

WAO41561
 date: July 24, 1996

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subject: Revised Ranges and Probability Distributions of K_{ds} for Dissolved Pu, Am, U, Th, and Np in the Culebra for the PA Calculations to Support the WIPP CCA

REVISIONS OF PREVIOUSLY SUBMITTED RANGES OF MATRIX K_{ds}

After Brush (1996) submitted ranges and probability distributions of matrix K_{ds} for dissolved Pu, Am, U, Th, and Np in the Culebra, we discovered two errors in the procedures used to calculate them.

First, Triay and her group at LANL used a density of 1.00 g/ml instead of her measured brine densities to calculate empirical K_{ds} for Pu, Am, U, Th, and Np in the absence of organic ligands. Therefore, she reported K_{ds} somewhat higher than the actual values (compare Tables B-1, B-2, B-3, B-4, C-1, C-2, C-3, C-4, D-1, D2, D-3, D-4, E-1, E-2, E-3, E-4, F-1, F-2, F-3, and F-4 in Appendices B through F of this and the previous memorandum). However, she calculated the concentrations of the organic ligands in Table G-1 and the K_{ds} in Tables G-2, G3, G-4, G-5, G-6, and G-7 (see Appendix G) correctly and did not revise them.

Second, Brady and his colleagues at SNL and LANL used incorrect values for the mass of dolomite to calculate mechanistic K_{ds} for Pu, Am, U, and Np. He thus reported K_{ds} significantly higher than the actual values (compare Tables B-5, C-6, D-5, and F-5 in this and the original submission). However, he calculated the K_{ds} for Nd (Table C-5) correctly.

After Triay and Brady revised their results, we used the same methods described above to re-establish the ranges and distributions of K_{ds} shown in Table 1 of this memorandum. Appendices B through F contain detailed descriptions of these methods, including all of the *revised* empirical-sorption data, the *revised* mechanistic-sorption data, and the *original* column-transport data considered and included or excluded. (Actually, Lucero and his colleagues at SNL revised the results of their transport study with intact Culebra cores twice

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prior to submission of the original ranges and distributions by Brush (1996).

Comparison of Table 1 in Brush (1996) and Table 1 in this memorandum reveals that revising the empirical and mechanistic K_d s changed many, but not all, of the upper and lower limits of these ranges. We did not change the (uniform) probability distributions of any of the ranges (see Methods Used to Establish Probability Distributions of Matrix K_d s below).

We realize that it is too late for performance-assessment (PA) personnel to re-run their transport calculations with the revised ranges. However, PA can still use these K_d s to assess the impact of the erroneous values on their calculations. *Based on our discussions with them, we do not expect any significant impact.*

The remainder of this memorandum is essentially identical to Brush (1996), except that we have revised the K_d s as necessary (see the tables listed above in Appendices B through F) and the parameters used to describe the extent of the ranges (see Methods Used to Establish Probability Distributions of Matrix K_d s), and inserted the word "revised" as appropriate.

INTRODUCTION

This memorandum contains revised ranges and probability distributions of matrix distribution coefficients (K_d s) for dissolved Pu, Am, U, Th, and Np under conditions expected during transport in the Culebra Dolomite member of the Rustler Formation. In this memorandum, a matrix K_d is the equilibrium ratio of the mass of Pu, Am, U, Th, or Np adsorbed on the solid phase(s) per unit mass of solid(s) divided by the concentration of that element in the aqueous phase (see, for example, Freeze and Cherry, 1979). PA personnel required K_d s for Pu, Am, U, and Th for their calculations to support the Waste Isolation Pilot Plant (WIPP) Compliance Certification Application (CCA) (see Ramsey, 1996). (We will include this memorandum, the original ranges and distributions submitted by Brush (1996), and all of the other memoranda cited herein in the parameter and analysis records packages for these revised K_d s.) Actually, PA required K_d s for various isotopes of these elements, but Ramsey (1996) did not specify them. However, Garner (1996) stated that PA needed K_d s for ^{239}Pu , ^{241}Am , ^{234}U , and ^{230}Th . It is reasonable to assume that, in view of the small differences among the masses of different isotopes of these elements, one can apply a K_d determined for one isotope to any other isotope of the same element. We are resubmitting K_d s for Np in case PA requires them for sensitivity calculations to show that omitting this element did not affect the long-term performance of the repository significantly.

We, the Sandia-National-Laboratories (SNL), and SNL-subcontractor personnel working on or familiar with the dissolved-actinide Retardation

Research Program (RRP) or related aspects of PA, established the ranges and distributions submitted by Brush (1996) from results obtained by the RRP through May 31, 1996. In this memorandum, we have used the same methods along with the revised empirical and mechanistic sorption data to establish the revised ranges and distributions shown in Table 1 (see Revisions of Previously Submitted Ranges of Matrix K_{ds} above). Both the original and the revised ranges and distributions pertain to dolomite-rich rock in the matrix (intact rock between the fractures) of the Culebra. (We use the terms "matrix" and "fractures" in a general sense, corresponding to transport pathways with relatively low and high transmissivities, respectively. Our use of these terms is consistent with the double-porosity conceptual model of the Culebra proposed by L. Meigs and her colleagues at SNL and its subcontractors.) Neither the original nor the revised ranges and distributions include K_{ds} for the clay-rich rock associated with fracture surfaces and dispersed in the matrix of the Culebra. We believe that, based on Swards (1991) and Swards et al. (1991, 1992) and recent, yet-to-be published studies of Culebra mineralogy, clay minerals such as corrensite (an ordered mixture of chlorite and saponite) are present on fracture surfaces and in the matrix of the Culebra at concentrations high enough to increase the retardation of Pu, Am, U, Th, and Np relative to that observed in laboratory studies with dolomite-rich rock (see Description of Laboratory Studies Used to Determine Matrix K_{ds} below). However, we have not included K_{ds} for clay minerals in these ranges and distributions because we do not have sufficient laboratory data for clay-rich rock under expected Culebra conditions at this time. Furthermore, we have not taken any credit for sorption by clay minerals on fractures. We believe that omitting K_{ds} for clays is conservative.

FRACTURE-SURFACE K_{ds}

We recommend that PA personnel set the fracture-surface K_{ds} (actually, K_{as}) for Pu, Am, U, Th, and Np in the Culebra equal to zero. A distribution coefficient expressed on a per-unit-surface-area basis, or K_a , is the equilibrium ratio of the mass of Pu, Am, U, Th, or Np adsorbed on the solid phase(s) per unit area of solid(s) divided by the concentration of that element in the aqueous phase (Freeze and Cherry, 1979). We also recommend that PA not include sorption by a discrete layer of material associated with fracture surfaces. Setting these K_{as} to zero will not affect the predicted retardation of actinide elements by the Culebra because: (1) we have not taken credit for sorption by clay minerals on fracture surfaces; (2) the surface area of the dolomite-rich rock lining the fractures is very small relative to that of the dolomite-rich rock in the matrix. WIPP Performance Assessment Department (1992) discussed sorption on fractures in detail.

REVISED MATRIX K_d s

This section briefly describes the laboratory studies used to determine matrix K_d s for dissolved Pu, Am, U, Th, and Np, and the modeling study used to predict the oxidation-state distributions of these elements under conditions expected in the Culebra. It then discusses the methods used to establish revised ranges and probability distributions of these K_d s.

Description of Laboratory Studies
Used to Determine Matrix K_d s

The RRP carried out several laboratory studies of the sorption of Pu, Am, U, Th, and Np by dolomite-rich rock from the Culebra. Papenguth and Behl (1996) described these studies in detail. These studies used different experimental methods and considered the effects of several factors on actinide sorption in the Culebra. The results used to establish revised ranges and probability distributions of matrix K_d s for Pu, Am, U, Th, and Np in the Culebra appear in Appendices B through F, respectively, of this memorandum. (These lengthy appendices are available on request to anyone who did not receive them.) Detailed descriptions of these laboratory studies and the complete results will appear as SNL and/or SNL subcontractor reports after submission of the CCA.

I. Triay and her group at Los Alamos National Laboratory (LANL) carried out an empirical study of the sorption of Pu(V), Am(III), U(VI), Th(IV), and Np(V) by samples of dolomite-rich rock from the Culebra. Triay used four synthetic fluids, Brine A, ERDA-6, AISinR, and H-17, for her experiments with dolomite-rich rock. Brine A, described by Molecke (1983), simulated fluids equilibrated with K- and Mg-bearing minerals in overlying potash-rich zones in the Salado Formation prior to entering WIPP disposal rooms. It is also similar to intergranular Salado brines at or near the stratigraphic horizon of the repository. These brines could accumulate in WIPP disposal rooms after filling and sealing, and flow from the repository into the Culebra in the event of human intrusion into the repository. ERDA-6 simulates brines that occur in isolated but occasionally large reservoirs in the underlying Castile Formation (Popielak et al., 1983). These brines could flow through the repository and into the Culebra in the event of human intrusion. AISinR simulates brine sampled from the Culebra in the WIPP Air Intake Shaft (AIS). H-17 simulates Culebra brine from the H-17 Hydropad. Triay also studied the effects of the partial pressure of CO_2 (and, hence, dissolved CO_2 concentration and, to some extent, pH) on sorption. She carried out experiments on the bench top (in contact with atmospheric CO_2 , which contains about 0.035% CO_2) and in glove boxes with atmospheres containing 0.24, 1.4, and 4.1% CO_2 . The CO_2 partial pressures in these runs were $10^{-3.5}$, $10^{-2.73}$, $10^{-1.98}$, and $10^{-1.50}$ atm, respectively, the range of P_{CO_2} calculated for Culebra groundwaters by Siegel et al. (1991). Furthermore, Triay studied the effects of dissolved actinide concentration on sorption. These experiments yielded sorption

isotherms, plots of the quantity of radionuclide sorbed by the solid phase or phases versus the final dissolved radionuclide concentration, or plots of K_{ds} versus the final dissolved radionuclide concentration. (We will include these isotherms in the parameter and analysis records packages for these revised K_{ds} .) These plots in turn provided information on the nature of the reaction(s) responsible for removal of radionuclides from solution. Finally, Triay studied the effects of equilibration time (3-days and 1-, 3-, 6-, or 8-weeks) and direction of reaction (sorption or desorption) on sorption. Triay crushed the samples, selected the 75-to-500- μm size fraction (significantly larger than the mean dolomite grain diameter of about 2 μm), washed these subsamples with dilute HCl to remove crystallographically strained surfaces, fine particles of dolomite, and Fe- and Mn-oxyhydroxides, and pretreated them with the same type of brine to be used for the actual experiment for periods of time for the most part identical to those of the sorption and desorption runs. Triay carried out each of the pretreatments and the actual experiments with 20 ml of brine and 1 g of rock. During the runs that yielded the K_{ds} used by PA, she used one actinide element at a time. At the end of her runs, Triay separated the aqueous and solid phases by sequential filtration to 0.2 μm , analyzed the solutions by liquid scintillation counting (LSC), and determined K_{ds} from the differences between the initial and the final radionuclide concentrations in the solutions. She carried out most of her experiments, and all of the runs that yielded the K_{ds} used by PA, with samples of dolomite-rich rock taken from AIS core segments adjacent to those used for the column-transport study (see below). X-ray-diffraction analysis of this rock failed to detect clay minerals in most cases. Because the detection limit of this technique is about 1%, the rock that yielded the K_{ds} for PA contains a lower concentration of clay minerals than the Culebra as a whole (estimated, based on previously published and ongoing studies of Culebra mineralogy, to be about 1 to 5%). Triay also carried out a few experiments with dolomite from the H-19 Hydropad and clay-rich rock from the lower, unnamed member of the Rustler. (The clay minerals in the lower member are identical to those lining fracture surfaces and dispersed in the matrix of the Culebra.) This study yielded a large number of K_{ds} for actual samples of nearly pure Culebra dolomite and actinide-bearing synthetic fluids closely resembling those that could actually flow through the Culebra after human intrusion.

P. V. Brady and his colleagues at SNL and LANL carried out a mechanistic study of the sorption of Pu(V), Am(III), Nd(III) (a nonradioactive analog of Am(III) and Pu(III)), U(VI), Th(IV), and Np(V) from synthetic 0.05, 0.5, and 5 M NaCl solutions by samples of well characterized, pure dolomite from Norway. Brady used a limited-residence-time (1 min.) reaction vessel to minimize the extent of dolomite dissolution, actinide precipitation, and other reactions unrelated to sorption during his experiments. This allowed him to study the effects of pH (from about 3 or 4 to 9 or 10 in most cases), the CO_2 concentration of the headspace (atmospheric, 0.5, and 5%), and the concentrations of potentially significant cations and anions on sorption in the absence of complexities caused by other reactions. Brady crushed the samples, selected the <106- μm size

fraction, washed them with dilute HCl, and pretreated them overnight in an NaCl solution with the same concentration to be used for the actual experiments, and a solution-to-solid ratio of 100 ml per g of dolomite. He carried out the actual experiments with several actinide elements at a time, and a solution-to-solid ratio of 200 ml/g. After his runs, Brady separated the aqueous and solid phases with a 0.22- μm filter, analyzed the solutions by inductively coupled plasma emission/mass spectrometry, and determined K_{ds} from the differences between the initial and the final radionuclide concentrations in the solutions. Although this study did not yield K_{ds} for actual samples of Culebra rock nor for synthetic Culebra fluids, it did yield results that have proven highly useful for interpreting the results of the empirical sorption study at LANL, and for extending the empirical data to the basic conditions (pH values of about 9 to 10) expected to result from use of an MgO backfill in WIPP disposal rooms (see below).

D. A. Lucero and his colleagues at SNL studied actinide transport through intact, 5.7-inch-diameter cores obtained from the Culebra in the WIPP AIS. Lucero obtained the cores used for this study from 16-to-18-ft.-long horizontal boreholes aligned in the current direction of groundwater flow in the vicinity of the AIS (see Predictions of Actinide Oxidation States in the Culebra below) and stored them under conditions that minimized evaporation of pore water. Prior to his experiments, Lucero cut 4-to-20-inch sections from the original cores and potted them in Neoprene. He then placed the potted core sections in Al core holders, mounted them vertically in a glove box, and pressurized them to about 50 atm, the *in situ* pressure at the depths (716 and 721 ft.) from which these cores were obtained. Lucero carried out spike injections or, in a few experiments, continuous injections of Pu(V), Am(III), U(VI), Th(IV), and/or Np(V) by introducing synthetic AISinR or, in a few runs, synthetic ERDA-6 with low concentrations of the radionuclide(s) into a cavity cut in the top of each core. He then pumped additional brine through these cores at low flow rates (0.1 ml/min and, in a few runs, 0.05 ml/min) for periods of up to 237 days (equivalent to pumping up to 34.2 pore volumes of brine through these cores). These flow rates are at or close to the upper limit of the range of *in situ* fluid velocities. He collected the effluent continuously and analyzed it every 5 ml by γ spectrometry or LSC. He also used scanning γ emission tomography to image the cores. By injecting different radionuclides at different times and, in some cases, by using different brines, Lucero carried out multiple, sequential experiments with each core. Because this study quantified actinide sorption from fluids flowing through intact samples of Culebra rock, it complements the static empirical and mechanistic sorption studies with crushed Culebra rock or pure dolomite. However, this study did not yield K_{ds} directly. For U and Np, which were moderately retarded by sorption, the observed delays between the elution peaks of nonsorbed radionuclides (such as ^3H or ^{22}Na) and those of U and Np yielded discrete values for the retardation factor R, which were then used, along with porosities determined with the nonsorbing tracers, to calculate K_{ds} . For Pu, Am, and Th, which were strongly retarded, Lucero did not observe breakthrough, even after pumping brine through these cores for 61, 118, and 211 days (Pu and Am)

and 133, 146, and 237 days (Th), equivalent to 8.83, 17.0, and 30.4 pore volumes (Pu and Am) and 19.1, 21.0, and 34.2 pore volumes (Th). Therefore, he was only able to calculate minimum values of R and K_d for these elements. These minimum values depend on factors such as the initial concentration of each radionuclide, the volume of brine pumped through the core, and the analytical detection limit for the radionuclide in addition to the extent of retardation.

Predictions of Actinide Oxidation States in the Culebra

Because oxidation state significantly affects the chemical behavior, including sorption, of the actinide elements, predictions of the oxidation-state distributions of Pu, U, and Np in the Culebra were necessary to establish ranges and probability distributions of matrix K_d s for use in the PA calculations. For Pu, U, and Np, the following oxidation states are possible in low-temperature, geochemical systems: Pu(III), Pu(IV), Pu(V), and Pu(VI); U(IV) and U(VI); and Np(IV), Np(V), and Np(VI). For Am and Th, only one oxidation state, Am(III) or Th(IV), respectively, is possible.

We have used experimentally based predictions of the oxidation-state distributions of Pu, U, and Np in WIPP disposal rooms from the Actinide Source Term Program (ASTP) to specify the oxidation states of these elements in the Culebra. Based on a laboratory study carried out under expected WIPP conditions by D. Clark and his colleagues at LANL and previously published results obtained for applications other than the WIPP Project, ASTP personnel predicted that Pu will speciate as Pu(III) or Pu(IV), but not as Pu(V) nor Pu(VI), that U will speciate as U(IV) and U(VI), and that Np will speciate as Np(IV) and Np(V), but not as Np(VI), in deep (Castile and Salado) brines in the repository. To evaluate the applicability of these predictions to the Culebra, H. W. Stockman of SNL carried out a modeling study of the oxidation states of Pu, U, and Np in the Culebra (see below). This study showed that Culebra fluids are poorly poised (have limited capacity to either oxidize or reduce actinide elements). Therefore, it was reasonable to use the oxidation-state distributions of Pu, U, and Np predicted for WIPP disposal rooms to specify the oxidation states of these elements in the Culebra. Using the ASTP predictions for the Culebra ensured consistency between the oxidation-state distributions of these elements in WIPP disposal rooms and at the point of injection of deep (Castile or Salado) brines into the Culebra following human intrusion into the repository. This in turn obviated the need to specify redox reactions in the Culebra, and the need to incorporate possible, concomitant dissolution and/or precipitation reactions in SECO, the PA code for Culebra flow and transport.

ASTP and PA personnel calculated solubilities for *either* Pu(III), U(IV), and Np(IV), *or* Pu(IV), U(VI), and Np(V) in any given vector. PA specified the oxidation states of these elements by sampling "oxstat," a parameter with a uniform probability distribution of 0 to 1. If the sampled value of oxstat was 0.5 or less, PA used the solubilities predicted for Pu(III), U(IV), and Np(IV). (These

solubilities were also sampled parameters.) If oxstat was greater than 0.5, PA used solubilities for Pu(IV), U(VI), and Np(V). We recommended that PA use the ranges and distributions of K_{ds} for the oxidation states of Pu, U, and Np sampled for each vector.

This approach was equivalent to assuming that the oxidation-state distributions of Pu, U, and Np predicted for WIPP disposal rooms will be maintained along the *entire* off-site transport pathway in the Culebra. (Previous PA calculations have predicted that, in the absence of climatic change, fluid will flow from the point of injection into the Culebra to the south or the southeast, and that the distance from the point of injection to the boundary of the Land Withdrawal Area will be about 2.5 or 3 km.) This assumption was certainly reasonable at the point of injection of deep brines into the Culebra and for some, perhaps significant, distance along the flow path. Because, in general, redox equilibrium is not observed in low-temperature aqueous solutions (see, for example, Lindberg and Runnells, 1984), the oxidation states of Pu, U, and Np predicted for the repository *could* persist along the entire flow path in the Culebra. At some point, however, the oxidation-state distributions of these elements *might* equilibrate with ambient conditions in the Culebra.

To evaluate the applicability of ASTP predictions to the Culebra, Stockman used the EQ3/6 geochemical software package (Daveler and Wolery, 1992; Wolery, 1992a, 1992b; Wolery and Daveler, 1992) to predict the oxidation-state distributions of Pu, U, and Np after mixing deep (Castile and Salado) brines containing these elements with Culebra brines. Stockman made various assumptions as to: (1) which naturally occurring or waste-derived dissolved species will control redox conditions in the deep brines after injection into the Culebra; (2) which naturally occurring dissolved or solid species control redox conditions in Culebra brines; (3) whether to use the data base in EQ3/6, or to modify it based on recently published studies of actinide chemistry. By calculating oxidation-state distributions of Pu, U, and Np before and after mixing deep brines with Culebra brines *under all possible combinations of these assumptions*, Stockman showed that Culebra fluids are poorly poised (have limited capacity to either oxidize or reduce actinide elements). Therefore, it is reasonable to assume that the oxidation-state distributions of Pu, U, and Np predicted for WIPP disposal rooms will be maintained along the entire off-site transport pathway.

Predictions of Brine Mixing in the Culebra

Brine composition could also affect the sorptive behavior of actinide elements in the Culebra. Therefore, predictions of the extent to which deep (Castile and Salado) and Culebra brines mix in the Culebra would have been necessary to specify weighting factors to combine the ranges and probability distributions of matrix K_{ds} for dissolved Pu, Am, U, Th, and Np established for deep and Culebra

brines and obtain an overall range and distribution for a given element or elemental oxidation state.

Opinions differ significantly on the extent to which deep and Culebra brines will mix in the Culebra. One extreme of a range of possibilities is that, because of the density difference between deep and Culebra brines and/or limited spreading due to heterogeneity, a "slug" of deep brine will flow along the entire off-site transport pathway without significant mixing. The other extreme is that, because of relatively high heterogeneity, hydrodynamic dispersion will result in rapid mixing, and the composition of the injected fluid will resemble that of Culebra groundwater on the order of hundreds of meters from the point of injection.

We submitted these ranges and distributions to PA concurrently with the submission of Culebra hydrologic parameters by personnel from Geohydrology Department 6115. Therefore, we were unable to carry out brine-mixing calculations with the current hydrologic parameters prior to establishing these ranges and distributions. In the absence of mixing calculations, E. J. Nowak, Manager of Chemical & Disposal Room Processes Department 6831, instructed us to take the following, conservative approach: (1) establish *separate* ranges and distributions for deep and the Culebra brines for each actinide element or elemental oxidation state; (2) recommend that PA personnel use the range and distribution that results in less retardation for each element or elemental oxidation state.

Methods Used to Establish Revised Ranges of Matrix K_d s

This subsection briefly describes the methods used to establish revised ranges of matrix K_d s for dissolved Pu, Am, U, Th, and Np under conditions expected in the Culebra. We carried out most of the work described in this subsection at a meeting held April 1 and 2, 1996, here at the BDM Building. Sixteen SNL and SNL-subcontractor personnel working on or familiar with the RRP or related aspects of PA participated in all or part of this meeting. Two US DOE Carlsbad Area Office and Carlsbad-Technical-and-Administrative-Contractor personnel observed all or part of it. Appendix A (see below) contains the invitation to, agenda for, and list of the participants and observers at this meeting. (This and the other six appendices are available on request to anyone who did not receive them with this memorandum.) Detailed descriptions, including all of the revised empirical-sorption, revised mechanistic-sorption, and original column-transport data considered and included or excluded, appear in Appendices B through F, respectively. Appendix G contains the original results of experiments on the effects of four organic ligands on these K_d s.

At this meeting, we decided to establish *experimentally obtained* ranges for Am(III), U(VI), Th(IV), and Np(V), and to use the experimentally obtained ranges for Am(III) and Th(IV), and the oxidation-state analogy to establish ranges for Pu(III), and Pu(IV), U(IV), and Np(IV). Based on the ASTP predictions of

oxidation-state distributions for Pu, U, and Np in WIPP disposal rooms and Stockman's predictions for the Culebra *under most of the possible combinations of assumptions* (see Predictions of Actinide Oxidation States in the Culebra above), we *did not* plan to establish an experimentally obtained range for Pu(V), nor to use the experimentally obtained range for U(VI) and the oxidation-state analogy to establish ranges for Pu(VI) and Np(VI).

We established *separate* ranges for the deep (Castile and Salado) and the Culebra brines for each actinide element or elemental oxidation state (see Predictions of Brine Mixing in the Culebra above). However, we *did not* establish separate ranges for the two deep brines studied by Triay and her group in the LANL empirical sorption study (Brine A and ERDA-6) because the PA calculations carried out with the multiphase flow code Brine and Gas Flow to support the WIPP CCA have predicted that, in some vectors, the brine in WIPP disposal rooms will comprise mainly Castile brine; in other vectors, it will comprise mainly Salado brine; and in the rest, it will comprise various proportions of these and Culebra brines that will seep into the repository from above. (The latter brines will resemble Castile brines after reacting with Salado minerals.) Therefore, we established one range for Brine A and ERDA-6 to simulate these compositional variations. Similarly, the Culebra off-site transport pathway predicted by previous PA calculations (see Predictions of Actinide Oxidation States in the Culebra) contains groundwaters that resemble *both* Culebra fluids used by Triay (AISinR and H-17). Therefore, we established one range and distribution for these fluids to simulate possible compositional variations along the flow path.

For U(VI), Th(IV), and Np(V) (see Appendices D, E, and F), we used the following methods to establish separate, *experimentally obtained* ranges for the deep and the Culebra brines. First, we considered *all* of the 6-week sorption data from the empirical study by Triay, the only experiments in which she has extensively studied the effects of dissolved actinide concentration on sorption. Because these are the only experiments carried out using a range of dissolved radionuclide concentrations, they are the only runs for which sorption isotherms have provided information on the nature of the reaction(s) responsible for removal of radionuclides from solution. (We will include these isotherms in the parameter and analysis records packages for these revised K_d s.) At the time of this meeting, Triay had not completed the 6-week desorption experiments. We would not, however, have included the results of the 6-week desorption runs, and did not include any data from the 3-day, nor the 1- nor 3-week desorption runs because these data could be artificially higher than those obtained from the sorption runs. Possible reasons for this include: (1) removal of a weakly sorbed actinide species concentrated in the aqueous phase by discarding the solution at the conclusion of a sorption experiment, thereby concentrating a strongly sorbed species prior to the start of a desorption run; (2) saturation of a sorption site with a high K_d followed by removal of the dissolved actinide after a sorption experiment, thereby resulting

in sorption of a higher proportion of the actinide on the sorption site with a high K_d during the desorption run.

To establish the *initial* ranges for the deep brines, we first considered *all* the data obtained from the 6-week sorption experiments carried out with Brine A and ERDA-6 on the bench top (in contact with ambient atmospheric CO_2). Atmospheric CO_2 has a partial pressure of about $10^{-3.5}$ atm, the lowest CO_2 partial pressure used in the LANL study. This partial pressure is equivalent to a CO_2 content of 0.033% in the LANL study. We did not use data from runs equilibrated with higher partial pressures of CO_2 for the initial ranges for the deep brines because we anticipate that an MgO backfill will be emplaced in WIPP disposal rooms to remove CO_2 . Next, we discarded the data from runs in which the difference between the activity of the radionuclide in a standard (the radionuclide-bearing brine with which runs were started) and that in a control (a run conducted identically to that of an actual run, but without any rock) exceeded 3σ , where the standard deviation σ equals the square root of the total number of LSC counts. Discarding these data yielded the *initial* ranges for deep brines:

To establish the *initial* ranges for the Culebra brines (AISinR and H-17), we first considered *all* the data obtained from the 6-week sorption experiments carried out on the bench top (0.033% CO_2) and in glove boxes with atmospheres containing 0.24 and 1.4% CO_2 . These three atmospheres had CO_2 partial pressures of $10^{-3.5}$, $10^{-2.73}$, and $10^{-1.98}$ atm, respectively. Siegel now considers this range more likely for groundwaters in the predicted off-site transport pathway than the previous range of $10^{-3.5}$ to $10^{-1.50}$ atm calculated for the Culebra as a whole by Siegel et al. (1991). We also discarded the data from runs in which the difference between the activity of the radionuclide in a standard and that in a control exceeded 3σ to obtain the *initial* ranges for Culebra brines.

We then compared these initial ranges with the data from the mechanistic sorption study by Brady and his colleagues at SNL and LANL. For the most part, we used Brady's data to extend Triay's empirical sorption data for the deep brines to the basic conditions expected to result from the use of an MgO backfill in WIPP disposal rooms. We assumed that, if mixing is sufficient to produce fluids with compositions similar to those of Culebra brines, the pH of these mixtures will also be similar to those of Culebra brines. Therefore, we *did not* use Brady's data to extend Triay's data for the Culebra brines to basic conditions. So far, Brady has reported data obtained with 0.05 and 0.5 M NaCl solutions, but not with 5 M NaCl. Therefore, we used only his data for 0.5 M NaCl and atmospheric CO_2 (the lowest CO_2 partial pressure used in this study) to extend Triay's data for the deep brines to basic conditions. This comparison yielded our *revised* ranges for the deep brines.

Next, we compared the revised ranges with the data from the transport study with intact Culebra cores by Lucero and his colleagues at SNL. Lucero carried out his experiments under ambient atmospheric conditions; therefore, the CO_2

content of these experiments was probably similar to that in the LANL bench-top runs. Because Lucero *did not* observe breakthrough of Th(IV) (nor of Pu(V) nor Am(III)), it was only possible to determine minimum values of K_d for Th(IV) (and for Pu(V) and Am(III)). This minimum K_d (and those for Pu(V)) are consistent with the ranges based on the empirical and mechanistic sorption studies. Lucero *did* observe breakthrough of U(VI) and Np(V) in his experiments. Therefore, it was possible to determine actual K_d s for these elements. In most cases, the K_d s determined for U(VI) and Np(V) from the transport study are less than the lower limits of the ranges obtained for these elements from the sorption studies. Therefore, we extended the ranges where necessary to obtain *final* ranges for U(VI) and Np(V) in the deep brines (Castile and Salado) and Culebra brines (see Table 1).

Finally we used the experimentally obtained ranges for Th(IV) and the oxidation-state analogy to establish ranges for Pu(IV), U(IV), and Np(IV).

We attempted to use the same methods to establish experimentally obtained ranges for Am(III) (see Appendix C). Inspection of the sorption isotherms for the 6-week LANL sorption data, however, revealed that the K_d s are proportional to the final dissolved Am(III) concentration. (We did not observe significant trends such as this in the isotherms for U(VI), Th(IV), nor Np(V)). These trends suggest that sorption of Am by the container walls, precipitation of an Am-bearing solid phase, coprecipitation of Am by another phase, incomplete separation of the aqueous and the solid phases at the end of an experiment, or some combination of these processes occurred in the runs with Am(III). Triay carried out additional posttest analyses of the brines from some of her 6-week sorption experiments with Am(III) to determine, if possible, what caused these trends, and to redetermine these K_d s. However, she continued to obtain data that displayed trends similar to those described above, and thus cannot rule out the occurrence of processes other than sorption. Therefore, we recommend using the *experimentally obtained* ranges for Pu(V) (Appendix B) for Am(III) by assuming that the K_d s for Am(III) are greater than or equal to those for Pu(V). This assumption is reasonable in view of results such as those in Figure 5 of Canepa (1992). In this case, the Am(III) K_d obtained for the Yucca Mountain Project is about one order of magnitude higher than that obtained for Pu(V) under the same conditions. (We will cite additional examples of differences between the K_d s for Am(III) and Pu(V) in future reports and presentations.) We *have not* used the oxidation-state analogy to justify the use of Pu(V) data for Am(III); instead, this approach is based on *differences* in the behavior of these oxidation states. Furthermore, we recommend using the range for Am(III) for Pu(III) (Table 1); for this recommendation, we invoke the oxidation-state analogy.

In June and July 1996, we repeated the procedures described above with the revised empirical-sorption, revised mechanistic-sorption, and original column-transport data (see Revisions of Previously Submitted Ranges of Matrix K_d s above).

Methods Used to Establish Probability Distributions of Matrix K_{ds}

M. S. Tierney, the PA Parameter Task Leader, provided guidance on establishing probability distributions of parameters for use in the PA calculations to support the CCA (see Tierney, 1996a; 1996b).

The RRP has studied the effects of several factors on sorption (see Description of Laboratory Studies Used to Determine Matrix K_{ds} , Predictions of Actinide Oxidation States in the Culebra, and Predictions of Brine Mixing in the Culebra above). Papenguth and Behl (1996) designed these studies to encompass the ranges of these factors expected in the Culebra. Therefore, the revised ranges of matrix K_{ds} established above correspond to the expected ranges of these factors in the Culebra. However, because of uncertainties about the extent to which deep (Castile and Salado) and Culebra brines will mix, there are uncertainties as to the probability distributions of these factors (especially brine type, the partial pressure of CO_2 , and the resulting pH) in the Culebra. Therefore, we *do not* recommend that PA use a Student t distribution based on the data included in these revised ranges, despite the fact that we included more than three data points for every range shown in Table 1.

Tierney (1996a) states that use of the uniform or log-uniform [probability] distribution "is appropriate when all that is known about a parameter is its range." Because we cannot specify probability distributions for the factors that affect sorption, we recommend that PA personnel use a uniform or a log-uniform distribution. Tierney (1996a) specifies use of a log-uniform distribution "when the range ... spans many orders of magnitude." Inspection of the revised ranges for deep and Culebra brines in Table 1 reveals that they span 1.30 and 2.65 orders of magnitude (deep and Culebra brines, respectively) for Pu(III) and Am(III); 1.15 orders of magnitude (deep brines only) for Pu(IV), U(IV), Th(IV), and Np(IV); 2.82 orders of magnitude (deep brines only) for U(VI); and 2.00 and 2.30 orders of magnitude (deep and Culebra brines, respectively) for Np(V). (Each of these values is the common logarithm of the maximum value of each range divided by its minimum value. We could not calculate this parameter for Th(IV) and Culebra brines because we were unable to establish this range; see Appendix E below. We could not calculate this parameter for the revised range for U(VI) and Culebra brines because its minimum value is 0.) Because these revised ranges all span three orders of magnitude or less, we recommend that PA use a uniform distribution instead of a log-uniform distribution for all of them.

Methods Used for Final Selection of the Revised Ranges of Matrix K_{ds}

We recommend the revised range and probability distribution of matrix K_{ds} for deep (Castile and Salado) or Culebra brines that results in less retardation for each element or elemental oxidation state (see Predictions of Brine Mixing in the Culebra above). Because we recommend a uniform distribution for *all* of the

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revised ranges (see Methods Used to Establish Probability Distributions of Matrix K_d s above), the *average* K_d that PA would sample for all of its vectors is the mean of the maximum and minimum values of each range. Therefore, we compared the means of the revised ranges for deep and Culebra brines to determine which range would result in less retardation for each element or elemental oxidation state. Inspection of the revised ranges in Table 1 reveals that the means are 210 and 2004.5 ml/g (deep and Culebra brines, respectively) for Pu(III) and Am(III); 5,350 ml/g (deep brines only) for Pu(IV), U(IV), Th(IV), and Np(IV); 10.015 and 30 ml/g (deep and Culebra brines, respectively) for U(VI); and 101 and 100.5 ml/g (deep and Culebra brines, respectively) for Np(V). (Each of these values is the sum of the maximum and the minimum values of each revised range divided by two; to facilitate this comparison, we *did not* round each result to one significant figure. We could not calculate this parameter for Th(IV) and Culebra brines because we could not establish this range; see Appendix E below.) Therefore, we recommend a revised range of 20 to 400 ml/g (the revised range for deep brines) for Pu(III) and Am(III); a revised range of 700 to 10,000 ml/g (deep brines) for Pu(IV), U(IV), Th(IV), and Np(IV); a revised range of 0.03 to 20 ml/g (deep brines) for U(VI); and a revised range of 1 to 200 ml/g (Culebra brines) for Np(V). In Table 1, the recommended ranges appear in bold font.

Because the ASTP decided to specify the oxidation states of Pu, U, and Np by sampling the "oxstat" parameter (see Predictions of Actinide Oxidation States in the Culebra), the revised range and distribution for each specified oxidation state would constitute the range and distribution for each of these elements during a given vector.

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Table 1. Revised Ranges of Matrix K_{ds} (ml/g) for Pu, Am, U, Th, and Np, and Dolomite-Rich Culebra Rock. Ranges in bold font to be used by PA. Oxidation state of Pu, U, and Np to be specified by the value of "oxstat" parameter sampled to calculate dissolved actinide concentrations in WIPP disposal rooms. All probability distributions are uniform (see text). Table compiled by L. H. Brush on April 3, 1996, based on results of meeting held April 1 and 2, 1996. Table checked by Brush and Y. Behl on April 3, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Behl on April 8, 1996. Table revised by Brush on July 6 and 10, 1996, based on information provided by LANL on June 28, 1996, and Brady (1996). Table checked by A. C. Peterson on July 18, 1996.

Oxidation State	Element				
	Pu	Am	U	Th	Np
VI	NA	NA	0.03 to 20 ^{A,C} 0 to 60 ^{B,C}	NA	NA
V	NA	NA	NA	NA	2 to 200; ^{A,C} 1 to 200 ^{B,C}
IV	700 to 10,000; ^{A,D} NE	NA	700 to 10,000; ^{A,E} NE	700 to 10,000; ^{A,C} NE	700 to 10,000; ^{A,G} NE
III	20 to 400; ^{A,H} 9 to 4,000 ^{B,H}	20 to 400; ^{A,I} 9 to 4,000 ^{B,I}	NA	NA	NA

A: range for deep (Castile and Salado) brines only (see text).

B: range for Culebra brines only (see text).

C: experimentally obtained range (see text).

D: experimentally obtained range for Th(IV) applied to Pu(IV) by oxidation-state analogy.

E: experimentally obtained range for Th(IV) applied to U(IV) by oxidation-state analogy.

F: experimentally obtained range for Th(IV) and deep brines applied to Th(IV) and Culebra brines.

G: experimentally obtained range for Th(IV) applied to Np(IV) by oxidation-state analogy.

H: experimentally obtained range for Pu(V) applied to Pu(III) (see text).

I: experimentally obtained range for Pu(V) applied to Am(III) (see text).

Table 1. Revised Ranges of Matrix K_d s (ml/g) for Pu, Am, U, Th, and Np, and Dolomite-Rich Culebra Rock. (continued).

NA: not applicable (element will not speciate in this oxidation state).
NE: not established for Culebra brines (see Appendix E).

July 24, 1996

APPENDIX A: MEETING TO ESTABLISH RANGES AND PROBABILITY
DISTRIBUTIONS OF ACTINIDE K_d s FOR THE WIPP PA
CALCULATIONS AND THE CCA

Invitation

March 25, 1996

Dear Colleague:

Attached is the agenda for the meeting to establish ranges and probability distributions of actinide K_d s for use in the long-term performance-assessment (PA) calculations to support the WIPP Compliance Certification Application (CCA). We will hold this meeting at the BDM Sandia Vista Building at 2301 Buena Vista SE in Albuquerque, NM, on Monday and Tuesday, April 1 and 2, 1996. Currently, we plan to meet in the Nuclear Waste Management Conference Room, the large conference room, all day Monday and Tuesday morning, and in Room 2105, a small conference room, on Tuesday afternoon. Because a key is required to enter the building in which the large conference room is located, I or someone else will meet you in the reception area of the Sandia Vista Building at 8:45 on Monday morning to take you to the large conference room if you do not have a key.

I view this as our main opportunity to reach consensus on the ranges and probability distributions of K_d s for Pu, Am, U, Th, and Np that we will submit to the US DOE's Carlsbad Area Office for their use in meeting the requirements of the Consultation and Cooperation (C & C) Agreement with the State of New Mexico, and then to PA personnel for their calculations to support the CCA.

Because most of you presented most of your results at the Retardation Research Program Review Meeting in Carlsbad last month, I have scheduled only one presentation for next week's meeting, Predictions of Actinide Oxidation States in the Culebra by Harlan Stockman of Sandia. However, please bring viewgraphs updated to include as many of your new data as possible for use in our discussions. Because you are very busy, please do not feel obligated to spend a lot of time making nice viewgraphs.

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Thank you very much in advance for taking time out of your busy schedule to participate in this meeting. I am looking forward to your input next week.

Best regards,

Larry Brush
WIPP Chemical & Disposal Room
Processes Department 6748

Distribution:

R. J. Lark, DOE/CAO
I. Triay, LANL
MS 0750 P. V. Brady (Org. 6118)
MS 0750 H. W. Stockman (Org. 6118)
MS 1320 E. J. Nowak (Org. 6831)
MS 1320 Y. Behl (Org. 6748)
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MS 1330 SWCF (Org. 6352), WBS 1.1.10.3.1 (2)

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Agenda

Monday and Tuesday, April 1 and 2, 1996
BDM Sandia Vista Building
2301 Buena Vista SE
Albuquerque, NM

Monday, April 1

9:00 - 9:30	Introduction	L. H. Brush, SNL
9:30 - 10:30	Predictions of Actinide Oxidation States in the Culebra	H. W. Stockman, SNL
10:30 - 10:45	Break	
10:45 - 11:45	Proposed Use of Ranges and Distributions of K_d s by PA	M. S. Tierney, SNL
11:45 - 13:00	Lunch	BDM Cafeteria
13:00 - 15:00	Discussion of Range and Distribution of K_d s for Pu(V)	All participants
15:00 - 15:15	Break	
15:15 - 17:15	Discussion of Range and Distribution of K_d s for Am(III) and Pu(III)	All participants

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Agenda (continued)

Tuesday, April 2

8:00 - 10:00	Discussion of Range and Distribution of K_d s for Th(IV), Pu(IV), and U(IV)	All participants
10:00 - 10:15	Break	
10:15 - 11:45	Discussion of Range and Distribution of K_d s for U(VI) and, if necessary, Pu(VI)	All participants
11:45 - 13:00	Lunch	BDM Cafeteria
13:00 - 13:30	Discussion of Range and Distribution of K_d s for U(VI) (continued)	All participants
13:30 - 13:45	Break	
13:45 - 15:45	Discussion of Range and Distribution of K_d s for Np(V)	All participants

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Participants

- Y. Behl, SciRes (SNL column transport study)
- P. V. Brady, SNL (Principal Investigator for the SNL/LANL mechanistic sorption study)
- L. H. Brush, SNL (Principal Investigator for the dissolved-actinide Retardation Research Program (RRP))
- R. V. Bynum, SAIC (Actinide Source Term Program management)
- C. Duffy, independent LANL contractor (LANL empirical sorption study)
- K. M. Economy, Ecodynamics (PA Culebra transport calculations)
- R. Holt, independent SNL contractor (characterization of clay minerals in the Culebra)
- E. J. Nowak, SNL (Manager, WIPP Chemical & Disposal Room Processes Department 6748)
- H. W. Papenguth, SNL (former Principal Investigator for the dissolved-actinide RRP)
- W. G. Perkins, SNL (Retardation Research Program management)
- M. D. Siegel, SNL (Principal Investigator for the Stanford mechanistic sorption study, brine mixing, and characterization of clay minerals in the Culebra)
- H. W. Stockman, SNL (predictions of actinide oxidation states in the Culebra)
- C. T. Stockman, SNL (predictions of actinide oxidation states in the Culebra)
- M. S. Tierney, SNL (Task Leader for the PA database)
- I. Triay, LANL (Group Leader, Chemical Science and Technology Group, and Principal Investigator for the LANL empirical sorption study)
- R. F. Weiner, SNL (Actinide Source Term Program)

Observers

- D. Hobart, Carlsbad Administrative and Technical Assistance Contractor (Actinide Source Term Program, Retardation Research Program)
- R. J. Lark, US DOE Carlsbad Area Office

APPENDIX B: RANGES AND PROBABILITY DISTRIBUTIONS OF
MATRIX K_d s FOR Pu(V) AND DOLOMITE-RICH
CULEBRA ROCK

Based on a laboratory study carried out under expected WIPP conditions and previously published results obtained for applications other than the WIPP Project, ASTP personnel have predicted that Pu will speciate as Pu(III) or Pu(IV), but not as Pu(V) nor Pu(VI), in deep (Castile and Salado) brines in the repository. Furthermore, a modeling study of the effects of mixing deep and Culebra brines on the oxidation states of Pu, U, and Np in the Culebra showed that Culebra fluids are poorly poised (see Predictions of Actinide Oxidation States in the Culebra above). Therefore, Pu will not speciate as Pu(V) in the Culebra. However, we could not establish experimentally obtained ranges of matrix K_d s for Am(III) (see Methods Used to Establish Ranges of Matrix K_d s above and Appendix C below). Instead, we established experimentally obtained ranges for Pu(V) and used them for Am(III) and Pu(III) by assuming that the K_d s for Am(III) and Pu(III) are greater than or equal to those for Pu(V).

To establish the *initial* ranges for Pu(V) and the deep brines, we first considered *all* of the data from the 6-week empirical sorption experiments carried out with Brine A and ERDA-6 on the bench top (0.033% CO₂) by Triay and her group at LANL (see Methods Used to Establish Ranges of Matrix K_d s for the reasons for considering these data). These runs were: #6004, #6024, #6044, #6064, and #6084 (see Table B-1 below), and #6005, #6025, #6045, #6065, and #6085 (Table B-2). Next, we discarded the data from #6025, #6045, and #6065, the runs in which the difference between the activity of the ²³⁹Pu in a standard and that in a control exceeded 3 σ , where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_d s.) Discarding the data from these three runs yielded an *initial* range of 19.1 ml/g (from #6004) to 387 ml/g (#6005) for Pu(V) and the deep brines.

To establish the *initial* ranges for Pu(V) and the Culebra brines, we first considered *all* of Triay's 6-week sorption data obtained with AISinR and H-17 on the bench top (0.033% CO₂) and in glove boxes with atmospheres containing 0.24 and 1.4% CO₂ (see Methods Used to Establish Ranges of Matrix K_d s). These were: #6006, #6026, #6046, #6066, #6086, #24006, #24026, #24046, #24066, #24086, #12006, #12026, #12046, #12066, and #12086 (Table B-3), and #6007, #6027, #6047, #6067, #6087, #24007, #24027, #24047, #24067, #24087, #12007, #12027, #12047, #12067, and #12087 (Table B-4). We then discarded the data from #6006, #24006, #24066, and #6007, the runs in which the difference between the activity of the ²³⁹Pu in a standard and that in a control exceeded 3 σ , to obtain the *initial* range of 8.70 ml/g (from #12007) to 3,517 ml/g (#12046) for Pu(V) and the Culebra brines.

Next, we compared these initial ranges with the data from the mechanistic sorption study by Brady and his colleagues at SNL and LANL. We used Brady's data to extend Triay's empirical sorption data for the deep brines to the basic conditions expected to result from the use of an MgO backfill in WIPP disposal rooms, *but not* to extend

Triay's data for the Culebra brines to basic conditions (see Methods Used to Establish Ranges of Matrix K_d s). Brady's data for 0.5 M NaCl, atmospheric CO_2 , and the highest pH value under these conditions are 82 and 69 ml/g at a pH of 9.9 (Table B-5). Because these values are *within* the initial range for Pu(V) and the deep brines (see above), and because we did not use this comparison to extend the initial range for Pu(V) and the Culebra brines to basic conditions, our *revised* ranges for Pu(V) remain 19.1 to 387 ml/g and 8.70 to 3,517 ml/g for the deep and Culebra brines, respectively.

We then compared both of these revised ranges with the data from the transport study with intact Culebra cores by Lucero and his colleagues at SNL. Lucero carried out his experiments under ambient atmospheric conditions; therefore, the CO_2 content of these experiments was probably similar to that in Triay's bench-top (0.033% CO_2) runs. Because Lucero *did not* observe breakthrough of Pu(V), it was only possible to determine a minimum K_d for this element. Lucero et al. (1996) submitted their results on March 28, 1996, (see Table B-6). Lucero and Brown (1996) and Brown (1996) then revised them on April 5 and 16, 1996, respectively (Tables B-7 and B-8). The minimum K_d s reported for experiments C-3, D3, and E-2 (Table B-8) *are consistent with the K_d s reported by Triay for Pu(V) and AlSinR in her experiments carried out on the bench top (0.033% CO_2)* (Table B-3). Because these values are consistent with the revised range for Pu(V) and the Culebra brines (see above), and because Lucero did not carry out any experiments with Pu(V) and the deep brines (Table B-8), our *final* ranges for Pu(V) remain 19.1 to 387 ml/g and 8.70 to 3,517 ml/g for the deep and Culebra brines, respectively. However, we rounded these ranges to 20 to 400 ml/g and 9 to 4,000 ml/g, respectively prior to inclusion in Table 1 above.

We recommend that PA personnel use a uniform probability distribution for both of these ranges (see Methods Used to Establish Probability Distributions of Matrix K_d s above).

Furthermore, we recommend that PA use the range of 20 to 400 ml/g (the range for deep brines) for Pu(V) because this range results in less retardation of this element than the range for Culebra brines (see Methods Used for Final Selection of the Range of Matrix K_d s for Use in PA Calculations above).

Finally, we recommend that PA use a range of 20 to 400 ml/g for Pu(III) and Am(III) (see Methods Used to Establish Ranges of Matrix K_d s and Appendix C).

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Table B-1. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Pu(V), Dolomite-Rich Culebra Rock, and Brine A (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. No K_d s in this table excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{239}Pu Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
Brine A	4.73×10^{-7} to 4.87×10^{-7}	19.1, #6004	19.9, #24004	26.8, #12004	23.8, #18004
Brine A	1.31×10^{-7} to 1.37×10^{-7}	46.1, #6024	219.2, #24024	32.4, #12024	30.2, #18024
Brine A	6.97×10^{-8} to 7.04×10^{-8}	23.5, #6044	29.0, #24044	36.9, #12044	33.2, #18044
Brine A	1.42×10^{-8} to 1.51×10^{-8}	22.9, #6064	25.6, #24064	54.6, #12064	26.9, #18064
Brine A	7.22×10^{-9} to 7.65×10^{-9}	24.0, #6084	25.6, #24084	26.2, #12084	25.4, #18084

Table B-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Pu(V); Dolomite-Rich Culebra Rock, and ERDA-6 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{239}Pu Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
ERDA-6	4.52 x 10 ⁻⁷ to 4.93 x 10 ⁻⁷	387, #6005	5,789, #24005	5,940, #12005	127, #18005
ERDA-6	1.29 x 10 ⁻⁷ to 1.35 x 10 ⁻⁷	3,297, #6025	5,460, #24025	5,853, #12025	172, #18025
ERDA-6	8.34 x 10 ⁻⁸ to 8.49 x 10 ⁻⁸	2,454, #6045	2,556, #24045	6,340, #12045	212, #18045
ERDA-6	1.49 x 10 ⁻⁸ to 1.53 x 10 ⁻⁸	569, #6065	958, #24065	1,657, #12065	143, #18065
ERDA-6	9.58 x 10 ⁻¹⁰ to 7.07 x 10 ⁻⁹	124, #6085	990, #24085	1,231, #12085	3,820, #18085

Table B-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Pu(V), Dolomite-Rich Culebra Rock, and AISinR (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{239}Pu Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
AISinR	1.77×10^{-7} to 4.17×10^{-7}	338, #6006	60.3, #24006	1,833, #12006	3,980, #18006
AISinR	1.05×10^{-7} to 1.17×10^{-7}	1,930, #6026	36.1, #24026	1,024, #12026	4,905, #18026
AISinR	5.72×10^{-8} to 5.86×10^{-8}	215, #6046	38.6, #24046	3,517, #12046	6,076, #18046
AISinR	1.11×10^{-8} to 1.15×10^{-8}	422, #6066	48.9, #24066	823, #12066	1,850, #18066
AISinR	5.66×10^{-9} to 6.11×10^{-9}	484, #6086	41.7, #24086	1,037, #12086	1,320, #18086

Table B-4. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Pu(V), Dolomite-Rich Culebra Rock, and H-17 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{239}Pu Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
H-17	4.72×10^{-7} to 4.81×10^{-7}	143, #6007	81.3, #24007	8.70, #12007	24.3, #18007
H-17	4.45×10^{-8} to 1.20×10^{-7}	174, #6027	141, #24027	12.1, #12027	30.5, #18027
H-17	5.71×10^{-8} to 6.17×10^{-8}	302, #6047	167, #24047	12.9, #12047	33.2, #18047
H-17	1.20×10^{-8} to 1.25×10^{-8}	233, #6067	165, #24067	22.9, #12067	39.7, #18067
H-17	6.21×10^{-9} to 6.29×10^{-9}	214, #6087	579, #24087	85.4, #12087	41.5, #18087

Table B-5. Effects of pH and P_{CO_2} on Matrix K_d s for Pu(V) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study). Sorption runs with Norwegian dolomite and 0.5 M NaCl. Data current as of March 31, 1996. Table retyped by L. H. Brush on April 24, 1996. Table checked by Y. Behl on April 28, 1996. Table revised by Brush on July 5, 1996, based on Brady (1996). Table checked by A. C. Peterson on July 15, 1996.

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
9.9	82	NA	NA
9.9	69	NA	NA
8.4	25	NA	NA
6.7	-8	NA	NA
6.2	6	NA	NA
5.8	6	NA	NA
5.2	6	NA	NA
4.6	25	NA	NA
4.1	-22	NA	NA
3.5	-8	NA	NA
3.1	-62	NA	NA

Table B-5. Effects of pH and P_{CO_2} on Matrix K_d s for Pu(V) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.9	NA	93	NA
8.5	NA	742	NA
7.3	NA	205	NA
7.2	NA	232	NA
7.0	NA	193	NA
6.9	NA	83	NA
6.6	NA	63	NA
6.2	NA	114	NA
5.3	NA	39	NA
4.0	NA	19	NA
3.1	NA	19	NA

Table B-5. Effects of pH and P_{CO_2} on Matrix K_d s for Pu(V) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.4	NA	NA	24
6.9	NA	NA	99
6.9	NA	NA	92
6.8	NA	NA	99
6.7	NA	NA	104
6.8	NA	NA	74
6.5	NA	NA	84
6.1	NA	NA	44
5.8	NA	NA	29
4.9	NA	NA	4
3.6	NA	NA	24

NA: not applicable.

Table B-6. Minimum Values of R and K_d for Pu(V) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-3	VPX-28-6C	AIS.	0.1	211	30.45	5,200	3.7 ^S	84	NA
D-3	VPX-25-8A	AIS.	0.1	118	17.02	1,140	9.1, ^S 5.3 ^D	46	NA
E-2	VPX-27-7A	AIS.	0.1	61	8.83	405	23, ^S 15.7 ^D	40	NA

AIS: AISinR.

D: dual porosity assumed.

NA: not available yet.

S: single porosity assumed.

Table B-7. Minimum Values of R and K_d for Pu(V) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-3	VPX-28-6C	AIS.	0.1	211	30.45	5,200	3.7 ^S	84	NA
D-3	VPX-25-8A	AIS.	0.1	118	17.02	1,140	9.1 ^S	46	NA
E-2	VPX-27-7A	AIS.	0.1	61	8.83	405	23 ^S	40	NA

AIS: AISinR.

NA: not available yet.

S: single porosity assumed.

Table B-8. Minimum Values of R and K_d for Pu(V) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y Behl on April 8, 1996. Table revised by Brush on April 17, 1996, based on Brown (1996).

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-3	VPX-28-6C	AIS.	0.1	211	30.45	5,200	3.7 ^S	84	NA
D-3	VPX-25-8A	AIS.	0.1	118	17.02	1,140	9.1 ^S	45	NA
E-2	VPX-27-7A	AIS.	0.1	61	8.83	405	23 ^S	40	NA

AIS: AISinR.

NA: not available yet.

S: single porosity assumed.

APPENDIX C: RANGES AND PROBABILITY DISTRIBUTIONS OF MATRIX K_d s FOR Am(III) AND DOLOMITE-RICH CULEBRA ROCK

For Am, only one oxidation state, Am(III), is possible in the Culebra (see Predictions of Actinide Oxidation States in the Culebra above). Therefore, we attempted to establish experimentally obtained ranges of matrix K_d s for Am(III), and use them and the oxidation-state analogy to establish ranges for Pu(III).

To establish the *initial* ranges for Am(III) and the deep brines, we first considered *all* of the data from the 6-week empirical sorption experiments carried out with Brine A and ERDA-6 on the bench top (0.033% CO₂) by Triay and her group at LANL (see Methods Used to Establish Ranges of Matrix K_d s above for the reasons for considering these data). These runs were: #6012, #6032, #6052, #6072, and #6092 (see Table C-1 below), and #6013, #6033, #6053, #6073, and #6093 (Table C-2). We discarded the data from #6012, #6032, #6013, #6033, #6073, and #6093, the runs in which the difference between the activity of the ²⁴³Am in a standard and that in a control exceeded 3 σ , where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_d s.) Even after discarding the results of these six runs, however, the defensibility of the remaining data is questionable because the K_d s retained for Brine A increase significantly as the final dissolved concentration of ²⁴³Am increases. (We will include these isotherms in the parameter and analysis records packages for these K_d s. However, this trend is also apparent in Table C-1.) Furthermore, the isotherm obtained by plotting the quantity of radionuclide sorbed by the solid phase or phases versus the final dissolved radionuclide concentration does not appear to pass through the origin. The K_d s are also proportional to the final dissolved ²⁴³Am concentration in the runs carried out in the glove box with an atmosphere containing 1.4% CO₂, and, based on the trends observed with *both* retained and discarded data, *appear* to increase similarly in the runs conducted in the glove boxes with atmospheres containing 0.24 and 4.1% CO₂ (Table C-1). Moreover, based on the trends observed with *both* retained and discarded data, these K_d s also *appear* proportional to the final dissolved ²⁴³Am concentration at all four CO₂ concentrations in the runs with ERDA-6 (Table C-2). These trends suggest that sorption of Am by the container walls, precipitation of an Am-bearing solid phase, coprecipitation of Am by another phase, incomplete separation of the aqueous and the solid phases at the end of an experiment, or some combination of these processes occurred in the runs with Am(III). We thought we had eliminated reactions other than sorption by the rock in these experiments because: (1) LANL personnel had filtered the brines sequentially, with a minimum filter size of 0.2 μ m, after these runs; (2) we had discarded results from the runs in which the difference between the activity of the radionuclide in the standard and that in the control exceeded 3 σ before examining these data; (3) the final Am(III) concentrations in these runs were less than the solubilities predicted by FMT for these brines. Triay carried out additional posttest analyses of the brines from her 6-week sorption experiments with Am(III) with 0.033% CO₂ to determine, if possible, what caused these trends, and to redetermine these K_d s. She did not attempt any additional posttest analyses of the brines from experiments conducted in the glove boxes because she had removed them from these glove boxes after

the original runs, thus exposing them to conditions different from those during the runs. Triay first recounted the brines to determine if mistaken sample identification or improper data entry had caused the trends described above. She then refiltered, centrifuged, and/or ultracentrifuged the brines to remove any suspended particles, and recounted them. Finally, she recalculated the K_{ds} using the controls instead of the standards to specify the initial dissolved ^{243}Am concentration. Despite these efforts, the data continued to display trends similar to those described above.

The 6-week LANL sorption experiments carried out with Am(III) and the Culebra brines (AISinR and H-17) yielded the same trends described above for the deep brines (compare Tables C-3 and C-4 with Tables C-1 and C-2). Therefore, we could not use them to establish a range for Am(III).

We did not use the data from the mechanistic sorption study by Brady and his colleagues at SNL and LANL, nor the column transport study by Lucero and his colleagues at SNL to establish a range for Am(III) for several reasons. First, Brady had used pure Norwegian dolomite and pure NaCl solutions, not actual Culebra dolomite and synthetic Culebra fluids. (Although we used his data to *extend* the initial ranges established with Triay's empirical data to the basic conditions expected to result from the use of an MgO backfill in WIPP disposal rooms, we *did not* believe this would be defensible in the absence of *any* empirical data for actual Culebra dolomite and synthetic Culebra fluids.) Furthermore, Brady did not report data for Am(III) with atmospheric and 0.5% CO_2 (see Table C-6), the headspace concentrations corresponding to CO_2 partial pressures within the range that Siegel now considers likely for groundwaters in the Culebra off-site transport pathway (see Methods Used to Establish Ranges of Matrix K_{ds}), above a pH of about 5 or 6. Moreover, although Brady *did* report data for Nd(III) with atmospheric and 0.5% CO_2 at neutral or nearly neutral values of pH (Table C-5), he also obtained them with pure Norwegian dolomite and pure NaCl solutions, not actual Culebra dolomite and synthetic Culebra fluids. Finally, because Lucero *did not* observe breakthrough of Am(III), it is only possible to determine minimum K_{ds} for this element (Tables C-7 through C-9). These minimum values are significantly lower than actual Am(III) K_{ds} typically obtained for applications other than the WIPP Project (see below).

Therefore, we recommend using the *experimentally obtained* ranges for Pu(V) (see Table 1 and Appendix B above) for Am(III) by assuming that the K_{ds} for Am(III) are greater than or equal to those for Pu(V). This assumption is reasonable in view of results such as those in Figure 5 of Canepa (1992). In this case, the Am(III) K_d obtained for the Yucca Mountain Project is about one order of magnitude higher than that obtained for Pu(V) under the same conditions. (We will cite additional examples of differences between the K_{ds} for Am(III) and Pu(V) in future reports and presentations.) We *have not* used the oxidation-state analogy to justify the use of Pu(V) data for Am(III); instead, this approach is based on *differences* in the behavior of these oxidation states. Furthermore, we recommend using the range for Am(III) for Pu(III); for this recommendation, we *have* used the oxidation-state analogy.

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Table C-1. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Am(III), Dolomite-Rich Culebra Rock, and Brine A (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{243}Am Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
Brine A	1.10×10^{-7} to 1.24×10^{-7}	811, #6012	876, #24012	1,109, #12012	1,061, #18012
Brine A	5.45×10^{-8} to 6.18×10^{-8}	779, #6032	937, #24032	955, #12032	902, #18032
Brine A	1.15×10^{-8} to 1.24×10^{-8}	429, #6052	436, #24052	465, #12052	502, #18052
Brine A	5.86×10^{-9} to 6.25×10^{-9}	278, #6072	299, #24072	329, #12072	291, #18072
Brine A	1.25×10^{-9} to 1.31×10^{-9}	57.1, #6092	64.3, #24092	73.0, #12092	65.4, #18092

Table C-2: Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Am(III), Dolomite-Rich Culebra Rock, and ERDA-6 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{243}Am Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
ERDA-6	1.11×10^{-7} to 1.24×10^{-7}	4,717, #6013	8,056, #24013	9,061, #12013	4,393, #18013
ERDA-6	6.08×10^{-8} to 7.25×10^{-8}	4,288, #6033	3,992, #24033	6,818, #12033	1,748, #18033
ERDA-6	1.04×10^{-8} to 1.17×10^{-8}	1,389, #6053	1,351, #24053	1,692, #12053	1,013, #18053
ERDA-6	5.19×10^{-9} to 5.96×10^{-9}	822, #6073	737, #24073	699, #12073	633, #18073
ERDA-6	1.20×10^{-9} to 1.61×10^{-9}	177, #6093	228, #24093	209, #12093	217, #18093

Table C-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Am(III), Dolomite-Rich Culebra Rock, and ASInR (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{243}Am Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
ASInR	9.59×10^{-8} to 1.06×10^{-7}	1,740, #6014	709, #24014	618, #12014	493, #18014
ASInR	5.41×10^{-8} to 5.95×10^{-8}	1,616, #6034	577, #24034	656, #12034	490, #18034
ASInR	9.03×10^{-9} to 1.02×10^{-8}	907, #6054	738, #24054	424, #12054	423, #18054
ASInR	4.70×10^{-9} to 5.96×10^{-9}	634, #6074	621, #24074	334, #12074	324, #18074
ASInR	1.22×10^{-9} to 1.36×10^{-9}	185, #6094	141, #24094	129, #12094	NR, #18094

NR: not reported.

Table C-4. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Am(III), Dolomite-Rich Culebra Rock, and H-17 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{243}Am Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
H-17	4.01×10^{-8} to 4.86×10^{-8}	1,445, #6015	1,190, #24015	626, #12015	497, #18015
H-17	2.38×10^{-8} to 4.14×10^{-8}	1,038, #6035	1,017, #24035	565, #12035	440, #18035
H-17	8.76×10^{-9} to 9.39×10^{-9}	793, #6055	760, #24055	454, #12055	576, #18055
H-17	5.67×10^{-9} to 6.19×10^{-9}	752, #6075	568, #24075	380, #12075	349, #18075
H-17	1.36×10^{-9} to 1.54×10^{-9}	69.2, #6095	170, #24095	172, #12095	141, #18095

Table C-5. Effects of pH and P_{CO_2} on Matrix K_d s for Nd(III) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study). Sorption runs with Norwegian dolomite and 0.05 M NaCl. Data current as of March 31, 1996. Table retyped by L. H. Brush on April 24, 1996. Table checked by Y. Behl on April 28, 1996.

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
9.08	2,864.3	NA	NA
8.41	1,619.2	NA	NA
7.52	1,225.2	NA	NA
6.72	1,141.4	NA	NA
6.49	571.49	NA	NA
6.19	497.91	NA	NA
5.74	546.24	NA	NA
5.25	272.78	NA	NA
4.63	241.5	NA	NA
4.2	279.24	NA	NA
3.75	202.2	NA	NA
3.35	141.3	NA	NA

Table C-5. Effects of pH and P_{CO_2} on Matrix K_d s for Nd(III) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
7.08	NA	538.93	NA
6.81	NA	403.05	NA
6.45	NA	261.86	NA
6.26	NA	386.81	NA
5.92	NA	149.45	NA
5.18	NA	84.721	NA
4.35	NA	55.485	NA
3.64	NA	51.358	NA

Table C-5. Effects of pH and P_{CO_2} on Matrix K_d s for Nd(III) and Pure Dolomite
(SNL/LANL Mechanistic Sorption Study) (continued)

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.33	NA	NA	226.71
6.24	NA	NA	179.19
6.15	NA	NA	182.28
6.01	NA	NA	169.89
5.88	NA	NA	168.9
5.76	NA	NA	111.58
5.54	NA	NA	72.6
5.21	NA	NA	206.36
3.42	NA	NA	34.636

NA: not applicable.

Table C-6. Effects of pH and P_{CO_2} on Matrix K_d s for Am(III) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study). Sorption runs with Norwegian dolomite and 0.5 M NaCl. Data current as of March 31, 1996. Table retyped by L. H. Brush on April 24, 1996. Table checked by Y. Behl on April 28, 1996. Table revised by Brush on July 5, 1996, based on Brady (1996). Table checked by A. C. Peterson on July 15, 1996.

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
9.9	NR	NA	NA
9.9	NR	NA	NA
8.4	NR	NA	NA
6.7	NR	NA	NA
6.2	NR	NA	NA
5.8	NR	NA	NA
5.2	NR	NA	NA
4.6	158	NA	NA
4.1	126	NA	NA
3.5	57	NA	NA
3.1	18	NA	NA

Table C-6. Effects of pH and P_{CO_2} on Matrix K_d s for Am(III) and Pure Dolomite
(SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.9	NA	NR	NA
8.5	NA	NR	NA
7.3	NA	NR	NA
7.2	NA	NR	NA
7.0	NA	NR	NA
6.9	NA	NR	NA
6.6	NA	NR	NA
6.2	NA	NR	NA
5.3	NA	226	NA
4.0	NA	13	NA
3.1	NA	31	NA

Table C-6. Effects of pH and P_{CO_2} on Matrix K_d s for Am(III) and Pure Dolomite
(SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.4	NA	NA	NR
6.9	NA	NA	NR
6.9	NA	NA	NR
6.8	NA	NA	NR
6.7	NA	NA	NR
6.8	NA	NA	NR
6.5	NA	NA	NR
6.1	NA	NA	NR
5.8	NA	NA	386
4.9	NA	NA	66
3.6	NA	NA	-2

NA: not applicable.

NR: not reported.

Table C-7. Minimum Values of R and K_d for Am(III) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-3	VPX-28-6C	AIS.	0.1	211	30.45	1,420	3.7 ^S	11	NA
D-3	VPX-25-8A	AIS.	0.1	118	17.02	350	9.1, ^S 5.3 ^D	14	NA
E-2	VPX-27-7A	AIS.	0.1	61	8.83	200	23, ^S 15.7 ^D	20	NA

AIS: AISinR.

D: dual porosity assumed.

NA: not available yet.

S: single porosity assumed.

Table C-8. Minimum Values of R and K_d for Am(III) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y. Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-3	VPX-28-6C	AIS.	0.1	211	30.45	1,420	3.7 ^S	11	NA
D-3	VPX-25-8A	AIS.	0.1	118	17.02	350	9.1 ^S	14	NA
E-2	VPX-27-7A	AIS.	0.1	61	8.83	200	23 ^S	20	NA

AIS: AISinR.

NA: not available yet.

S: single porosity assumed.

Table C-9. Minimum Values of R and K_d for Am(III) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y. Behl on April 8, 1996. Table revised by Brush on April 17, 1996, based on Brown (1996).

Run #	Solid- (core)	Brine	Flow rate (ml/ min)	Run Time (days)	Ef- fluent Vol. (L)	R_{min}	Poro- sity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/ g)
C-3	VPX- 28-6C	AIS.	0.1	211	30.45	1,420	3.7 ^S	23	NA
D-3	VPX- 25-8A	AIS.	0.1	118	17.02	350	9.1 ^S	14	NA
E-2	VPX- 27-7A	AIS.	0.1	61	8.83	200	23 ^S	20	NA

AIS: AISinR.

NA: not available yet.

S: single porosity assumed.

APPENDIX D: RANGES AND PROBABILITY DISTRIBUTIONS OF
MATRIX K_d s FOR U(VI) AND DOLOMITE-RICH
CULEBRA ROCK

Based on experimental results, ASTP personnel have predicted that U will speciate as U(IV) or U(VI) in deep (Castile and Salado) brines in WIPP disposal rooms. Furthermore, a modeling study of the effects of mixing deep and Culebra brines on the oxidation states of Pu, U, and Np in the Culebra showed that Culebra fluids are poorly poised (see Predictions of Actinide Oxidation States in the Culebra above). Therefore; we established experimentally obtained ranges of matrix K_d s for U(VI) and used the experimentally obtained ranges for Th(IV) (see Appendix E below) and the oxidation-state analogy to establish ranges for U(IV) (and Np(IV)).

To establish the *initial* ranges for U(VI) and the deep brines, we first considered *all* of the data from the 6-week empirical sorption experiments carried out with Brine A and ERDA-6 on the bench top (0.033% CO₂) by Triay and her group at LANL (see Methods Used to Establish Ranges of Matrix K_d s above for the reasons for considering these data). These runs were: #6008, #6028, #6048, #6068, and #6088 (see Table D-1 below), and #6009, #6029, #6049, #6069, and #6089 (Table D-2). Next, we discarded the data from #6008, #6028, #6048, #6068, and #6009, the runs in which the difference between the activity of the ²³³U in a standard and that in a control exceeded 3 σ , where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_d s). Discarding the data from these five runs yielded an *initial* range of 3.20 ml/g (from #6029) to 18.4 ml/g (#6088) for U(VI) and the deep brines.

To establish the *initial* ranges for U(VI) and the Culebra brines, we first considered *all* of Triay's 6-week sorption data obtained with AISinR and H-17 on the bench top (0.033% CO₂) and in glove boxes with atmospheres containing 0.24 and 1.4% CO₂ (see Methods Used to Establish Ranges of Matrix K_d s). These were: #6010, #6030, #6050, #6070, #6090, #24010, #24030, #24050, #24070, #24090, #12010, #12030, #12050, #12070, and #12090 (Table D-3), and #6011, #6031, #6051, #6071, #6091, #24011, #24031, #24051, #24071, #24091, #12011, #12031, #12051, #12071, and #12091 (Table D-4). We then discarded the data from #6010, #6050, #6070, #24010, #24030, #12010, #6011, #6031, #6051, #6071, #12011, and #12051, the runs in which the difference between the activity of the ²³³U in a standard and that in a control exceeded 3 σ , to obtain the *initial* range of -1.50 ml/g (from #12091) to 62.4 ml/g (#24091) for U(VI) and the Culebra brines. However, we set the lower limit of this range equal to 0 ml/g because there is no reason why a K_d could have a value less than 0.

Next, we compared these initial ranges with the data from the mechanistic sorption study by Brady and his colleagues at SNL and LANL. We used Brady's data to extend Triay's empirical sorption data for the deep brines to the basic conditions expected to result from the use of an MgO backfill in WIPP disposal rooms, *but not* to extend Triay's data for the Culebra brines to basic conditions (see Methods Used to Establish Ranges of Matrix K_d s). Brady's data for 0.5 M NaCl, atmospheric CO₂, and the highest

pH value under these conditions are 2 and 6 ml/g at a pH of 9.9 (Table D-5)... Because one of these values is *less than the lower limit* of the initial range for U(VI) and the deep brines (see above), we extended this range to obtain a *revised* range for U(VI) and deep brines of 2 to 18.4 ml/g. Because we did not use this comparison to extend the initial range for U(VI) and the Culebra brines to basic conditions, this *revised* range remains 0 to 62.4 ml/g.

We then compared both of these revised ranges with the data from the transport study with intact Culebra cores by Lucero and his colleagues at SNL. Lucero carried out his experiments under ambient atmospheric conditions; therefore, the CO₂ content of these experiments was probably similar to that in the LANL bench-top (0.033% CO₂) runs. Lucero *did* observe breakthrough of U(VI) in his experiments. Therefore, it was possible to determine actual K_ds for this element. Lucero et al. (1996) submitted their results on March 28, 1996, (see Table D-6). Lucero and Brown (1996) and Brown (1996) then revised them on April 5 and 16, 1996 (Tables D-7 and D-8, respectively). The K_d reported for Experiment C-7 with the deep brine ERDA-6 (Table D-8) is *less than the lower limit of the revised range of K_ds for U(VI) and the deep brines obtained from the empirical and mechanistic sorption studies* (see above). Therefore, we extended this range to obtain a *final* range for U(VI) and deep brines of 0.029 to 18.4 ml/g, and rounded it to 0.03 to 20 ml/g prior to inclusion in Table 1 above. Because Lucero's K_ds for U(VI) and the Culebra brine AISinR (B-3, B-6, C-2, D-5, and D-6 in Table D-8) are *within* the revised range for U(VI) and the Culebra brines (see above), our *final* range remains 0 to 62.4 ml/g, rounded to 0 to 60 ml/g for inclusion in Table 1.

We recommend that PA personnel use a uniform probability distribution for both of these ranges (see Methods Used to Establish Probability Distributions of Matrix K_ds above).

Finally, we recommend that PA use the range of 0.03 to 20 ml/g (the range for deep brines) for U(VI) because this range results in less retardation of this element than the range for Culebra brines (see Methods Used for Final Selection of the Range of Matrix K_ds for Use in PA Calculations above).

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Table D-1. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for U(VI), Dolomite-Rich Culebra Rock, and Brine A (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{233}U Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
Brine A	2.02×10^{-6} to 2.97×10^{-6}	10.5, #6008	4.00, #24008	1.00, #12008	0.600, #18008
Brine A	1.09×10^{-6} to 1.39×10^{-6}	14.1, #6028	2.40, #24028	1.00, #12028	2.20, #18028
Brine A	2.87×10^{-7} to 3.44×10^{-7}	16.7, #6048	4.40, #24048	1.20, #12048	2.10, #18048
Brine A	1.13×10^{-7} to 1.34×10^{-7}	13.9, #6068	5.70, #24068	0.800, #12068	1.90, #18068
Brine A	3.41×10^{-8} to 4.21×10^{-8}	18.4, #6088	4.00, #24088	-4.50, #12088	1.20, #18088

Table D-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for U(VI), Dolomite-Rich Culebra Rock, and ERDA-6 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{233}U Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
ERDA-6	3.38×10^{-6} to 3.56×10^{-6}	0.500, #6009	1.10, #24009	3.50, #12009	3.10, #18009
ERDA-6	1.18×10^{-6} to 1.27×10^{-6}	3.20, #6029	1.30, #24029	5.00, #12029	2.70, #18029
ERDA-6	3.10×10^{-7} to 3.31×10^{-7}	3.20, #6049	2.00, #24049	6.10, #12049	2.40, #18049
ERDA-6	1.19×10^{-7} to 1.27×10^{-7}	3.30, #6069	3.70, #24069	5.20, #12069	3.90, #18069
ERDA-6	3.39×10^{-8} to 3.80×10^{-8}	5.50, #6089	1.80, #24089	5.90, #12089	0.900, #18089

Table D-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for U(VI), Dolomite-Rich Culebra Rock, and AISinR (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{233}U Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
AISinR	3.13×10^{-6} to 3.45×10^{-6}	2.50, #6010	0.300, #24010	0.500, #12010	1.60, #18010
AISinR	1.10×10^{-6} to 1.19×10^{-6}	2.50, #6030	2.60, #24030	2.00, #12030	0.700, #18030
AISinR	2.89×10^{-7} to 3.42×10^{-7}	3.60, #6050	0.400, #24050	1.60, #12050	3.50, #18050
AISinR	9.70×10^{-8} to 1.17×10^{-7}	3.90, #6070	3.10, #24070	1.00, #12070	0.100, #18070
AISinR	2.87×10^{-8} to 3.56×10^{-8}	7.20, #6090	0.100, #24090	1.70, #12090	1.70, #18090

Table D-4. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for U(VI), Dolomite-Rich Culebra Rock, and H-17. (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{233}U Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
H-17	2.98×10^{-6} to 3.30×10^{-6}	3.30, #6011	0.300, #24011	-0.700, #12011	-0.300, #18011
H-17	1.20×10^{-6} to 1.46×10^{-6}	5.00, #6031	1.20, #24031	0.100, #12031	0.400, #18031
H-17	2.63×10^{-7} to 3.61×10^{-7}	6.30, #6051	2.60, #24051	-1.60, #12051	2.00, #18051
H-17	9.71×10^{-8} to 1.23×10^{-7}	4.70, #6071	1.70, #24071	1.40, #12071	-1.10, #18071
H-17	2.72×10^{-8} to 3.72×10^{-8}	9.30, #6091	62.4, #24091	-1.50, #12091	2.70, #18091

Table D-5. Effects of pH and P_{CO_2} on Matrix K_d s for U(VI) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study). Sorption runs with Norwegian dolomite and 0.5 M NaCl. Data current as of March 31, 1996. Table retyped by L. H. Brush on April 24, 1996. Table checked by Y. Behl on April 28, 1996. Table revised by Brush on July 5, 1996, based on Brady (1996). Table checked by A. C. Peterson on July 15, 1996.

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
9.9	6	NA	NA
9.9	2	NA	NA
8.4	1,538	NA	NA
6.7	958	NA	NA
6.2	669	NA	NA
5.8	1,137	NA	NA
5.2	495	NA	NA
4.6	495	NA	NA
4.1	524	NA	NA
3.5	468	NA	NA
3.1	379	NA	NA

Table D-5. Effects of pH and P_{CO_2} on Matrix K_d s for U(VI) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.9	NA	155	NA
8.5	NA	-22	NA
7.3	NA	8	NA
7.2	NA	24	NA
7.0	NA	57	NA
6.9	NA	169	NA
6.6	NA	222	NA
6.2	NA	91	NA
5.3	NA	354	NA
4.0	NA	322	NA
3.1	NA	844	NA

Table D-5. Effects of pH and P_{CO_2} on Matrix K_d s for U(VI) and Pure Dolomite
(SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.4	NA	NA	95
6.9	NA	NA	13
6.9	NA	NA	3
6.8	NA	NA	8
6.7	NA	NA	13
6.8	NA	NA	13
6.5	NA	NA	59
6.1	NA	NA	303
5.8	NA	NA	411
4.9	NA	NA	615
3.6	NA	NA	334

NA: not applicable.

Table D-6. Measured Values of R and Calculated Values of K_d for U(VI) in Intact Culebra Cores (SNL Column Transport Study). Values in bold font to be excluded from ranges and distributions because fits to elution data were inferior to those assuming single porosity and dual porosity with fracture retardation. Data current as of March 30, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity (%)	K_d (ml/g)	Range (\pm ml/g)
B-3	VPX-26-11A	AIS.	0.1	NA	NA	3.4; ^S	9.8 ^S	.084 ^S	.022 ^S
						1, 18.3; ^N	5.2 ^{DN}	0.68 ^{DN}	.67 ^{DN}
						3.1, 5.2 ^{DF}	5.2 ^{DF}	.039 ^{DF}	0.03 ^{DF}
B-6	VPX-26-11A	AIS.	0.05	NA	NA	13.1; ^S	4.8 ^S	0.25 ^S	0.07 ^S
						1, NA; ^{DN}	NA ^{DN}	NA ^{DN}	NA ^{DN}
						NA, NA ^{DF}	NA ^{DF}	NA ^{DF}	NA ^{DF}
C-2	VPX-28-6C	AIS.	0.1	21	2	10.4; ^S	5.7 ^S	0.23 ^S	0.08 ^S
						1, 260; ^{DN}	3.5 ^{DN}	3.9 ^{DN}	7 ^{DN}
						12.0, 0.6 ^{DF}	3.5 ^{DF}	0.17 ^{DF}	0.06 ^{DF}
C-7	VPX-28-6C	ER.-6	0.1	13	2	2.7; ^S	3.9 ^S	.029 ^S	.022 ^S
						1, 0.6; ^{DN}	2.1 ^{DN}	.069 ^{DN}	0.13 ^{DN}
						2.7, 0.76 ^{DF}	2.1 ^{DF}	.016 ^{DF}	.005 ^{DF}

Table D-6. Measured Values of R and Calculated Values of K_d for U(VI) in Intact Culebra Cores (SNL Column Transport Study) (continued)

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity (%)	K_d (ml/g)	Range (\pm ml/g)
D-5	VPX-25-8A	AIS.	0.1	13	2	21, ^S	17.3 ^S	1.50 ^S	0.38 ^S
						1, 184, ^{DN}	7.1 ^{DN}	5.6 ^{DN}	5.5 ^{DN}
						NA, NA ^{DF}	7.1 ^{DF}	NA ^{DF}	NA ^{DF}
D-6	VPX-25-8A	AIS.	0.05	60	2	10.1, ^S	15.5 ^S	0.61 ^S	0.15
						1, NA, ^{DN}	7.1 ^{DN}	NA ^{DN}	NA ^{DN}
						12.3, 71 ^{DF}	7.1 ^{DF}	0.35 ^{DF}	0.19 ^{DF}

AIS: AISinR.

DF: dual porosity and fracture retardation assumed.

DN: dual porosity and no fracture retardation assumed.

ER-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

Table D-7. Measured Values of R and Calculated Values of K_d for U(VI) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 30, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y. Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity (%)	K_d (ml/g)	Range (\pm ml/g)
B-3	VPX-26-11A	AIS.	0.1	NA	NA	3.4 ^S	9.8 ^S	0.084 ^S	NA ^S
B-6	VPX-26-11A	AIS.	0.05	NA	NA	13 ^S	4.8 ^S	0.25 ^S	NA ^S
C-2	VPX-28-6C	AIS.	0.1	21	2	10.4 ^S	5.7 ^S	0.23 ^S	NA ^S
C-7	VPX-28-6C	ER.-6	0.1	13	2	2.7 ^S	3.9 ^S	0.029 ^S	NA ^S
D-5	VPX-25-8A	AIS.	0.1	13	2	21 ^S	17.3 ^S	1.5 ^S	NA ^S
D-6	VPX-25-8A	AIS.	0.05	60	2	10 ^S	15.5 ^S	0.61 ^S	NA ^S

AIS: AISinR.

ER.-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

Table D-8. Measured Values of R and Calculated Values of K_d for U(VI) in Intact Culebra Cores. (SNL Column Transport Study). Data current as of March 30, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996 based on Lucero and Brown (1996). Table checked by Y. Behl on April 8, 1996. Table revised by Brush on April 17, 1996, based on Brown (1996).

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity (%)	K_d (ml/g)	Range (\pm ml/g)
B-3	VPX-26-11A	AIS.	0.1	NA	NA	3.4 ^S	9.8 ^S	0.10 ^S	NA ^S
B-6	VPX-26-11A	AIS.	0.05	NA	NA	13 ^S	4.8 ^S	0.25 ^S	NA ^S
C-2	VPX-28-6C	AIS.	0.1	21	2	10.4 ^S	5.7 ^S	0.23 ^S	NA ^S
C-7	VPX-28-6C	ER.-6	0.1	13	2	2.7 ^S	3.9 ^S	0.029 ^S	NA ^S
D-5	VPX-25-8A	AIS.	0.1	13	2	21 ^S	17.3 ^S	1.5 ^S	NA ^S
D-6	VPX-25-8A	AIS.	0.05	60	2	10 ^S	15.5 ^S	0.61 ^S	NA ^S

AIS: AISinR.

ER.-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

APPENDIX E: RANGES AND PROBABILITY DISTRIBUTIONS OF
MATRIX K_d s FOR Th(IV) AND DOLOMITE-RICH
CULEBRA ROCK

For Th, only one oxidation state, Th(IV), is possible in the Culebra (see Predictions of Actinide Oxidation States in the Culebra above). Therefore, we established an experimentally obtained range of matrix K_d s for Th(VI), and used it and the oxidation-state analogy to establish ranges for Pu(IV), U(IV), and Np(IV).

To establish the *initial* ranges for Th(IV) and the deep brines, we first considered *all* of the data from the 6-week empirical sorption experiments carried out with Brine A and ERDA-6 on the bench top (0.033% CO₂) by Triay and her group at LANL (see Methods Used to Establish Ranges of Matrix K_d s above for the reasons for considering these data). These runs were: #7011A and #7011B (see Table E-1 below), and #7007A, #7007B, #7008A, #7008B, #7009A, #7009B, #7010A, and #7010B (Table E-2). Next, we discarded the data from #7011A and #7011B, the runs in which the difference between the activity of the ²³⁰Th in a standard and that in a control exceeded 3 σ , where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_d s). Discarding the data from these two runs yielded an *initial* range of 726 ml/g (from #7010A) to 12,604 ml/g (#7008B) for Th(IV) and the deep brines.

For the *initial* ranges for Th(IV) and the Culebra brines, we first considered *all* of Triay's 6-week sorption data obtained with AISinR and H-17 on the bench top (0.033% CO₂) and in glove boxes with atmospheres containing 0.24 and 1.4% CO₂ (see Methods Used to Establish Ranges of Matrix K_d s). These were: #7012A, #7012B, #7054A, #7054B, #7026A, #7026B, #7040A, and #7040B (Table E-3), and #7013A, #7013B, #7055A, #7055B, #7027A, #7027B, #7041A, and #7041B (Table E-4). Unfortunately, we had to discard the data from *all* of these the runs because the difference between the activity of the ²³⁰Th in a standard and that in a control exceeded 3 σ . Therefore, we assumed that the *initial* range of 726 to 12,604 ml/g for Th(IV) and the deep brines does not differ significantly from that for Th(IV) and the Culebra brines.

Next, we attempted to compare these initial ranges with the data from the mechanistic sorption study by Brady and his colleagues at SNL and LANL. However, Brady *did not* obtain any usable results for Th because of one or more of the following reasons: (1) the walls of the containers used to prepare Th-bearing solutions sorbed essentially all of it prior to his experiments; (2) essentially all of the Th precipitated on the walls of these containers prior to his runs; (3) the walls of his apparatus sorbed essentially all of the Th during his runs; (4) essentially all of the Th precipitated on the dolomite and/or the apparatus during his runs. Therefore, our *revised* ranges for Th(IV) remained 726 to 12,604 ml/g for *both* the deep and Culebra brines.

We then compared the revised range with the data from the transport study with intact Culebra cores by Lucero and his colleagues at SNL. Lucero carried out his experiments under ambient atmospheric conditions; therefore, the CO₂ content of these

experiments was probably similar to that in the LANL bench-top (0.033% CO₂) runs. Because Lucero *did not* observe breakthrough of Th(IV), it was only possible to determine a minimum K_d for this element. Furthermore, the minimum K_d s calculated for Th are significantly lower than those calculated for Pu and Am, the other elements for which Lucero did not observe breakthrough (compare Tables B-8, C-9, and E-6), because: (1) the detection limit of γ -spectrometric analysis (one of the two methods used in this study) for ²²⁸Th in the effluent is much higher than those for ²⁴¹Pu and ²⁴¹Am because of the low yield of the ²²⁸Th γ emission; (2) although ²²⁸Th emits α particles detectable by LSC (the other analytical method used in this study), its daughter products have interfering α emissions; (3) lowering the detection limit for ²²⁸Th by observing the decay of its daughters, such as ²²⁴Ra, was not possible because of interference by identical daughters produced by the decay of ²³²U, which was used in all of the cores. Lucero et al. (1996) submitted their results on March 28, 1996, (Table E-5). Lucero and Brown (1996) then revised them on April 5, 1996 (Table E-6). The minimum K_d s reported for experiments C-2, C-5, and D-2 (Table E-6) *are consistent with the revised range obtained from the empirical and mechanistic sorption studies* (see above). Therefore, our *final* range remains 726 to 12,604, ml/g, rounded to 700 to 10,000 ml/g prior to inclusion in Table 1 above.

We recommend that PA personnel use a uniform probability distribution for this range (see Methods Used to Establish Probability Distributions of Matrix K_d s above).

Finally, based on the oxidation-state analogy, we recommend that PA use a range of 700 to 10,000 ml/g for Pu(IV), U(IV), and Np(IV) (see Table 1).

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Table E-1. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_{ds} for Th(IV), Dolomite-Rich Culebra Rock, and Brine A (LANL Empirical Sorption Study). Six -week sorption runs with VPX-25-8. K_{ds} in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 30 and April 3, 1996, based on information provided by LANL on March 28 and April 1, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by L. J. Storz on July 9, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Initial ^{230}Th Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
Brine A	ND	ND	ND	ND	ND
Brine A	ND	ND	ND	ND	ND
Brine A	ND	ND	ND	ND	ND
Brine A	ND	ND	ND	ND	ND
Brine A	ND	ND	ND	ND	ND
Brine A	ND	ND	ND	ND	ND
Brine A	NA	263, #7011A	173, #7053A	284, #7025A	583, #7039A
Brine A	NA	210, #7011B	191, #7053B	296, #7025B	593, #7039B
Brine A	ND	ND	ND	ND	ND
Brine A	ND	ND	ND	ND	ND

NA: not available yet.

ND: not determined.

Table E-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Th(IV), Dolomite-Rich Culebra Rock, and ERDA-6 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 30 and April 3, 1996, based on information provided by LANL on March 28 and April 1, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by L. J. Storz on July 9, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Initial ^{230}Th Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
ERDA-6	ND	ND	ND	ND	ND
ERDA-6	ND	ND	ND	ND	ND
ERDA-6	NA	4,486, #7007A	5,544, #7049A	10,877, #7021A	3,862, #7035A
ERDA-6	NA	4,432, #7007B	7,520, #7049B	13,402, #7021B	5,935, #7035B
ERDA-6	NA	5,585, #7008A	7,329, #7050A	7,286, #7022A	6,166, #7036A
ERDA-6	NA	12,604, #7008B	5,416, #7050B	6,534, #7022B	8,080, #7036B
ERDA-6	NA	1,831, #7009A	1,378, #7051A	11,848, #7023A	5,721, #7037A
ERDA-6	NA	2,371, #7009B	3,139, #7051B	6,110, #7023B	38,346, #7037B
ERDA-6	NA	726, #7010A	1,621, #7052A	High, #7024A	306, #7038A
ERDA-6	NA	1,092, #7010B	1,497, #7052B	949, #7024B	2,398, #7038B

Table E-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_{ds} for Th(IV), Dolomite-Rich Culebra Rock, and ERDA-6 (LANL Empirical Sorption Study) (continued).

NA: not available yet.

ND: not determined.

Table E-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Th(IV), Dolomite-Rich Culebra Rock, and AISinR (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 30 and April 3, 1996, based on information provided by LANL on March 28 and April 1, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by L. J. Storz on July 9, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Initial ^{230}Th Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
AISinR	ND	ND	ND	ND	ND
AISinR	ND	ND	ND	ND	ND
AISinR	ND	ND	ND	ND	ND
AISinR	ND	ND	ND	ND	ND
AISinR	ND	ND	ND	ND	ND
AISinR	ND	ND	ND	ND	ND
AISinR	NA	High, #7012A	10,439, #7054A	4,451, #7026A	55,454, #7040A
AISinR	NA	High, #7012B	16,375, #7054B	6,871, #7026B	High, #7040B
AISinR	ND	ND	ND	ND	ND
AISinR	ND	ND	ND	ND	ND

NA: not available yet.

ND: not determined.

Table E-4. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Th(IV), Dolomite-Rich Culebra Rock, and H-17 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 30 and April 3, 1996, based on information provided by LANL on March 28 and April 1, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by L. J. Storz on July 9, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Initial ^{230}Th Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
H-17	ND	ND	ND	ND	ND
H-17	ND	ND	ND	ND	ND
H-17	ND	ND	ND	ND	ND
H-17	ND	ND	ND	ND	ND
H-17	ND	ND	ND	ND	ND
H-17	ND	ND	ND	ND	ND
H-17	NA	11,005, #7013A	6,902, #7055A	High, #7027A	13,140, #7041A
H-17	NA	High, #7013B	High, #7055B	21,581, #7027B	12,961, #7041B
H-17	ND	ND	ND	ND	ND
H-17	ND	ND	ND	ND	ND

NA: not available yet.

ND: not determined.

Table E-5. Minimum Values of R and K_d for Th(IV) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-2	VPX-28-6C	AIS.	0.1	237	34.15	35	5.7 ^S 3.5 ^D	0.87	NA
C-5	VPX-28-6C	ER.-6	0.1	146	20.98	22	3.9 ^S 2.3 ^D	0.36	NA
D-2	VPX-25-8A	AIS.	0.1	133	19.12	8.5	8.2 ^S 5.5 ^D	0.25	NA

AIS: AISinR.

D: dual porosity assumed.

ER.-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

Table E-6. Minimum Values of R and K_d for Th(IV) in Intact Culebra Cores (SNL Column Transport Study). Data current as of March 26, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y. Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R_{min}	Porosity (%)	$K_{d, min}$ (ml/g)	Range (\pm ml/g)
C-2	VPX-28-6C	AIS.	0.1	237	34.15	35	5.7 ^S	0.87	NA
C-5	VPX-28-6C	ER.-6	0.1	146	20.98	22	3.9 ^S	0.36	NA
D-2	VPX-25-8A	AIS.	0.1	133	19.12	8.5	8.2 ^S	0.25	NA

AIS: AISinR.

ER.-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

APPENDIX F: RANGES AND PROBABILITY DISTRIBUTIONS OF
MATRIX K_{ds} FOR Np(V) AND DOLOMITE-RICH
CULEBRA ROCK

Based on experimental results, ASTP personnel have predicted that Np will speciate as Np(IV) or Np(V), but not as Np(VI), in deep (Castile and Salado) brines in WIPP disposal rooms. Furthermore, a modeling study of the effects of mixing deep and Culebra brines on the oxidation states of Pu, U, and Np in the Culebra showed that Culebra fluids are poorly poised (see Predictions of Actinide Oxidation States in the Culebra above). Therefore; we established experimentally obtained ranges of matrix K_{ds} for Np(V) and used the experimentally obtained ranges for Th(IV) (see Appendix E above) and the oxidation-state analogy to establish ranges for Np(IV) (and U(IV)).

For the *initial* ranges for Np(V) and the deep brines, we first considered *all* of the data from the 6-week empirical sorption experiments carried out with Brine A and ERDA-6 on the bench top (0.033% CO₂) by Triay and her group at LANL (see Methods Used to Establish Ranges of Matrix K_{ds} above for the reasons for considering these data). These runs were: #6020, #6040, #6060, and #6080 (see Table F-1 below), and #6021, #6041, #6061, #6081 (Table F-2). Next, we discarded the data from #6040, #6021, and #6041, the runs in which the difference between the activity of the ²³⁷Np in a standard and that in a control exceeded 3 σ , where σ is the standard deviation (see Methods Used to Establish Ranges of Matrix K_{ds}). Discarding the data from these three runs yielded an *initial* range of 7.30 ml/g (from #6020) to 40.0 ml/g (#6061) for Np(V) and the deep brines.

For the *initial* ranges for Np(V) and the Culebra brines, we first considered *all* of Triay's 6-week sorption data obtained with AISinR and H-17 on the bench top (0.033% CO₂) and in glove boxes with atmospheres containing 0.24 and 1.4% CO₂ (see Methods Used to Establish Ranges of Matrix K_{ds}). These were: #6022, #6042, #6062, #6082 #24022, #24042 #24062, #24082, #12022, #12042, #12062, and #12082 (Table F-3), and #6023, #6043, #6063, #6083, #24023, #24043, #24063, #24083, #12023, #12043, #12063, and #12083 (Table F-4). We then discarded the data from #24042 and #24082, the runs in which the difference between the activity of the ²³⁷Np in a standard and that in a control exceeded 3 σ , to obtain the *initial* range of 2.00 ml/g (from #12022) to 159 ml/g (#6042) for Np(V) and the Culebra brines.

Next, we compared these initial ranges with the data from the mechanistic sorption study by Brady and his colleagues at SNL and LANL. We used Brady's data to extend Triay's empirical sorption data for the deep brines to the basic conditions expected to result from the use of an MgO backfill in WIPP disposal rooms, *but not* to extend Triay's data for the Culebra brines to basic conditions (see Methods Used to Establish Ranges of Matrix K_{ds}). Brady's data for 0.5 M NaCl, atmospheric CO₂, and the highest pH value under these conditions are 178 and 187 ml/g at a pH of 9.87 and 9.88, respectively (Table F-5). Because these values are *greater than the upper limit* of the initial range for Np(V) and the deep brines (see above), we extended this range to obtain a

revised range for Np(V) and deep brines of 7.30 to 187 ml/g. Because we did not use this comparison to extend the initial range for Np(V) and the Culebra brines to basic conditions, this revised range remains 2.00 to 159 ml/g.

We then compared both of these revised ranges with the data from the transport study with intact Culebra cores by Lucero and his colleagues at SNL. Lucero carried out his experiments under ambient atmospheric conditions; therefore, the CO₂ content of these experiments was probably similar to that in the LANL bench-top (0.033% CO₂) runs. Lucero *did* observe breakthrough of Np(V) in his experiments. Therefore, it was possible to determine actual K_{ds} for this element. Lucero et al. (1996) submitted their results on March 28, 1996, (see Table F-6), Lucero and Brown (1996) then revised them on April 5, 1996 (Table F-7). The K_d reported for Experiment C-7 with the deep brine ERDA-6 (Table F7) is less than the lower limit of the revised range of K_{ds} for Np(V) and the deep brines obtained from the empirical and mechanistic sorption experiments (see above). Therefore, we extended this range to obtain a final range for Np(V) and deep brines of 2.0 to 187 ml/g, and rounded it to 2 to 200 ml/g prior to inclusion in Table 1 above. Because Lucero's K_{ds} for Np(V) and the Culebra brine AISinR (C-6, D-2, and D4 in Table F-7), are also less than the lower limit of the revised range for Np(V) and the Culebra brines obtained from the sorption studies (see above), we extended this range to obtain a final range of 1.0 to 159 ml/g, rounded to 1 to 200 ml/g (Table 1).

We recommend that PA personnel use a uniform probability distribution for both of these ranges (see Methods Used to Establish Probability Distributions of Matrix K_{ds} above).

Furthermore, we recommend that PA use the range of 1 to 200 ml/g (the range for Culebra brines) for Np(V) because this range results in less retardation of this element than the range for deep brines (see Methods Used for Final Selection of the Range of Matrix K_{ds} for Use in PA Calculations above).

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Table F-1. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Np(V), Dolomite-Rich Culebra Rock, and Brine A (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{237}Np Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
Brine A	ND	ND	ND	ND	ND
Brine A	1.13×10^{-5} to 1.15×10^{-5}	7.30, #6020	4.20, #24020	189, #12020	319, #18020
Brine A	5.92×10^{-6} to 1.08×10^{-5}	13.4, #6040	26.8, #24040	9.90, #12040	7.50, #18040
Brine A	1.17×10^{-6} to 4.88×10^{-6}	17.1, #6060	126, #24060	17.9, #12060	18.4, #18060
Brine A	5.59×10^{-7} to 5.93×10^{-7}	31.5, #6080	27.3, #24080	30.8, #12080	22.7, 18080

ND: not determined.

Table F-2. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_{ds} for Np(V), Dolomite-Rich Culebra Rock, and ERDA-6 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_{ds} in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{237}Np Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
ERDA-6	ND	ND	ND	ND	ND
ERDA-6	6.26×10^{-6} to 1.41×10^{-5}	183, #6021	203, #24021	472, #12021	427, #18021
ERDA-6	4.01×10^{-6} to 5.55×10^{-6}	46.4, #6041	152, #24041	129, #12041	99.2, #18041
ERDA-6	1.43×10^{-6} to 5.10×10^{-6}	40.0, #6061	236, #24061	137, #12061	25.1, #18061
ERDA-6	6.54×10^{-7} to 5.67×10^{-6}	26.7, #6081	11,782, #24081	High, #12081	High, #18081

ND: not determined.

Table F-3. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Np(V), Dolomite-Rich Culebra Rock, and AISinR (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{237}Np Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
AISinR	ND	ND	ND	ND	ND
AISinR	9.82×10^{-6} to 1.01×10^{-5}	5.00, #6022	3.60, #24022	2.00, #12022	2.10, #18022
AISinR	5.09×10^{-6} to 6.66×10^{-6}	159, #6042	11.6 , #24042	2.30, #12042	2.20, #18042
AISinR	1.01×10^{-6} to 1.07×10^{-6}	19.8, #6062	9.30, #24062	3.90, #12062	4.70, #18062
AISinR	5.72×10^{-7} to 1.15×10^{-6}	31.9, #6082	45.3 , #24082	9.60, #12082	10.1, #18082

ND: not determined.

Table F-4. Effects of Initial Radionuclide Concentration and P_{CO_2} on Matrix K_d s for Np(V), Dolomite-Rich Culebra Rock, and H-17 (LANL Empirical Sorption Study). Six-week sorption runs with VPX-25-8. No K_d s in this table excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of April 3, 1996. Table compiled by L. H. Brush on March 23 and 30, 1996, based on information provided by LANL on March 19 and 26, 1996. Table checked by Brush and S. Boone on April 3, 1996. Table revised by Brush on June 7, 1996, based on information provided by L. J. Storz on June 6, 1996. Table checked by Storz on June 10, 1996. Table revised by Storz on July 1, 1996, based on information provided by LANL on June 28, 1996. Table checked by A. C. Peterson on July 10, 1996.

Brine	Range of Initial ^{237}Np Conc. (M)	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 0.24% CO_2	K_d (ml/g), 1.4% CO_2	K_d (ml/g), 4.1% CO_2
H-17	ND	ND	ND	ND	ND
H-17	5.56×10^{-7} to 1.10×10^{-5}	47.6, #6023	17.3, #24023	2.70, #12023	1.30, #18023
H-17	5.56×10^{-6} to 6.89×10^{-6}	14.3, #6043	12.1, #24043	2.90, #12043	2.20, #18043
H-17	1.11×10^{-6} to 1.15×10^{-6}	36.5, #6063	23.5, #24063	42.8, #12063	4.20, #18063
H-17	5.65×10^{-7} to 1.15×10^{-5}	40.1, #6083	7.30, #24083	3.40, #12083	6.00, #18083

ND: not determined.

Table F-5. Effects of pH and P_{CO_2} on Matrix K_d s for Np(V) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study). Sorption runs with Norwegian dolomite and 0.5 M NaCl. Data current as of March 31, 1996. Table retyped by L. H. Brush on April 24, 1996. Table checked by Y. Behl on April 28, 1996. Table revised by Brush on July 5, 1996, based on Brady (1996). Table checked by A. C. Peterson on July 15, 1996.

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
9.9	187	NA	NA
9.9	178	NA	NA
8.4	64	NA	NA
6.7	11	NA	NA
6.2	11	NA	NA
5.8	-1	NA	NA
5.2	11	NA	NA
4.6	11	NA	NA
4.1	11	NA	NA
3.5	11	NA	NA
3.1	-1	NA	NA

Table F-5. Effects of pH and P_{CO_2} on Matrix K_d s for Np(V) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.9	NA	16	NA
8.5	NA	124	NA
7.3	NA	70	NA
7.2	NA	49	NA
7.0	NA	49	NA
6.9	NA	31	NA
6.6	NA	16	NA
6.2	NA	31	NA
5.3	NA	16	NA
4.0	NA	16	NA
3.1	NA	31	NA

Table F-5. Effects of pH and P_{CO_2} on Matrix K_d s for Np(V) and Pure Dolomite (SNL/LANL Mechanistic Sorption Study) (continued).

pH (standard units)	K_d (ml/g), atmospheric CO_2	K_d (ml/g), 0.5% CO_2	K_d (ml/g), 5% CO_2
6.4	NA	NA	-11
6.9	NA	NA	20
6.9	NA	NA	40
6.8	NA	NA	20
6.7	NA	NA	20
6.8	NA	NA	20
6.5	NA	NA	20
6.1	NA	NA	3
5.8	NA	NA	3
4.9	NA	NA	20
3.6	NA	NA	3

NA: not applicable.

Table F-6. Measured Values of R and Calculated Values of K_d for Np(V) in Intact Culebra Cores (SNL Column Transport Study). Values in bold font to be excluded from ranges and distributions because fits to elution data were inferior to those assuming single porosity and dual porosity with fracture retardation. Data current as of March 30, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity	K_d (ml/g)	Range (\pm ml/g)
C-5	VPX-28-6C	ER.-6	0.1	13	2	30.8; ^S	3.9 ^S	0.51 ^S	0.29 ^S
						1,			
						166;^{DN}	2.3 ^{DN}	1.65^{DN}	1.0^{DN}
C-6	VPX-28-6C	AIS.	0.1	13	2	7.0,			
						103^{DF}	2.3 ^{DF}	0.06 ^{DF}	0.03 ^{DF}
C-7	VPX-28-6C	ER.-6	0.1	13	2	58.5; ^S	4.5 ^S	1.12 ^S	0.26 ^S
						1,			
						301;^{DN}	1.85 ^{DN}	2.4^{DN}	1.4^{DN}
D-2	VPX-25-8A	AIS.	0.1	12	2	22,			
						158^{DF}	1.85 ^{DF}	.169 ^{DF}	.048 ^{DF}
C-7	VPX-28-6C	ER.-6	0.1	13	2	119; ^S	3.9 ^S	2.0 ^S	0.8 ^S
						1,			
						910;^{DN}	2.1 ^{DN}	8.3^{DN}	11.9^{DN}
D-2	VPX-25-8A	AIS.	0.1	12	2	169,			
						0^{DF}	2.1 ^{DF}	1.53 ^{DF}	38 ^{DF}
D-2	VPX-25-8A	AIS.	0.1	12	2	47; ^S	8.2 ^S	1.64 ^S	0.58 ^S
						1,			
						1670;^N	5.5 ^{DN}	40^{DN}	6^{DN}
D-2	VPX-25-8A	AIS.	0.1	12	2	6.6,			
						NA^{DF}	5.5 ^{DF}	NA ^{DF}	NA ^{DF}

Table F-6: Measured Values of R and Calculated Values of K_d for Np(V) in Intact Culebra Cores (SNL Column Transport Study) (continued).

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity	K_d (ml/g)	Range (\pm ml/g)
D-4	VPX-25-8A	AIS.	0.1	13	2	39, ^S 1, 340, ^{DN} 17.5, 154 ^{DF}	10.0 ^S 4.8 ^{DN} 4.8 ^{DF}	1.65 ^S 7.1 ^{DN} 0.34 ^{DF}	0.22 ^S 4.2 ^{DN} 0.07 ^{DF}

AIS: AISinR.

DF: dual porosity and fracture retardation assumed.

DN: dual porosity and no fracture retardation assumed.

ER.-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

Table F-7. Measured Values of R and Calculated Values of K_d for Np(V) in Intact Culébra Cores (SNL Column Transport Study). Data current as of March 30, 1996. Table compiled by L. H. Brush on March 30, 1996, based on Lucero et al. (1996). Table checked by Brush on March 31, 1996. Table revised by Brush on April 6, 1996, based on Lucero and Brown (1996). Table checked by Y. Behl on April 8, 1996.

Run #	Solid (core)	Brine	Flow rate (ml/min)	Run Time (days)	Ef-fluent Vol. (L)	R	Porosity	K_d (ml/g)	Range (\pm ml/g)
C-6	VPX-28-6C	AIS.	0.1	13	2	59 ^S	4.5 ^S	1.1 ^S	NA
C-7	VPX-28-6C	ER.-6	0.1	13	2	120 ^S	3.9 ^S	2.0 ^S	NA
D-2	VPX-25-8A	AIS.	0.1	12	2	47 ^S	8.2 ^S	1.6 ^S	NA
D-4	VPX-25-8A	AIS.	0.1	13	2	39 ^S	10.0 ^S	1.6 ^S	NA

AIS: AISinR.

ER.-6: ERDA-6.

NA: not available yet.

S: single porosity assumed.

APPENDIX G: EFFECTS OF ORGANIC LIGANDS ON RANGES AND PROBABILITY DISTRIBUTIONS OF MATRIX K_d s FOR Pu(V), Am(III), U(VI), Th(IV), Np(V), AND DOLOMITE-RICH CULEBRA ROCK

Triay and her group at LANL carried out two sets of experiments on the effects of four organic ligands (acetate, citrate, ethylenediaminetetraacetic acid or EDTA, and lactate) on the K_d s for dissolved Pu(V), Am(III), U(VI), Th(IV), and Np(V) under conditions expected in the Culebra. Brush (1990) concluded that these and six other organic and two inorganic ligands could affect the solubilities of the actinide elements in TRU waste. Therefore, he estimated the concentrations of these 12 ligands in three quantities of brine that could resaturate WIPP disposal rooms after filling and sealing. Since 1990, the ASTP has reduced the number of organic ligands of concern from twelve to four (acetate, citrate, EDTA, and oxalate). Triay carried out experiments with acetate, citrate, EDTA, and lactate because the ASTP had not eliminated lactate from consideration yet, and because Triay concluded that oxalate would be extremely insoluble given the dissolved Ca concentrations expected in WIPP brines. Triay conducted the first set of runs with ERDA-6 and H17, and acetate, citrate, EDTA, and lactate all present at concentrations as close as possible to the "minimum" and "maximum" concentrations estimated by Brush (1990) (see Table G-1 below). Soon after Triay started their preliminary experiments, Weiner (1996) used the quantities of acetate, citrate, EDTA, and oxalate in TRU waste estimated by Drez (1996) to predict the concentrations of these organic ligands in brines in the repository (Table G-1).

Tables G-2, G-3, G-4, G-5, and G-6 give the results of the preliminary experiments with ERDA-6 and H-17, and Pu(V), Am(III), U(VI), Th(IV), and Np(V), respectively. At low concentrations, acetate, citrate, EDTA, and lactate have little or no effect on the K_d s for these elements (compare the results for "low-concentration organics" to those for "none," the runs without any organic ligands present.) In fact, for Pu(V) and ERDA-6 in contact with ambient atmospheric or (about 0.033%) CO₂; Am(III), ERDA-6, and 0.033% CO₂; and U(VI), ERDA-6, and 0.033% CO₂, low concentrations of these organic ligands actually *increase* the K_d s relative to those obtained without any organic ligands. However, at high concentrations, these organic ligands significantly *decrease* the K_d s for all of these elements. Note that the low and the high concentrations of acetate, citrate, and EDTA used in these preliminary runs bracket the predicted concentrations of these organic ligands (Table G-1).

Triay used ERDA-6 and H-17, which contain 19 and 74.1 mM Mg, respectively, for this set of experiments. However, ASTP personnel have predicted the effects of acetate, citrate, EDTA, and oxalate on the solubilities of the actinide elements by assuming that all of these organic ligands will dissolve in intergranular Salado brine as it accumulates in WIPP disposal rooms. Novak (1996) used FMT to predict that the Mg concentration in SPC brine (Brine A modified by omitting minor and trace constituents, and used by the ASTP to simulate Salado brine in several experimental and modeling studies) will be 454 mM after equilibration with halite, anhydrite; the actinide elements and the organic ligands in TRU waste, and an MgO backfill. This Mg concentration is significantly higher than that of ERDA-6 before or after equilibration with this backfill (19 and 48 mM, respectively) and significantly higher than that of H-17 (74.1 mM). Because we hoped that competition among Mg and Pu, Am, U, Th, and Np for the binding sites on these organic ligands

would mitigate the effects of these organics on the K_d s for these elements, Triay carried out an additional set of experiments with acetate, citrate, EDTA, and lactate at low, intermediate, and high concentrations (see Table G-1) and with Brine A modified to simulate the composition of Salado brine after equilibration with an MgO backfill.

Table G-7 shows the results of these experiments. Low concentrations of organics significantly decreased the K_d s for Th relative to those obtained without any organics, but had much less effect on the K_d s for the other elements. Intermediate concentrations of organics significantly decreased the K_d s for all of the elements except U(VI). High concentrations significantly decreased the K_d s for all five of these elements.

However, we *have not* revised the ranges and probability distributions of K_d s for Pu, Am, U, Th, and Np shown in Table 1 (see above) because large quantities of other metals (see below) will be present to form complexes with these organic ligands, thus preventing them from forming complexes with the actinide elements and decreasing the K_d s for the actinides in the Culebra. (These other metals will also prevent these organic ligands from increasing the solubilities of the actinide elements in WIPP disposal rooms.) These other metals include Fe, large quantities which will be present in WIPP disposal rooms in steel waste containers (drums and boxes) and as steels, stainless steels, and other Fe-base materials in the waste; Mg, large quantities of which will be emplaced in the repository as an MgO backfill to remove microbially produced CO_2 (but will be present as MgCO_3 and/or $\text{Mg}(\text{OH})_2$, and magnesium oxychloride after reaction with CO_2 and/or brine); and Cr, Mn, Ni, Pb, and V, which will be present in lesser but still sufficient quantities in steel drums and boxes, and in steels, stainless steels, and other Fe-base alloys in the waste, and in other waste constituents. Preliminary modeling of the equilibria among dissolved and solid-phase Pu and Am, Fe, Mg, and Ni, and EDTA imply that, under the conditions expected in WIPP disposal rooms, Ni would form complexes with 99.8% of the EDTA expected to be present in the repository, thus preventing it from complexing significant quantities of Pu and Am. A detailed description of these calculations, and any additional modeling or laboratory studies of these competitive equilibria, will appear elsewhere.

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Table G-1. Concentrations of Organic Ligands in Experiments with ERDA-6, H-17, and Modified Brine A, and Predicted Concentrations of Organic Ligands in Brines in WIPP Disposal Rooms. Table compiled by L. H. Brush on May 10, 1996, based on information provided by LANL on April 25, 1996. Table checked by L. J. Storz on May 17, 1996.

Organic Ligand	Low Conc.	High Conc.	Low Conc.	Intermediate Conc.	High Conc.	Predicted Conc. in WIPP (mM)
	(ERDA-6 and H-17) (mM)	(ERDA-6 and H-17) (mM)	(Modified Brine A) (mM)	(Modified Brine A) (mM)	(Modified Brine A) (mM)	
Acetate	0.195 (ERDA-6)	19.5172 (ERDA-6)	0.489	4.89	48.9	1.062
	0.195 (H-17)	19.5172 (H-17)				
Citrate	0.0340 (ERDA-6)	3.4002 (ERDA-6)	0.03417	0.3417	3.417	0.465
	0.0340 (H-17)	3.4002 (H-17)				
EDTA	0.000146 (ERDA-6)	0.0146 (ERDA-6)	0.00011	0.0011	0.011	0.00416
	0.000146 (H-17)	0.0146 (H-17)				
Lactate	0.00761 (ERDA-6)	0.7610 (ERDA-6)	0.02088	0.2088	2.088	Not predicted
	0.00796 (H-17)	0.7956 (H-17)				
Oxalate	NU	NU	NU	NU	NU	7.404

NU: Not used because LANL expected Ca-oxalate to precipitate from these brines at very low oxalate concentrations.

Table G-2. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Pu(V) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study). One-week sorption runs with H-19, B-4, Box 7. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Still counting new controls for underlined samples. Data current as of May 30, 1996. Table compiled by L. H. Brush on May 16, 1996, based on information provided by LANL on May 15, 1996. Table checked by L. J. Storz on May 16 and 17, 1996. Table revised by Brush on May 31 and June 1, 1996, based on information provided by LANL on May 30 and 31, 1996. Table checked by L. J. Storz on June 10, 1996. Table re-checked by A. C. Peterson on July 16, 1996.

Brine	Additive	K_d , (ml/g), 0.033% CO_2	K_d (ml/g), 4.1% CO_2
ERDA-6	None	157, #JRF O-131	<u>217</u> , #JRF O-181
ERDA-6	None	158, #JRF O-132	<u>223</u> , #JRF O-182
ERDA-6	Avg. without organics	158	<u>220</u>
ERDA-6	Low-conc. organics	787, #JRF O-139	171, #JRF O-189
ERDA-6	Low-conc. organics	142, #JRF O-140	184, #JRF O-190
ERDA-6	Avg. w. low-conc. org.	464	178
ERDA-6	High-conc. organics	6.44, #JRF O-137	10.3, #JRF O-187
ERDA-6	High-conc. organics	7.48, #JRF O-138	9.10, #JRF O-188
ERDA-6	Avg. w. high-conc. org.	6.96	9.70

Table G-2. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Pu(V) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study) (continued).

Brine	Additive	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 4.1% CO_2
H-17	None	18.4, #JRF O-31	<u>8.51</u> , #JRF O-81
H-17	None	19.8, #JRF O-32	<u>9.19</u> , #JRF O-82
H-17	Avg. without organics	19.1	<u>8.85</u>
H-17	Low-conc. organics	9.50, #JRF O-39	4.45, #JRF O-89
H-17	Low-conc. organics	17.0, #JRF O-40	7.73, #JRF O-90
H-17	Avg. w. low-conc. org.	13.2	6.09
H-17	High-conc. organics	1.39, #JRF O-37	0.315, #JRF O-87
H-17	High-conc. organics	0.934, #JRF O-38	0.515, #JRF O-88
H-17	Avg. w. high-conc. org.	1.16	0.415

Table G-3. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Am(III) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study). One-week sorption runs with H-19, B-4, Box 7. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Still counting new controls for underlined samples. Data current as of May 30, 1996. Table compiled by L. H. Brush on May 16, 1996, based on information provided by LANL on May 15, 1996. Table checked by L. J. Storz on May 16 and 17, 1996. Table revised by Brush on May 31 and June 1, 1996, based on information provided by LANL on May 30 and 31, 1996. Table checked by L. J. Storz on June 10, 1996. Table rechecked by A. C. Peterson on July 16, 1996.

Brine	Additive	K_d , (ml/g), 0.033% CO_2	K_d , (ml/g), 4.1% CO_2
ERDA-6	None	199, #JRF O-141	<u>2,890</u> , #JRF O-191
ERDA-6	None	1,220, #JRF O-142	<u>2,160</u> , #JRF O-192
ERDA-6	Avg. without organics	710	<u>2,525</u>
ERDA-6	Low-conc. organics	1,390 #JRF O-161	1,680, #JRF O-199
ERDA-6	Low-conc. organics	1,470, #JRF O-171	1,880, #JRF O-200
ERDA-6	Avg. w. low-conc. org.	1,430	1,780
ERDA-6	High-conc. organics	10.6 , #JRF O-147	7.40, #JRF O-197
ERDA-6	High-conc. organics	7.84 , #JRF O-151	5.05, #JRF O-198
ERDA-6	Avg. w. high-conc. org.	9.22	6.22

Table G-3. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Am(III) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study) (continued).

Brine	Additive	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 4.1% CO_2
H-17	None	533, #JRF O-41	379, #JRF O-91
H-17	None	549, #JRF O-42	391, #JRF O-92
H-17	Avg. without organics	541	385
H-17	Low-conc. organics	503, #JRF O-49	311, #JRF O-99
H-17	Low-conc. organics	497, #JRF O-50	299, #JRF O-100
H-17	Avg. w. low-conc. org.	500	305
H-17	High-conc. organics	7.79, #JRF O-47	3.58, #JRF O-97
H-17	High-conc. organics	7.37, #JRF O-48	3.75, #JRF O-98
H-17	Avg. w. high-conc. org.	7.58	3.66

Table G-4. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for U(VI) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study). One-week sorption runs with H19, B-4, Box 7. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Still counting new controls for underlined samples. Negative K_d s set to 0.00 before determining the mean. Data current as of May 30, 1996. Table compiled by L. H. Brush on May 16, 1996, based on information provided by LANL on May 15, 1996. Table checked by L. J. Storz on May 16 and 17, 1996. Table revised by Brush on May 31 and June 1, 1996, based on information provided by LANL on May 30 and 31, 1996. Table checked by L. J. Storz on June 10, 1996. Table rechecked by A. C. Peterson on July 16, 1996.

Brine	Additive	K_d , (ml/g), 0.033% CO_2	K_d , (ml/g), 4.1% CO_2
ERDA-6	None	-0.148, #JRF O-111	<u>-0.296</u> , #JRF O-159
ERDA-6	None	0.220, #JRF O-112	<u>0.275</u> , #JRF O-160
ERDA-6	Avg. without organics	0.110	<u>0.138</u>
ERDA-6	Low-conc. organics	<u>1.83</u> , #JRF O-119	<u>-0.0367</u> , #JRF O-168
ERDA-6	Low-conc. organics	<u>-0.371</u> , #JRF O-120	<u>-0.933</u> , #JRF O-169
ERDA-6	Avg. w. low-conc. org.	<u>0.915</u>	<u>0.00</u>
ERDA-6	High-conc. organics	<u>-0.631</u> , #JRF O-117	<u>-0.475</u> , #JRF O-166
ERDA-6	High-conc. organics	<u>-0.638</u> , #JRF O-118	<u>-0.948</u> , #JRF O-167
ERDA-6	Avg. w. high-conc. org.	<u>0.000</u>	<u>0.00</u>

Table G-4. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for U(VI) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study) (continued).

Brine	Additive	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 4.1% CO_2
H-17	None	-2.11, #JRF O-11	-1.69, #JRF O-61
H-17	None	-1.79, #JRF O-12	-0.323, #JRF O-62
H-17	Avg. without organics	0.00	0.00
H-17	Low-conc. organics	-1.27, #JRF O-19	-0.601, #JRF O-69
H-17	Low-conc. organics	-1.67, #JRF O-20	-1.44, #JRF O-70
H-17	Avg. w. low-conc. org.	0.00	0.00
H-17	High-conc. organics	-1.77, #JRF O-17	-1.81, #JRF O-67
H-17	High-conc. organics	-1.51, #JRF O-18	-1.67, #JRF O-68
H-17	Avg. w. high-conc. org.	0.00	0.00

Table G-5. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Th(IV) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study). One-week sorption runs with H-19, B-4, Box 7. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Still counting new controls for underlined samples. Data current as of May 30, 1996. Table compiled by L. H. Brush on May 16, 1996, based on information provided by LANL on May 16, 1996. Table checked by L. J. Storz on May 16 and 17, 1996. Table revised by Brush on May 31 and June 1, 1996, based on information provided by LANL on May 30 and 31, 1996. Table checked by L. J. Storz on June 10, 1996. Table re-checked by A. C. Peterson on July 16, 1996.

Brine	Additive	K_d , (ml/g), 0.033% CO_2	K_d , (ml/g), 4.1% CO_2
ERDA-6	None	120, #JRF O-101	<u>153,</u> #JRF O-148
ERDA-6	None	98.6, #JRF O-102	<u>169,</u> #JRF O-149
ERDA-6	Avg. without organics	109	<u>161</u>
ERDA-6	Low-conc. organics	101, #JRF O-109	157, #JRF O-157
ERDA-6	Low-conc. organics	99.9, #JRF O-110	166, #JRF O-158
ERDA-6	Avg. w. low-conc. org.	100	162
ERDA-6	High-conc. organics	30.0, #JRF O-107	55.0, #JRF O-155
ERDA-6	High-conc. organics	32.8, #JRF O-108	63.2, #JRF O-156
ERDA-6	Avg. w. high-conc. org.	31.4	59.1

Table G-5. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Th(IV) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study) (continued).

Brine	Additive	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 4.1% CO_2
H-17	None	15.0, #JRF O-1	<u>12.0</u> , #JRF O-51
H-17	None	16.6, #JRF O-2	<u>11.3</u> , #JRF O-52
H-17	Avg. without organics	15.8	<u>11.6</u>
H-17	Low-conc. organics	13.8, #JRF O-9	9.72, #JRF O-59
H-17	Low-conc. organics	14.4, #JRF O-10	9.20, #JRF O-60
H-17	Avg. w. low-conc. org.	14.1	9.46
H-17	High-conc. organics	5.72, #JRF O-7	0.874, #JRF O-57
H-17	High-conc. organics	8.04, #JRF O-8	1.06, #JRF O-58
H-17	Avg. w. high-conc. org.	6.88	0.967

Table G-6. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Np(V) and Dolomite-Rich Culebra Rock (LANL Empirical Sorption Study). One-week sorption runs with H-19, B-4, Box 7. K_d s in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Still counting new controls for underlined samples. Data current as of May 30, 1996. Table compiled by L. H. Brush on May 16, 1996, based on information provided by LANL on May 15, 1996. Table checked by L. J. Storz on May 16 and 17, 1996. Table revised by Brush on May 31 and June 1, 1996, based on information provided by LANL on May 30 and 31, 1996. Table checked by L. J. Storz on June 10, 1996. Table re-checked by A. C. Peterson on July 16, 1996.

Brine	Additive	K_d , (ml/g), 0.033% CO_2	K_d , (ml/g), 4.1% CO_2
ERDA-6	None	96.5, #JRF O-121	<u>136</u> , #JRF O-170
ERDA-6	None	87.6, #JRF O-122	<u>148</u> , #JRF O-172
ERDA-6	Avg. without organics	92.0	<u>142</u>
ERDA-6	Low-conc. organics	<u>83.6</u> , #JRF O-129	<u>175</u> , #JRF O-179
ERDA-6	Low-conc. organics	<u>79.1</u> , #JRF O-130	<u>147</u> , #JRF O-180
ERDA-6	Avg. w. low-conc. org.	<u>81.4</u>	<u>161</u>
ERDA-6	High-conc. organics	<u>63.9</u> , #JRF O-127	<u>131</u> , #JRF O-177
ERDA-6	High-conc. organics	<u>63.3</u> , #JRF O-128	<u>113</u> , #JRF O-178
ERDA-6	Avg. w. high-conc. org.	<u>63.6</u>	<u>122</u>

Table G-6. Effects of Brine, Organic Ligands, and P_{CO_2} on Matrix K_d s for Np(V) and Dolomite-Culebra Rock (LANL Empirical Sorption Study) (continued).

Brine	Additive	K_d (ml/g), 0.033% CO_2	K_d (ml/g), 4.1% CO_2
H-17	None	5.17, #JRF O-21	<u>0.905</u> , #JRF O-71
H-17	None	4.37, #JRF O-22	<u>1.06</u> , #JRF O-72
H-17	Avg. without organics	4.77	<u>0.983</u>
H-17	Low-conc. organics	4.86, #JRF O-29	1.33, #JRF O-79
H-17	Low-conc. organics	4.44, #JRF O-30	0.694, #JRF O-80
H-17	Avg. w. low-conc. org.	4.65	1.01
H-17	High-conc. organics	1.45, #JRF O-27	-0.236, #JRF O-77
H-17	High-conc. organics	1.67, #JRF O-28	-0.433, #JRF O-78
H-17	Avg. w. high-conc. org.	1.56	0.00

Table G-7. Effects of Organic Ligands on Matrix K_{ds} (ml/g) for Pu(V), Am(III), U(VI), Th(IV), and Np(V), Dolomite-Rich Culebra Rock, and Modified Brine A (LANL Empirical Sorption Study). One-week sorption runs with H-19, B-4, Box 7. K_{ds} in bold font excluded from ranges and distributions because of unacceptable differences between standards and controls. Data current as of May-30, 1996. Table compiled by L. H. Brush on May 16, 1996, based on information provided by LANL on May 15, 1996. Table checked by L. J. Storz on May 16, 1996. Table revised by Brush on May 31, 1996, based on information provided by LANL on May 30, 1996. Table checked by L. J. Storz on June 10, 1996. Table re-checked by A. C. Peterson on July 16, 1996.

Additive	Element and Oxidation State				
	Pu(V)	Am(III)	U(VI)	Th(IV)	Np(V)
None	8.73, #JRF-233	528, #JRF-243	19.3, #JRF-213	11,300, #JRF-203	22.7, #JRF-223
None	10.1, #JRF-234	501, #JRF-244	19.1, #JRF-214	10,700, #JRF-204	17.1, #JRF-224
Avg. without organics	9.42	514	19.2	11,000	19.9
Low-conc. organics	7.69, #JRF-239	355, #JRF-249	12.4, #JRF-219	1.70, #JRF-209	11.9, #JRF-229
Low-conc. organics	8.84, #JRF-240	325, #JRF-250	17.2, #JRF-220	6.47, #JRF-210	10.5, #JRF-230
Avg. w. low-conc. organics	8.26	340	14.8	4.08	11.2
Intermed.-conc. organics	5.03, #JRF-237	67.6, #JRF-247	16.6, #JRF-217	1.05, #JRF-207	6.25, #JRF-227
Intermed.-conc. organics	5.06, #JRF-238	36.7, #JRF-248	16.8, #JRF-218	6.29, #JRF-208	5.89, #JRF-228
Avg. w. inter.-conc. org.	5.04	52.2	16.7	3.67	6.07

Table G-7. Effects of Organic Ligands on Matrix K_{ds} (ml/g) for Pu(V), Am(III), U(VI), Th(IV), and Np(V), Dolomite-Rich Culebra Rock, and Modified Brine A (LANL Empirical Sorption Study) (continued).

Additive	Element and Oxidation State				
	Pu(V)	Am(III)	U(VI)	Th(IV)	Np(V)
High-conc. organics	2.55, #JRF-235	2.34, #JRF-245	10.1, #JRF-215	0.469, #JRF-205	1.93, #JRF-225
High-conc. organics	2.22, #JRF-236	2.05, #JRF-246	8.01, #JRF-216	0.467, #JRF-206	2.49, #JRF-226
Avg. w. high-conc. org.	2.38	2.20	9.06	0.468	2.21

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Subject: Transcription Review of Tables B-1, B-2, B-3, B-4, C-1, C-2, C-3, C-4, D-1, D-2, D-3, D-4, F-1, F-2, F-3, F-4, G-2, G-3, G-4, G-5, G-6, and G-7 in "Ranges and Probability Distributions of K_d S for Dissolved Pu, Am, U, Th, and Np in the Culebra for the PA Calculations to Support the WIPP CCA" by L.J. Storz on June 10, 1996.

The subject review by L.J. Storz was performed to verify that the values used in these tables were correctly transcribed from the original data sheets furnished by Los Alamos National Laboratory.

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