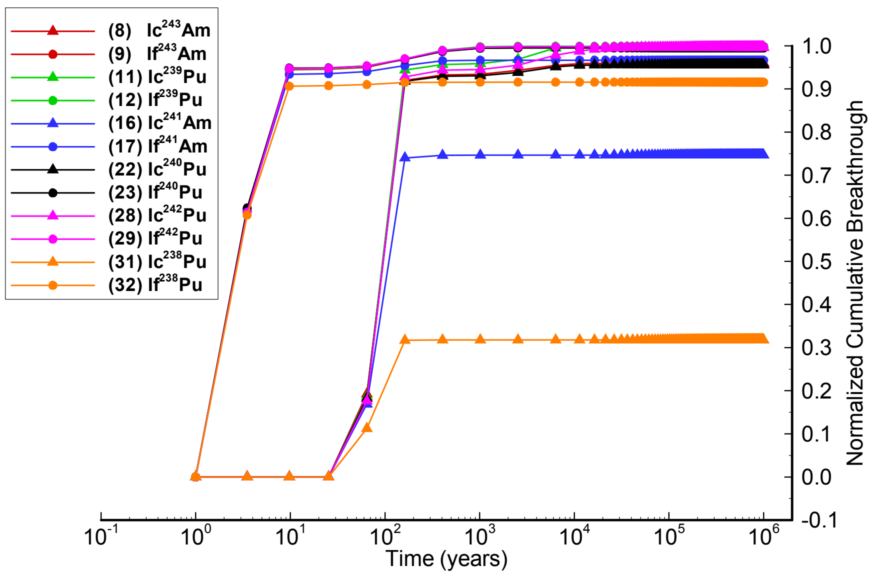
Two output DTNs from the analyses presented in the parent document were revised as a result of the analyses presented in this ERD. The two revised DTNs are: MO0705TRANSTAT.000 REV 02 and LA0506BR831371.002 REV 01. For both DTNs, the results and files from the supplemental analyses presented in this ERD were added to the files and results of the parent report. Thus, the work from the parent documents was unchanged in the two DTNs.

III.1 Breakthrough Curves Evaluation

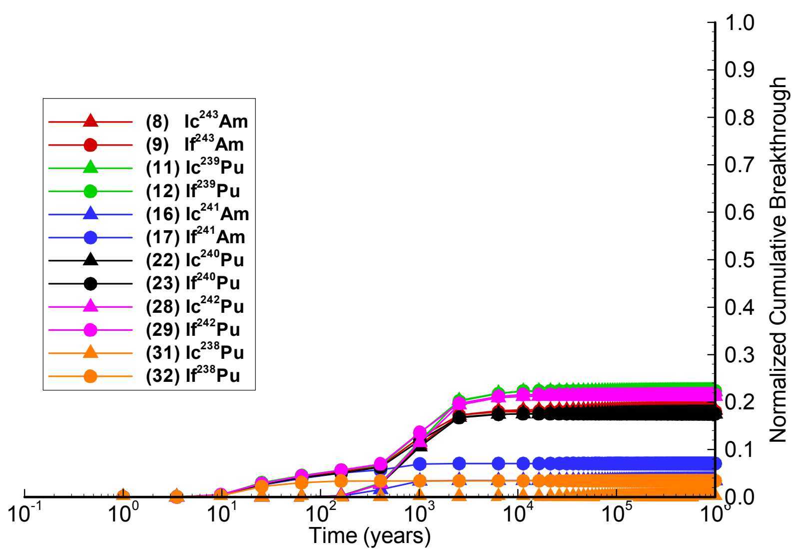
The results below replace the work in the third paragraph of MDL-NBS-HS-000020 REV 02 AD 02, Section 6.6.2.2[b]. Comparisons of breakthrough curves for 12 colloidal species (Ic and If species of ^{243}Am, ^{239}Pu,^{241}Am, ^{240}Pu, ^{242}Pu, and ^{238}Pu) released from both the locations are illustrated in Figure 6.6.2-6[c]. Note that the numbering of the sections and figures is intentionally consistent with the parent document. Figure 6.6.2-6[c] has four separate graphs; plots (a) and (b) present simulation results for the case including colloid filtration for the northern and southern release locations, respectively. The other two plots (c) and (d) present the simulation results for the case without colloid filtration for the northern and southern release locations, respectively. The simulation results for the case including colloid filtration (plots (a) and (b)) show that, as expected, radionuclides that are irreversibly attached to “fast” colloids (If species), which are not affected by matrix diffusion and retardation, have the shortest breakthrough times. At the northern location, within about 10 years after release, over 90% of the irreversible fast colloids travel through the unsaturated zone. Radionuclides that are irreversibly attached to “slow” colloids (Ic species), which undergo retardation due to colloid attachment/detachment processes, move more slowly than their corresponding fast colloid counterparts. The transport time of the irreversible slow colloids depends on the colloid retardation factor, a parameter that is explored more fully in MDL-NBS-HS-000020 REV 02 AD 02, Section 6.8.2[b]. Compared to the fast colloids released at the northern location, the first arrival times for the southern release location are about one order of magnitude larger, due to the thickness of the interval of unfractured rock governed by slower matrix transport. The cumulative breakthroughs for most of these irreversible fast colloids in the northern location are close to unity (except for Ic^{238}Pu and Ic^{241}Am), whereas for the southern location, the cumulative breakthrough is significantly reduced for all radionuclides due to a combination of filtration at the interfaces of matrix units and radioactive decay. The filtration mechanism is more pronounced for the southern release location due to the prevalence of matrix-dominated flow in the south. In summary, most of the Ic and If colloidal species have very limited reduction due to decay in the unsaturated zone from the northern release location, whereas a larger proportion of the radionuclides decay or are subject to colloid filtration in the unsaturated zone before reaching the water table for the southern release location.

For the case without colloid filtration (plots (c) and (d)), the effect of removing colloid filtration is negligible in the northern area (compare plots (a) and (c)) because of the fast travel times. In the southern release area (compare plots (b) and (d)), the effect is more pronounced. Without filtration, a greater portion of the radionuclides attached to colloids will exit the flow system before they decay. The results presented in Figure 6.6.2-6[c](d) are explained by the differences in the half life of the elements. The shortest half life elements ^{238}Pu and ^{241}Am decay quickly and a small portion of Ic and If remain to exit the flow system. Longer lived elements such as ^{242}Pu show almost no decay before the Ic and If portions exit the flow system. The normalized cumulative breakthrough for Ic and If^{239}Pu results from a long half life and ingrowth from the decay of Ic and If^{243}Am.

(a)



(b)

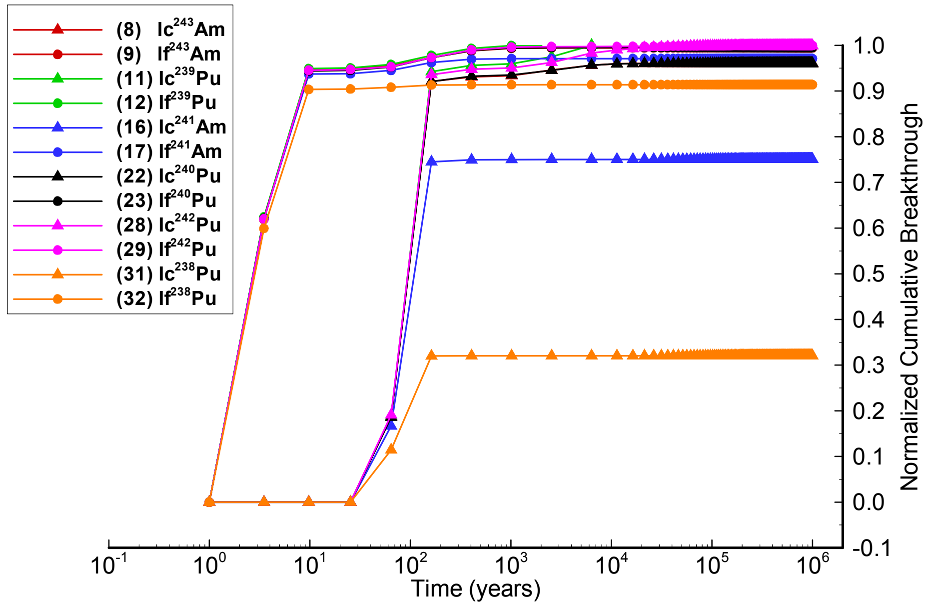


Output DTN: MO0705TRANSTAT.000 REV 02.

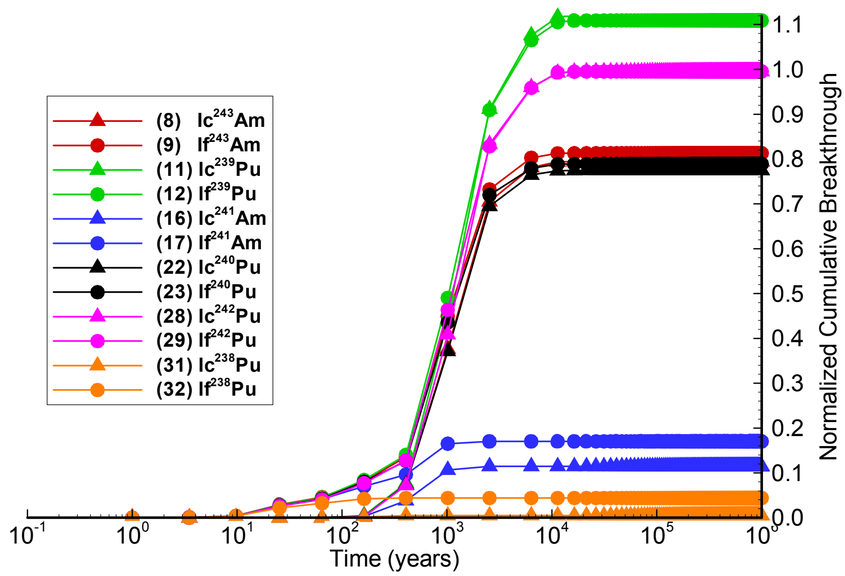
NOTE: Northern Release Location (top) (a) and Southern Release Location (bottom) (b).

Figure 6.6.2-6[c] (a) and (b). Normalized Cumulative Breakthrough Curves of 6 Irreversible Fast Colloids and 6 Irreversible Slow Colloids for the Glacial-Transition 10th Percentile Infiltration Condition and Representative Parameter Values, with Colloid Filtration

(c)



(d)



Output DTN: MO0705TRANSTAT.000 REV 02.

NOTE: Northern Release Location (top) (c) and Southern Release Location (bottom) (d).

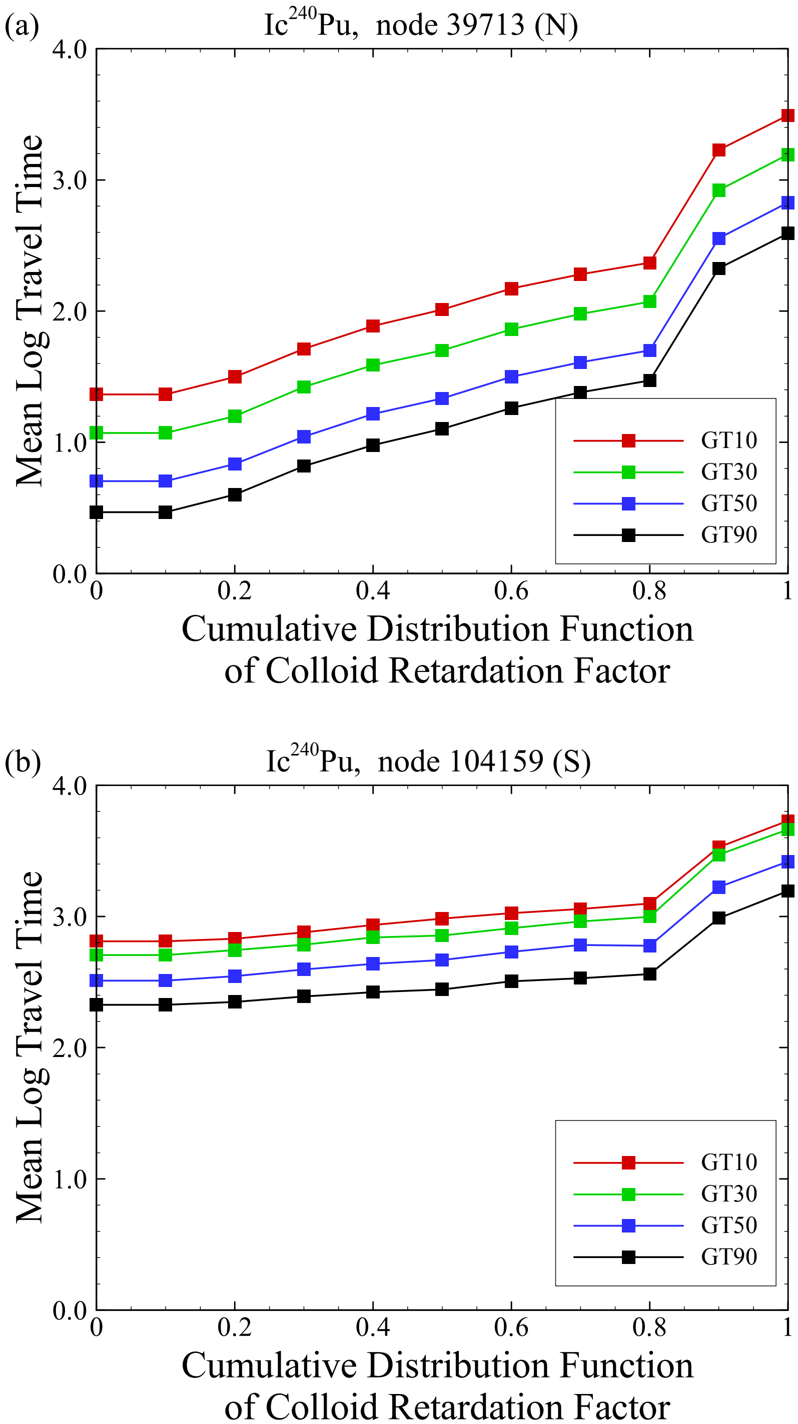
Figure 6.6.2-6[c] (c) and (d). Normalized Cumulative Breakthrough Curves of 6 Irreversible Fast Colloids and 6 Irreversible Slow Colloids for the Glacial-Transition 10th Percentile Infiltration Condition and Representative Parameter Values, without Colloid Filtration

III.2 Uncertainty Evaluation

This section presents additional analyses that examine the influence of uncertainty with and without colloid filtration. This work replaces the last paragraph and the last two figures of MDL-NBS-HS-000020 REV 02 AD 02, Section 6.8.2[b].

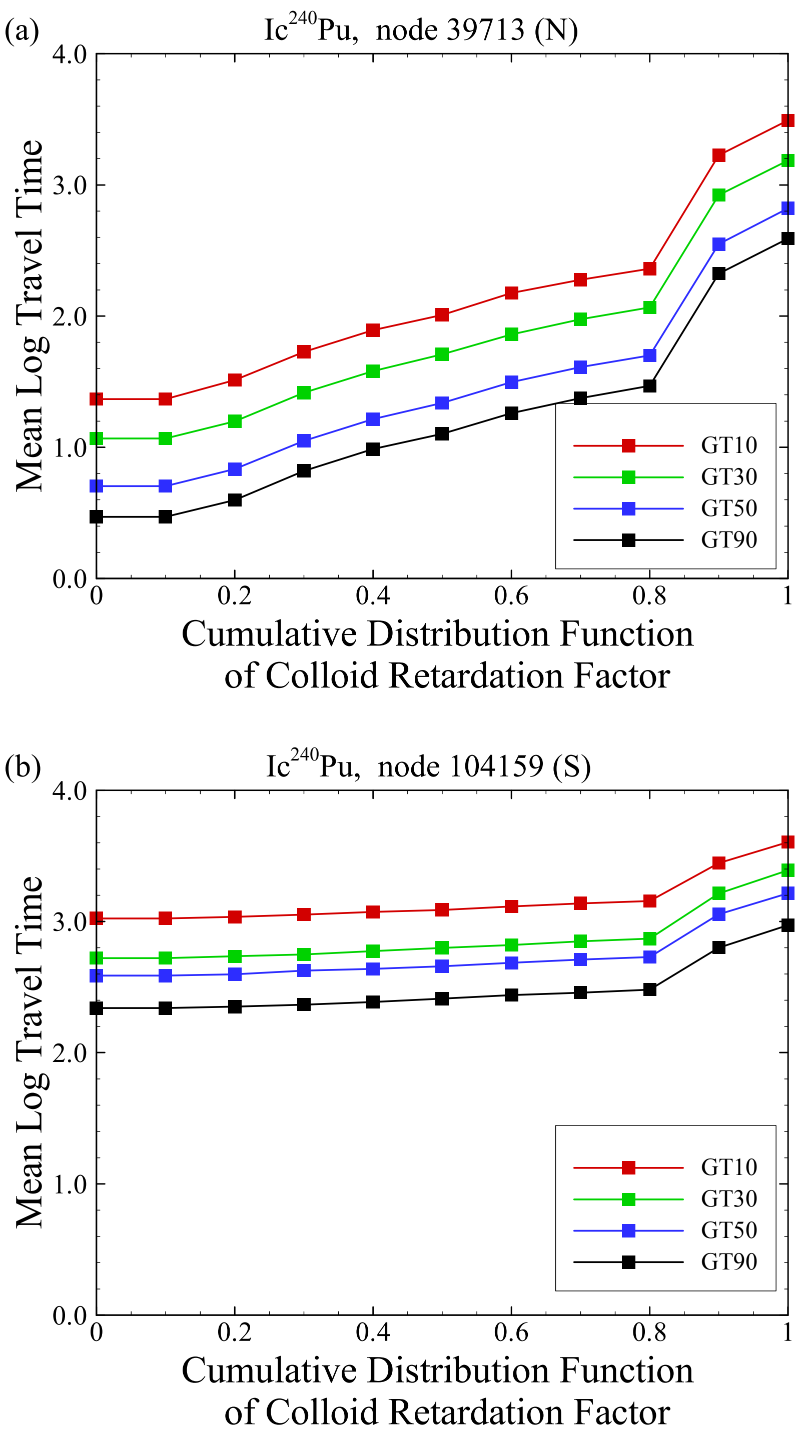
The following set of analyses examines the influence of uncertainty in the value of the colloid retardation factor R_{coll} for the irreversible Ic species of ^{240}Pu. Figure 6.8.2-23[c](#1) (with colloid filtration) and Figure 6.8.2-23[c](#2) (without colloid filtration) show the results of the mean travel time as a function of R_{coll} for the four glacial-transition flow fields, for the northern (top) and southern (bottom) release locations. Similar plots for the decay fraction C/C_0 are shown in Figure 6.8.2-24[c](#1) (with colloid filtration) and Figure 6.8.2-24[c](#2) (without colloid filtration). For the with filtration versions of both figures, the results are slightly different than the corresponding figures in Addendum 01 of the parent document, but the conclusions in that document are still valid.

Comparing the results with and without colloid filtration, the results without colloid filtration are slightly different than the corresponding figures in Addendum 01 of MDL-NBS-HS-000020 REV 02 AD 02, but the conclusions reached in that document are still valid. For the northern release location, travel times are larger for either lower fluid flow rates or larger values of R_{coll}. The southern release location, with its interval of matrix-dominated transport, has generally larger travel times and a smaller impact of fracture retardation of colloids, since this effect "competes with" the matrix transport time for importance. For either release location, the decay fraction is close to unity for this species of ^{240}Pu except for the highest values of R_{coll} in the uncertainty distribution. For other Ic species with shorter half lives, a larger effect of R_{coll} uncertainty on the decay fraction would be expected. There is very little impact of colloid filtration on the travel times of Ic species of Pu through the flow system. As was observed above, the effects are relatively larger in the southern release location than in the northern release location.



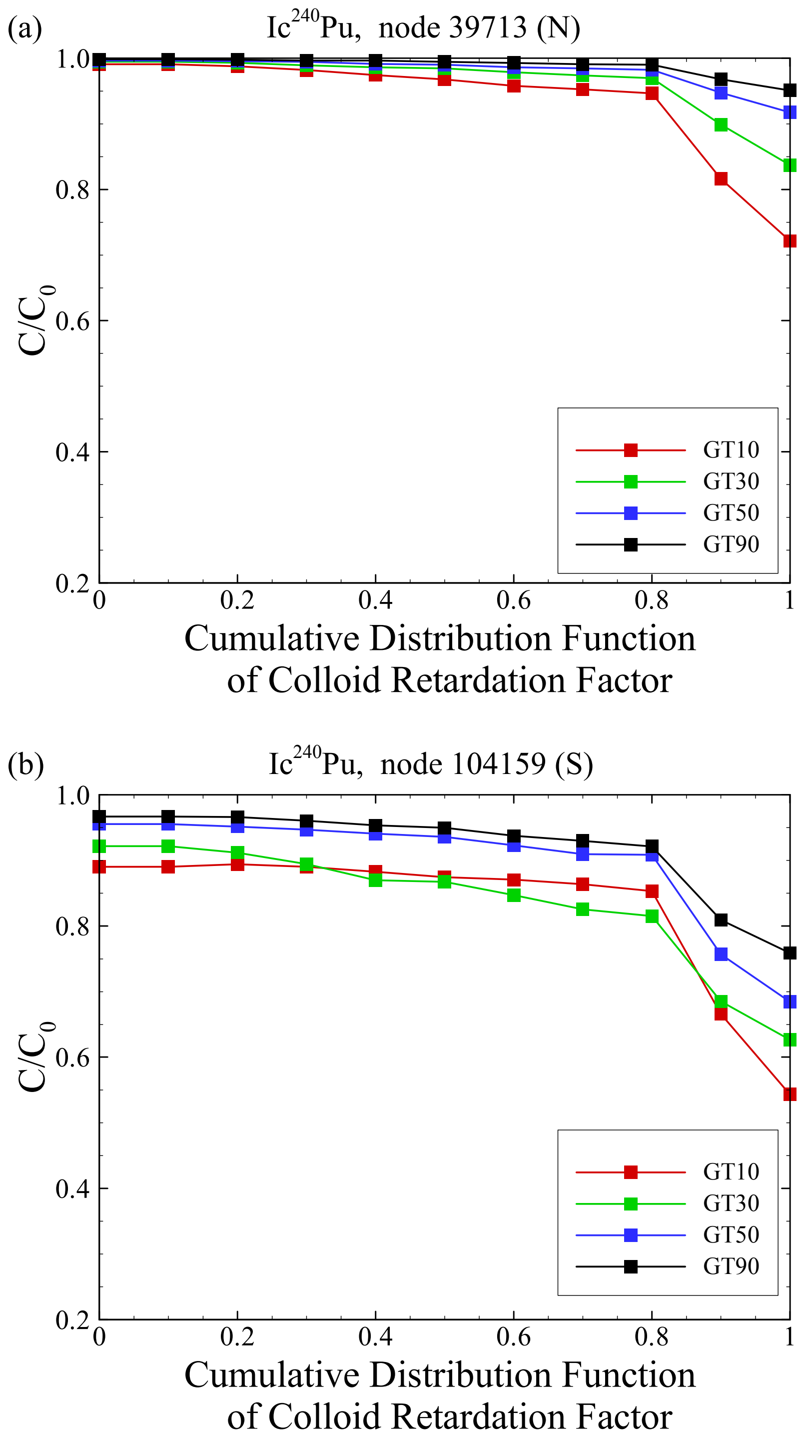
Output DTN: MO0705TRANSTAT.000 REV 02.

Figure 6.8.2-23[c](#1).Mean Travel Time of $Ic^{240}Pu$ as a Function of Colloid Retardation Factor for the Glacial-Transition Climate Condition, with Colloid Filtration: (a) is the northern release location and (b) is the southern release location



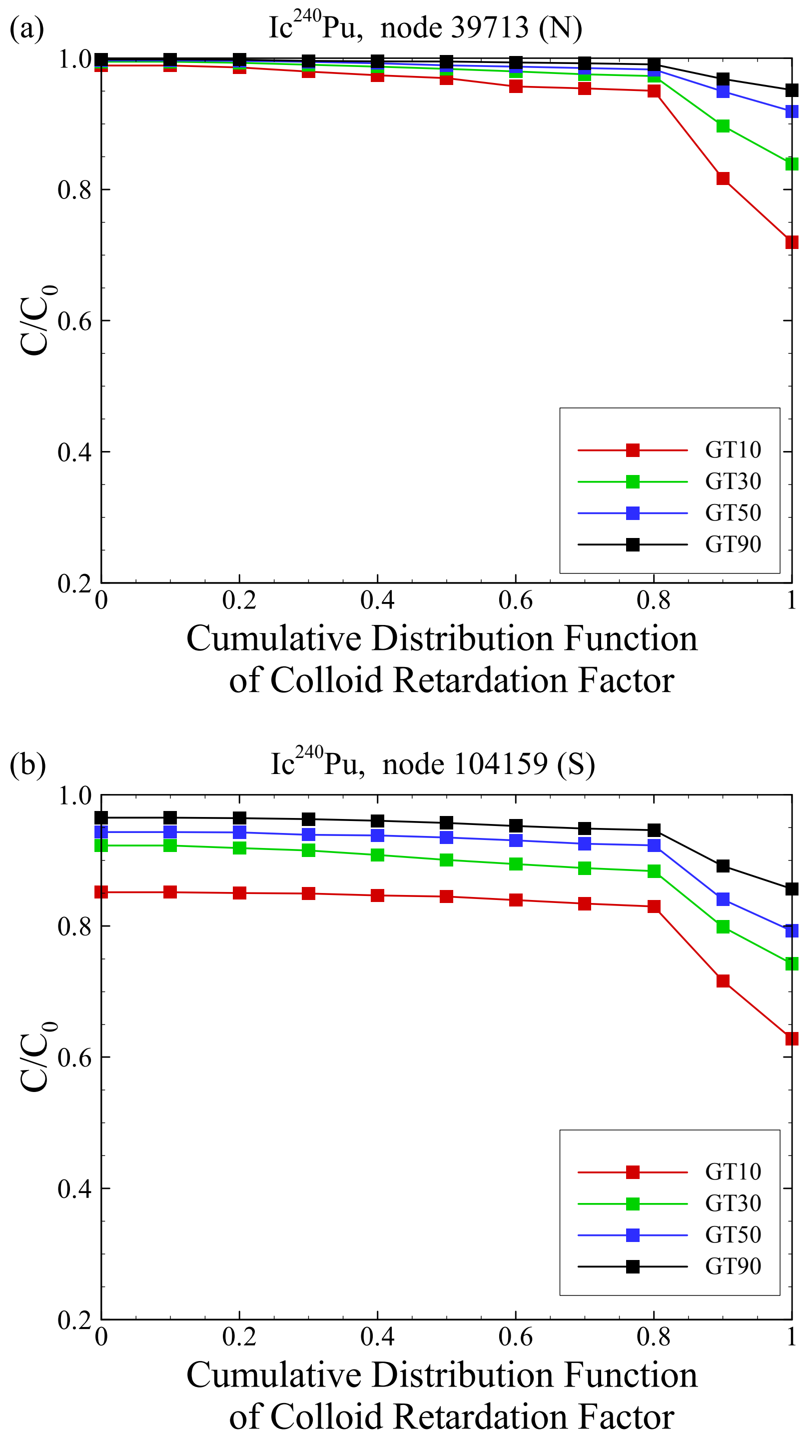
Output DTN: MO0705TRANSTAT.000 REV 02.

Figure 6.8.2-23[c](#2).Mean Travel Time of Ic^{240}Pu as a Function of Colloid Retardation Factor for the Glacial-Transition Climate Condition, without Colloid Filtration: (a) is the northern release location and (b) is the southern release location



Output DTN: MO0705TRANSTAT.000 REV 02.

Figure 6.8.2-24[c](#1). Normalized Concentration of $Ic^{240}Pu$ (Decay Fraction, Computed from Travel Time Distributions) as a Function of Colloid Retardation Factor for the Glacial-Transition Climate Condition, with Colloid Filtration: (a) is the northern release location and (b) is the southern release location



Output DTN: MO0705TRANSTAT.000 REV 02.

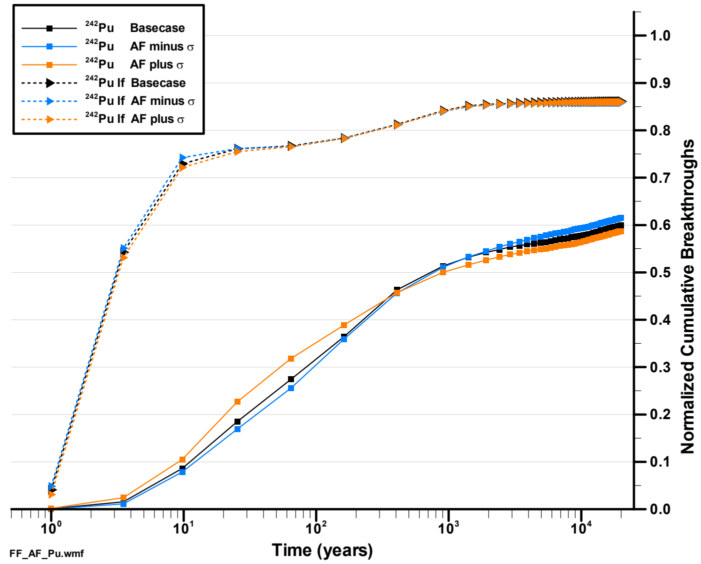
Figure 6.8.2-24[c](#2). Normalized Concentration of $Ic^{240}Pu$ (Decay Fraction, Computed from Travel Time Distributions) as a Function of Colloid Retardation Factor for the Glacial-Transition Climate Condition, without Colloid Filtration: (a) is the northern release location and (b) is the southern release location

III.3 Sensitivity Analysis

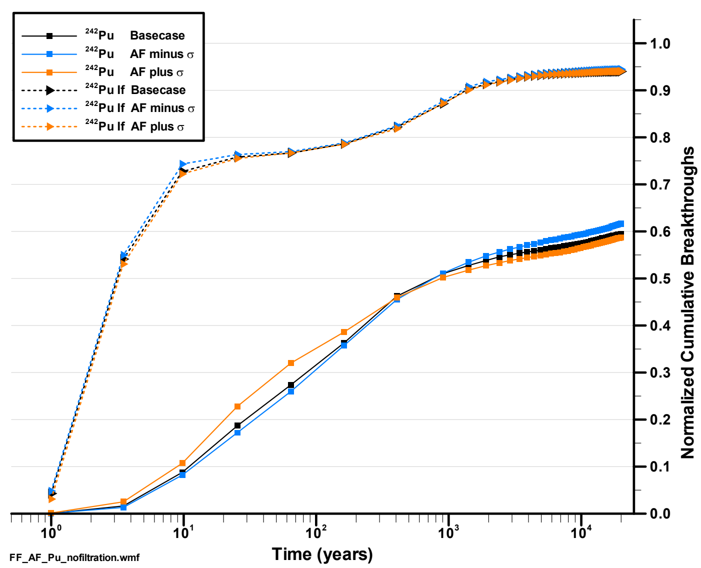
The final set of analyses show the sensitivity studies to flow parameter uncertainty. This work was originally presented in MDL-NBS-HS-000020 REV 02, Section 6.6.3. The discussion in the original section of the parent document is still valid because the work presented in the ERD does not replace the work in the parent section, but supplements the analysis by including cases "without colloid filtration." Note that these results are for comparison purposes only. Actual radionuclide mass flux reaching the water table will depend on release rates and locations, and is simulated in the TSPA-LA model.

As noted earlier, figure numbers correspond to the section of the parent document. Figure 6-26[c] contains the results of simulations varying the value of the van Genuchten parameter α for the fracture continuum. The upper plot (a) includes colloid filtration while plot (b) is without colloid filtration. For the dissolved species, the results are the same as expected. For the irreversibly sorbed radionuclide If^{242}Pu, the normalized cumulative breakthrough increased from about 0.86 to 0.94. Comparing the two groups of results (with and without colloid filtration), the case without colloid filtration shows more breakthrough at later time, but the conclusions reached in the parent report are still valid.

(a)



(b)

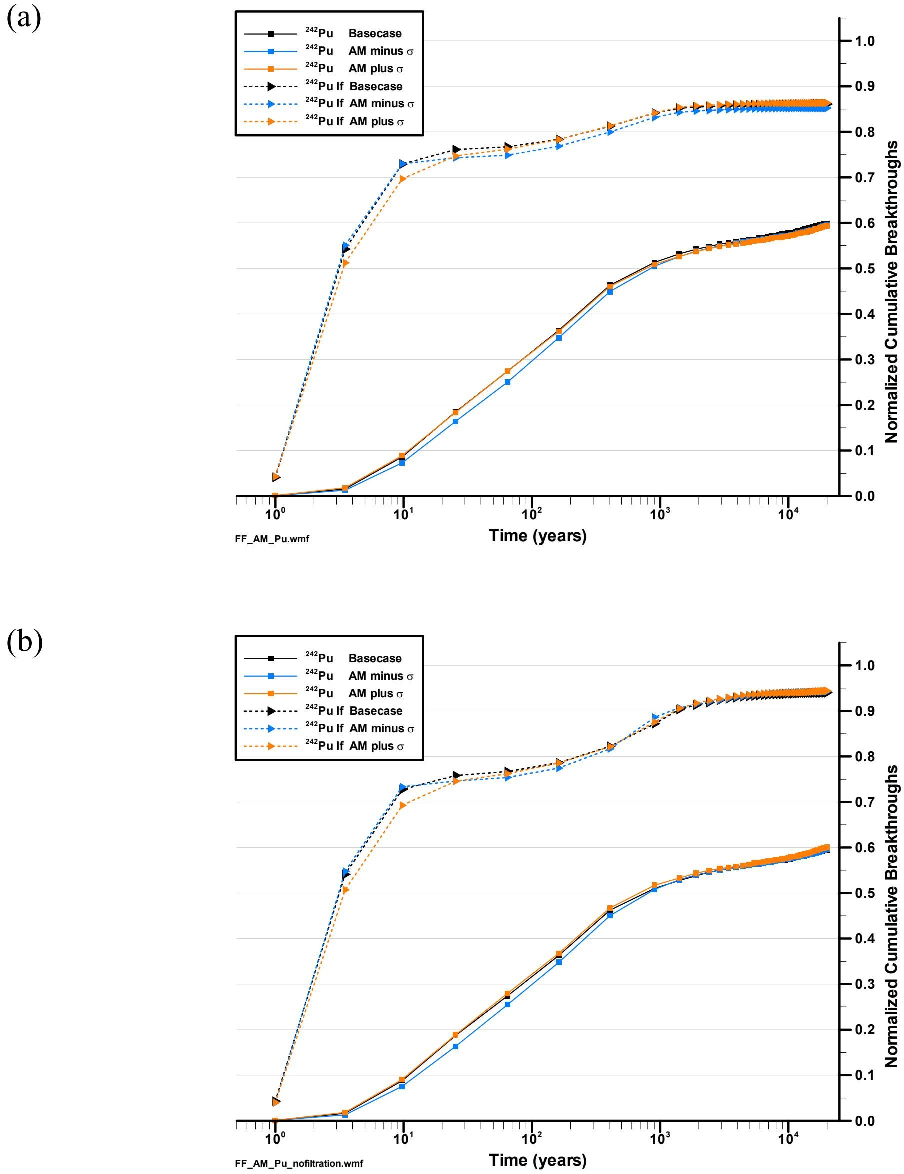


Output DTN: LA0506BR831371.002 REV 01

Note: (top (a): with colloid filtration; bottom (b): without colloid filtration).

Figure 6-26[c]. Base-Case Model Normalized Mass Flux at the Water Table for Different Species of ^{242}Pu, Glacial-Transition Mean Infiltration Scenario, for Different Values (Plus and Minus One Standard Deviation (σ) from the Base Case) of the van Genuchten α Parameter for the Fracture Continuum, and Elevated Water Table

Figure 6-28[c] shows similar results for the case of varying the van Genuchten parameter α for the matrix continuum. The results for both the case including colloid filtration and the case without indicate that the van Genuchten parameter α for the matrix continuum has very little impact on predicted transport of radionuclides.



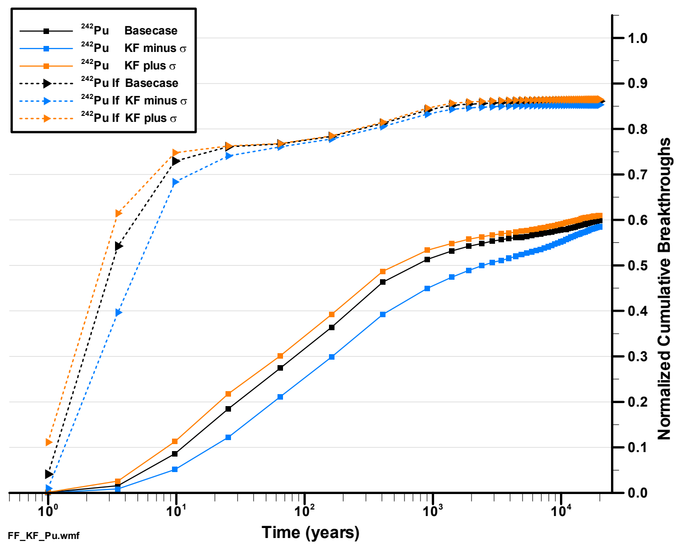
Output DTN: LA0506BR831371.002 REV 01

Note: (top (a): with colloid filtration; bottom (b): without colloid filtration).

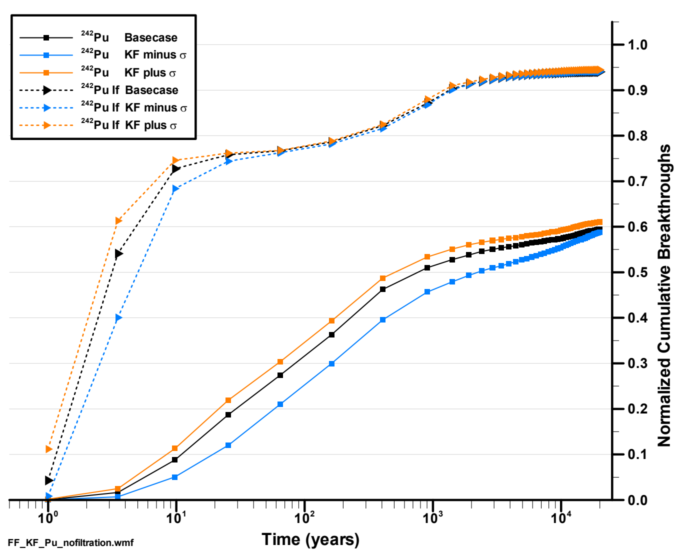
Figure 6-28[c]. Base-Case Model Normalized Mass Flux at the Water Table for Different Species of ^{242}Pu, Glacial-Transition Mean Infiltration Scenario, for Different Values (Plus and Minus One Standard Deviation (σ) from the Base Case) of the van Genuchten α Parameter for the Matrix Continuum, and Elevated Water Table

The impact of changing the absolute permeability of the fracture continuum is shown in Figure 6-30[c]. The case including colloid filtration (a) has slightly less normalized cumulative breakthrough than for the case (b) without colloid filtration. The difference in the late time normalized cumulative breakthrough (about 0.86 versus 0.94) is the same as the previous two figures and shows that without colloid filtration a slightly greater amount of irreversibly sorbed radionuclides will exit the flow system.

(a)



(b)



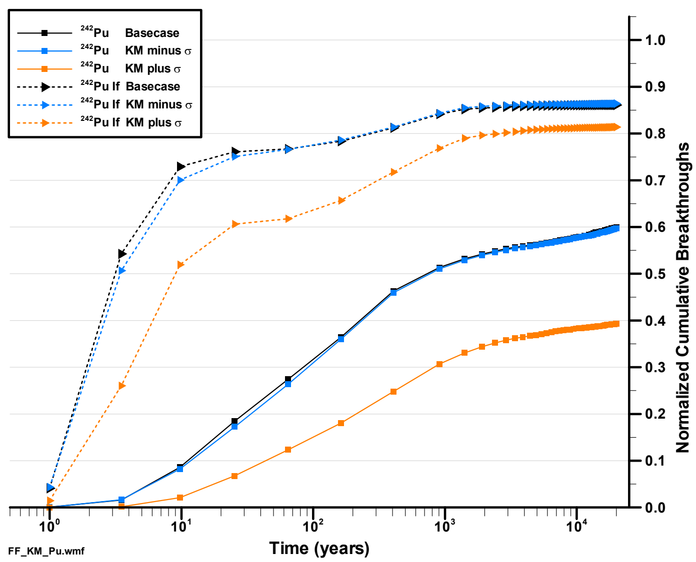
Output DTN: LA0506BR831371.002 REV 01

Note: (top (a): with colloid filtration; bottom (b): without colloid filtration).

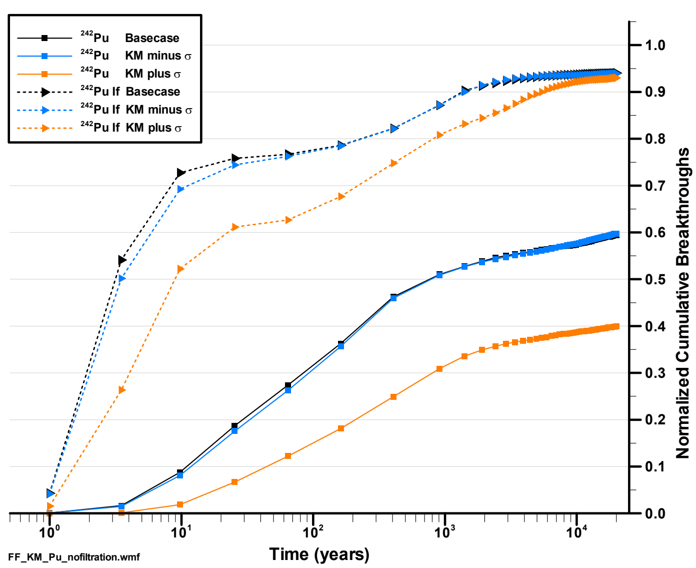
Figure 6-30[c]. Base-Case Model Normalized Mass Flux at the Water Table for Different Species of ^{242}Pu, Glacial-Transition Mean Infiltration Scenario, for Different Values (Plus and Minus One Standard Deviation (σ) from the Base Case) of the Absolute Permeabilities of the Fracture Continuum, and Elevated Water Table

The final comparison is presented in Figure 6-32[c], where the sensitivity of predicted transport to varying the absolute permeability of the matrix rocks is presented. The case including colloid filtration (a) is compared with the case without colloid filtration (b). As in the previous figures, colloid filtration has no impact on the dissolved species. As well, the late time normalized cumulative breakthrough increased to about 0.94 for the case without colloid filtration. One final observation is that in the case including colloid filtration (a), increasing the absolute permeability increased the travel time and produced a different normalized cumulative breakthrough at the end of the simulation. Without colloid filtration (b), the travel times are also longer, but by the end of the simulation, the normalized cumulative breakthrough are nearly the same.

(a)



(b)



Output DTN: LA0506BR831371.002 REV 01

Note: (top (a): with colloid filtration; bottom (b): without colloid filtration).

Figure 6-32[c]. Base-Case Model Normalized Mass Flux at the Water Table for Different Species of ^{242}Pu, Glacial-Transition Mean Infiltration Scenario, for Different Values (Plus and Minus One Standard Deviation (σ) from the Base Case) of the Permeabilities of the Matrix Continuum, and Elevated Water Table

In summary, the simulations without colloid filtration have very little effect on the travel time of radionuclides. However, the mass of radionuclides irreversibly attached to colloids reaching the water table is always larger for the case without colloid filtration. Thus, simulations conducted without colloid filtration will be conservative with regard to dose when compared with cases that include colloid filtration.

IV Impact Evaluation

The issue identified in CR-12112 resulted in supplemental simulations that allowed for a comparison of the impact of the transport of irreversibly sorbed radionuclides with and without colloid filtration. These comparisons are presented above and discussed with respect to the corresponding figures in the parent report (Figures 6.6.2-6[b], 6.8.2-23[b], and 6.8.2-24[b] of MDL-NBS-HS-000020 REV 02 AD 02, and Figures 6-26, 6-28, 6-30, and 6-32 of MDL-NBS-HS-000020 REV 02). As was demonstrated in Section III, the updates to the parent report described in this ERD do not impact the conclusions of the parent document. As was demonstrated in Section III, the breakthrough curves without colloid filtration differ only slightly from the breakthrough curves without colloid filtration. Furthermore, those breakthrough curves, as implemented in TSPA, will result in slightly higher dose. Therefore, there is no detrimental impact to the conclusions of MDL-NBS-HS-000020 REV 02 AD 02 or to any downstream technical documents.

The updates to the parent report described in this ERD have resulted in changes to several documents including the FEPs report (ANL-WIS-MD-000027 REV 00), the TSPA model report (MDL-WIS-PA-000005 REV 00 AD 01), *Postclosure Nuclear Safety Design Bases (*ANL-WIS-MD-000024 REV 01) and the SAR. A DIRS analysis of inputs from the parent report used as direct input in these four reports indicated no impact. In all cases, the conclusions of the downstream documents are unchanged, but the descriptions of the colloid filtration process are revised to be consistent with the no colloid filtration case. The corrected information is consistent with the implementation of the UZ transport model in the TSPA-LA and removal of colloid filtration from the model results in more conservative estimates of the dose.